J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

Regioselective Functionalization and Diels–Alder Cycloadditions of Exocyclic Dienes in Five-membered Heterocycles

Gustavo A. Monroy-Flores[1], Pablo Montoya[1], Ailyn N. García-González[1], Carlos H. Escalante[1], R. Uri Gutiérrez[1], R. Israel Hernández[1], Aydeé Fuentes-Benítes[1,2], Edson Barrera,[1] Omar Gómez-García[1], Francisco Delgado[1], Joaquín Tamariz[1,*]

[1]Departamento de Química Orgánica, Escuela Nacional de Ciencias Biológicas, Instituto Politécnico Nacional. Prol. Carpio y Plan de Ayala, S/N, 11340 México, D.F. México.
[2]Departamento de Química Orgánica, Facultad de Química, Universidad Autónoma del Estado de México, Paseo Colón/Paseo Tollocan S/N, 50000 Toluca, Estado de México, México.

***Corresponding author:** Joaquín Tamariz, email: jtamarizm@ipn.mx; jtamarizm@gmail.com

Received March 20th, 2024; Accepted October 17th, 2024.

DOI for the article: http://dx.doi.org/10.29356/jmcs.v69i4.2343

Supplementary Information

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

INDEX A

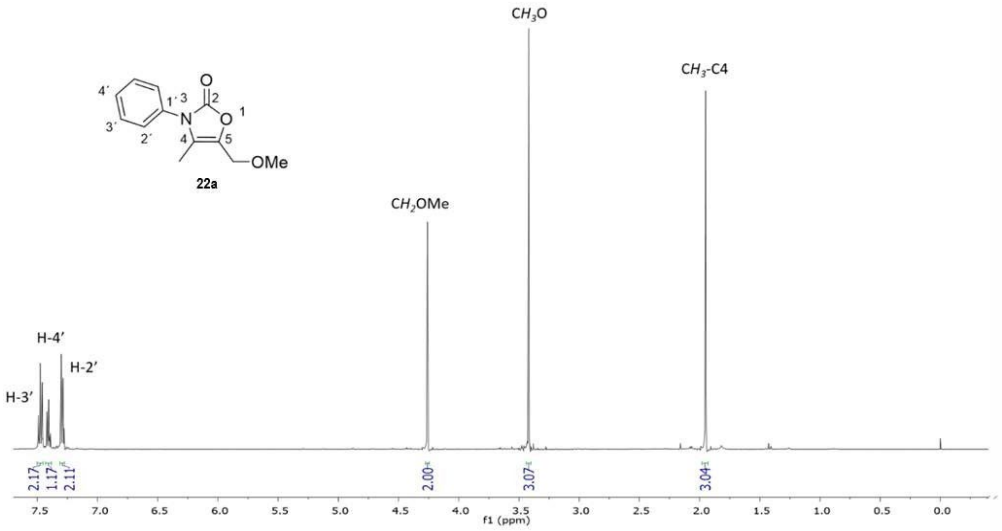

Fig. S1. ^{1}H NMR (500 MHz, CDCl3) spectrum of **22a**.

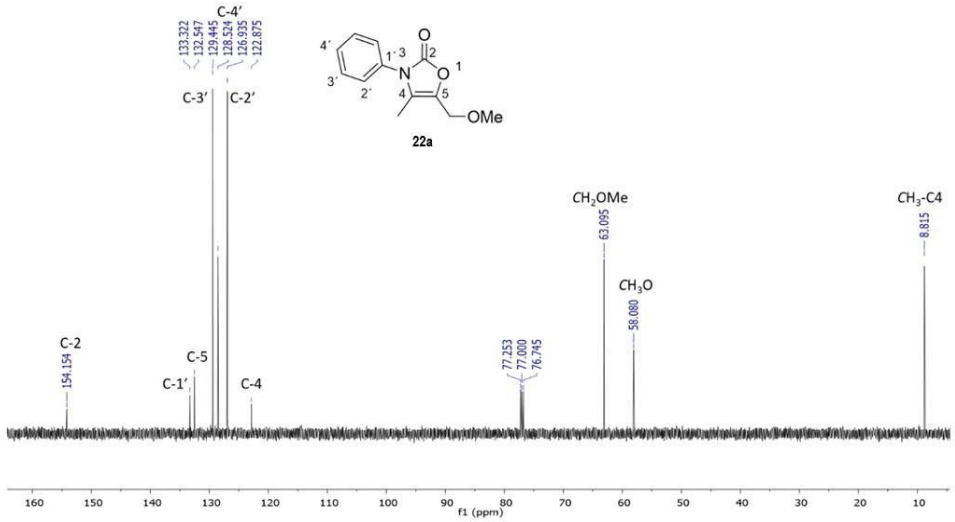

Fig. S2. ^{13}C NMR (125 MHz, CDCl3) spectrum of **22a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

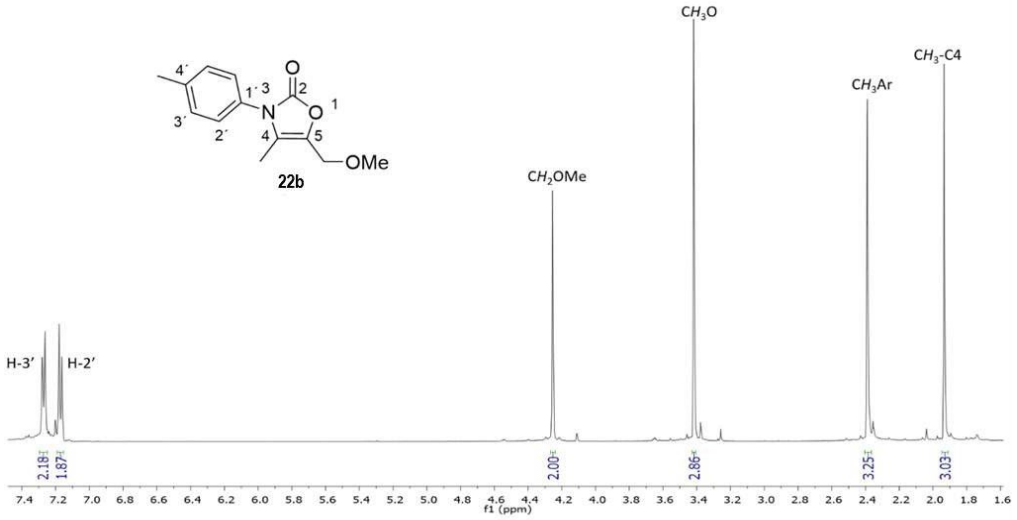

Fig. S3. ^{1}H NMR (500 MHz, CDCl3) spectrum of **22b**.

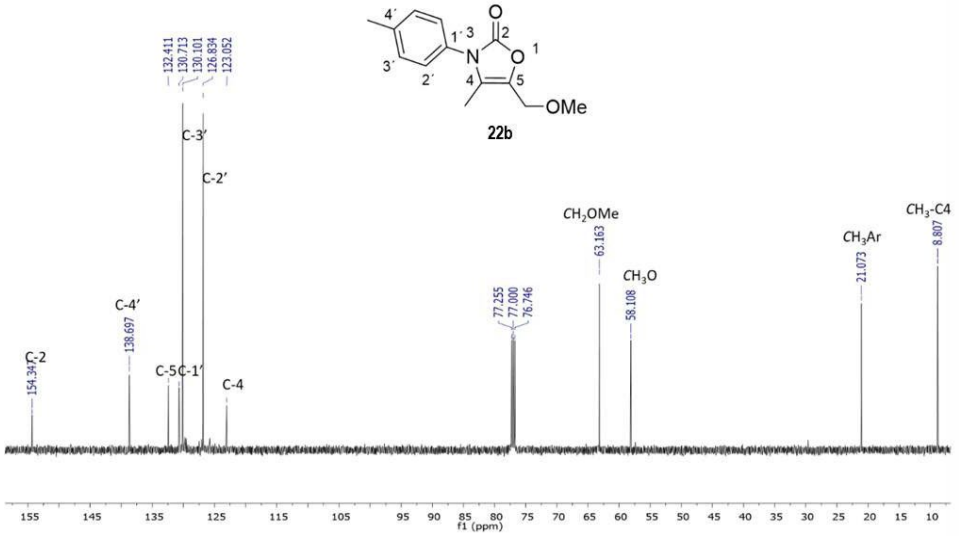

Fig. S4. ^{13}C NMR (125 MHz, CDCl3) spectrum of **22b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

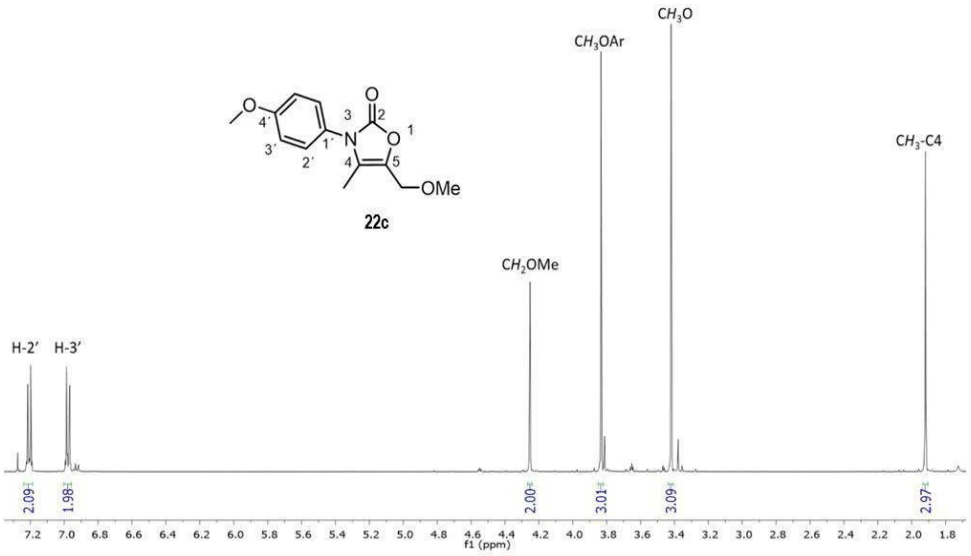

Fig. S5. ^{1}H NMR (500 MHz, CDCl3) spectrum of **22c**.

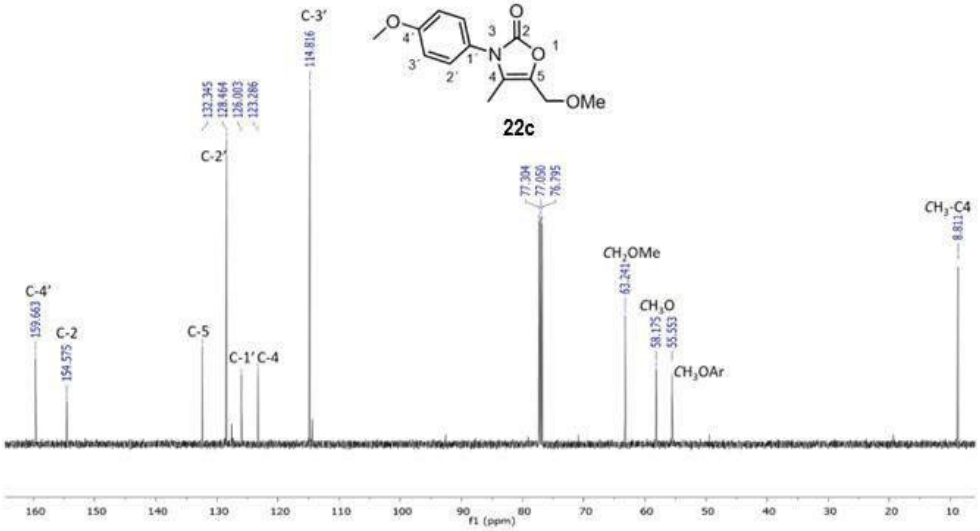

Fig. S6. ^{13}C NMR (125 MHz, CDCl3) spectrum of **22c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

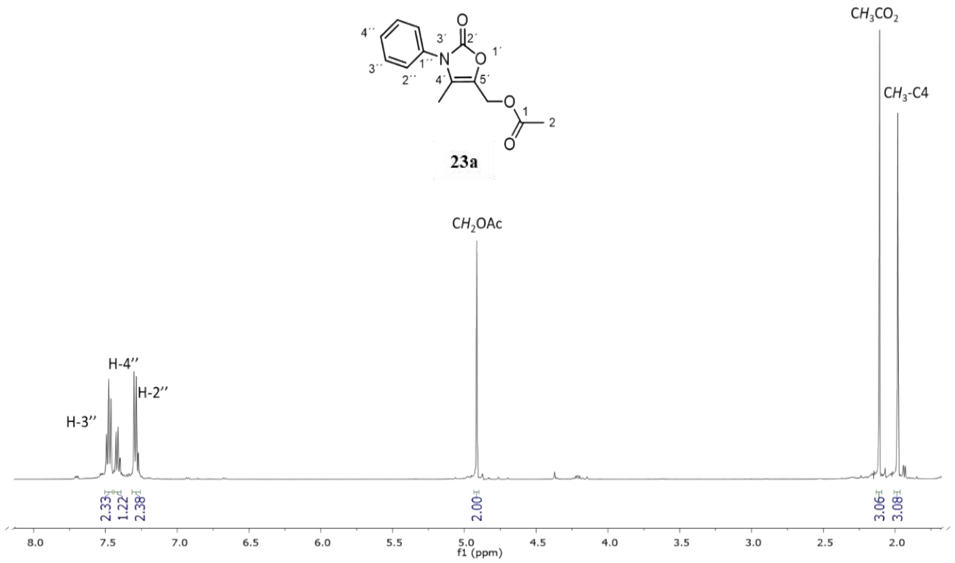

Fig. S7. ^{1}H NMR (500 MHz, CDCl3) spectrum of **23a**

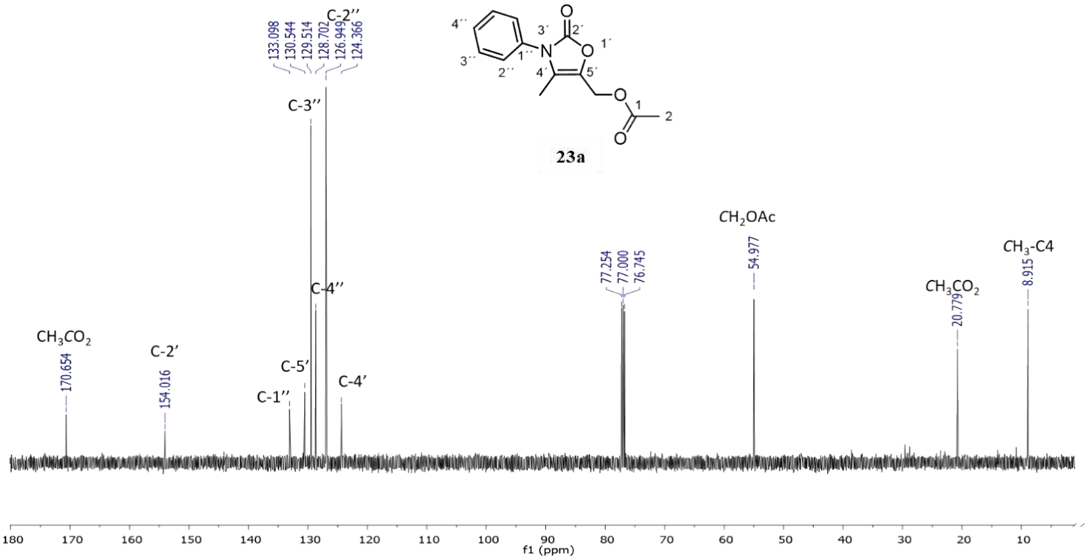

Fig. S8. ^{13}C NMR (125 MHz, CDCl3) spectrum of **23a**

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

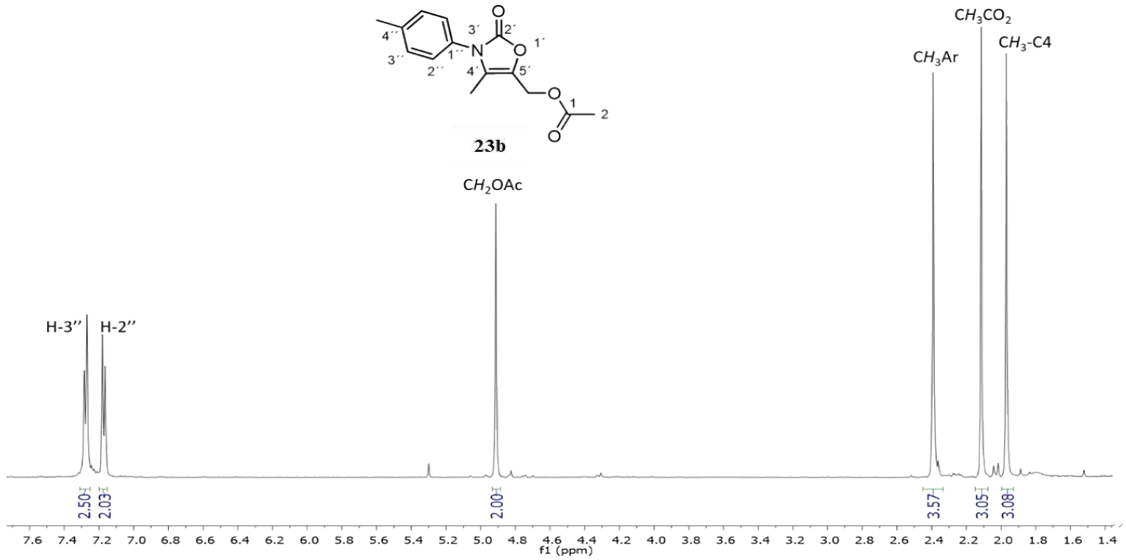

Fig. S9. ^{1}H NMR (500 MHz, CDCl3) spectrum of **23b**.

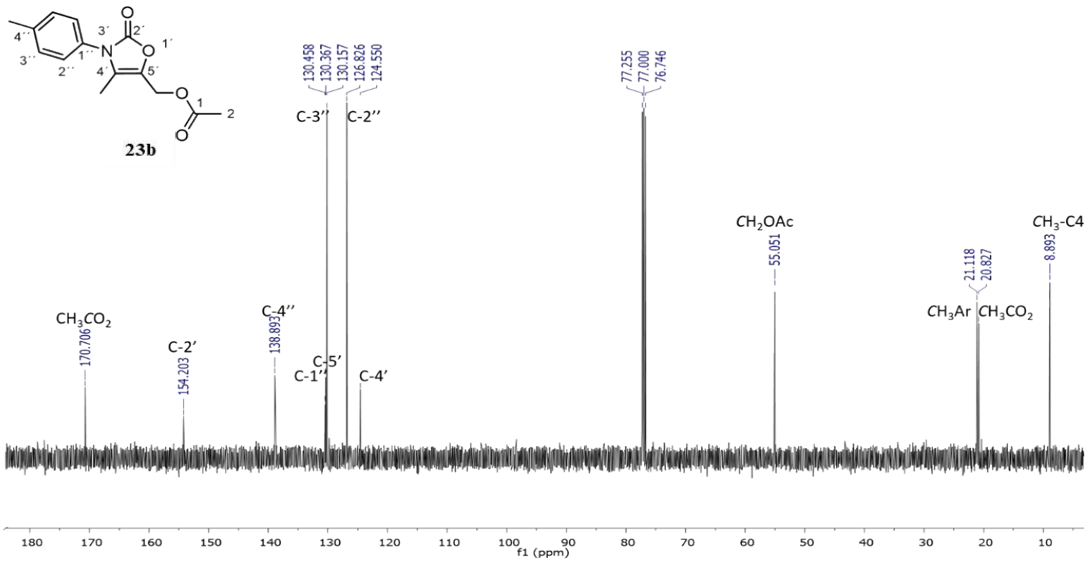

Fig. S10. ^{13}C NMR (125 MHz, CDCl3) spectrum of **23b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

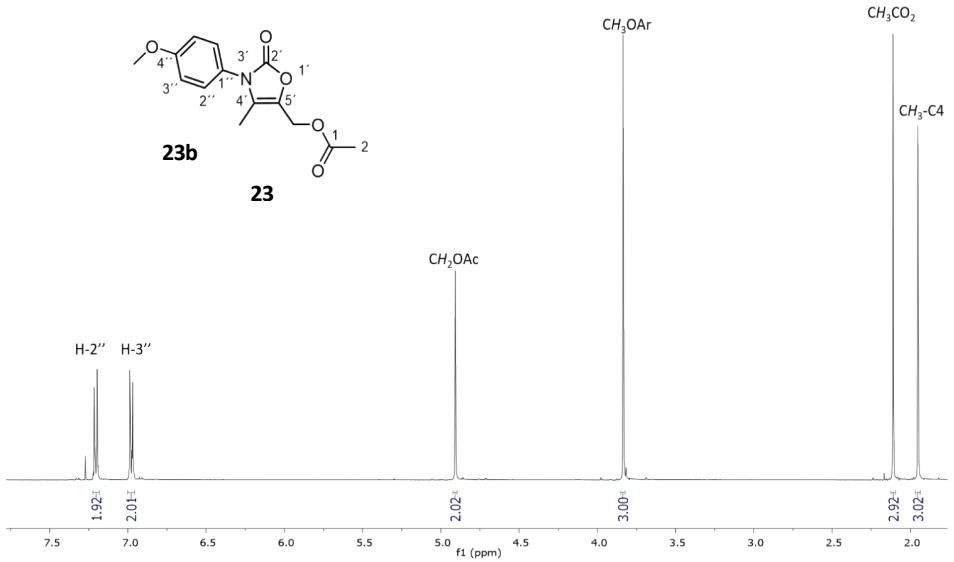

Fig. S11. ^{1}H NMR (500 MHz, CDCl3) spectrum of **23c**.

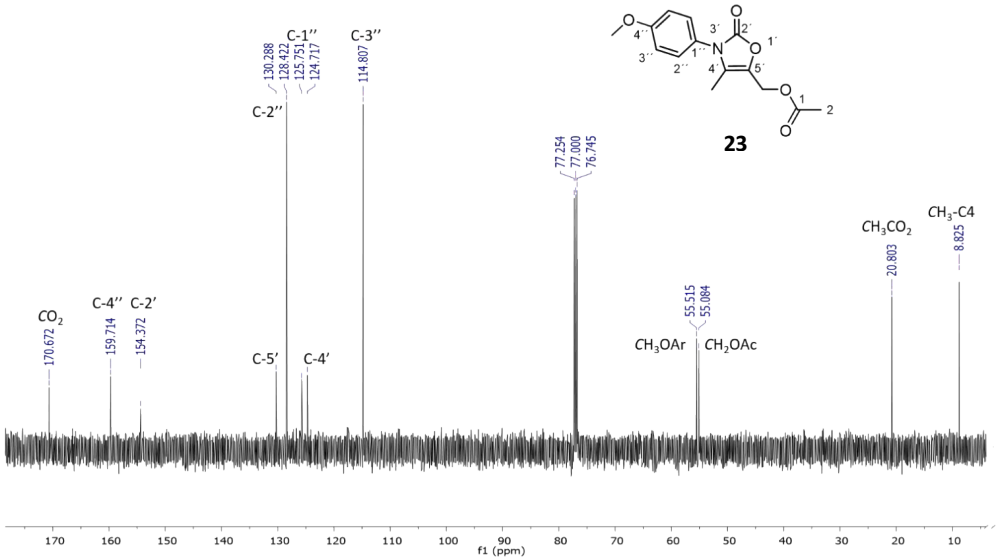

Fig. S12. ^{13}C NMR (125 MHz, CDCl3) spectrum of **23c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

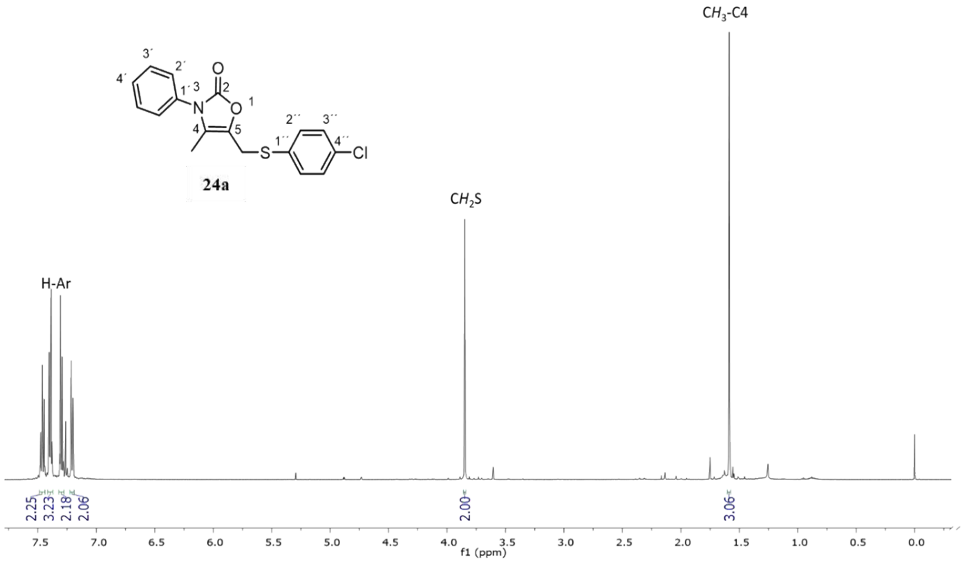

Fig. S13.[1]H NMR (500 MHz, CDCl3) spectrum of **24a**.

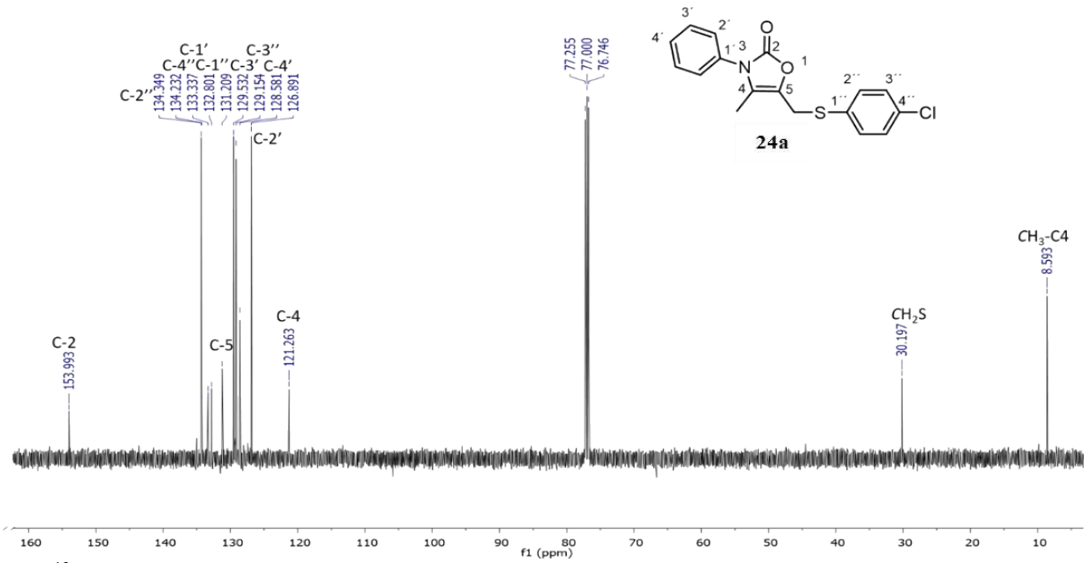

Fig. S14.[13]C NMR (125 MHz, CDCl3) spectrum of **24a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

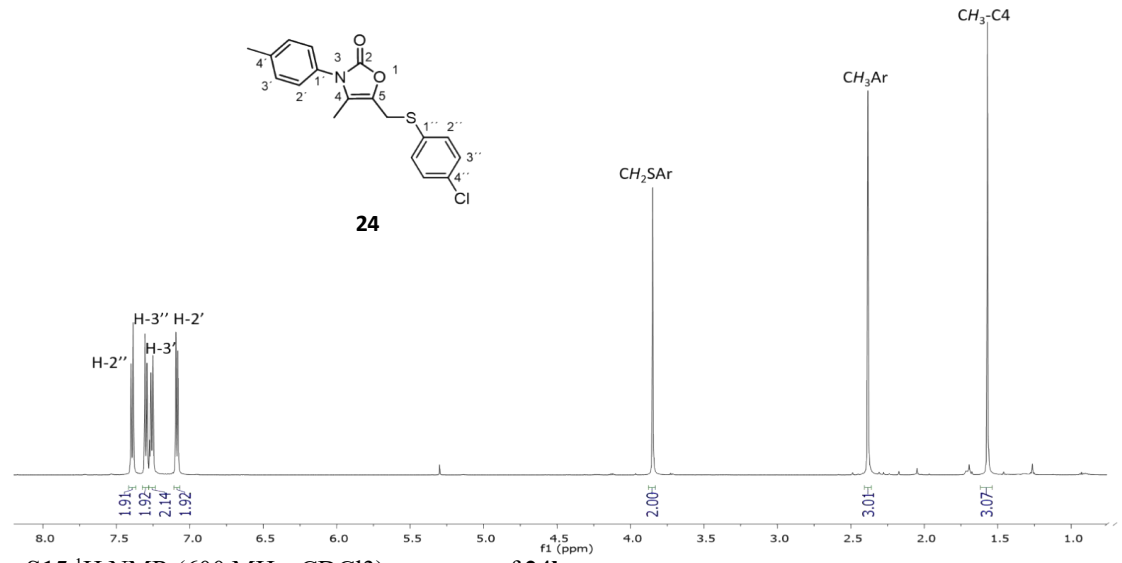

Fig. S15. ^{1}H NMR (600 MHz, CDCl3) spectrum of **24b**.

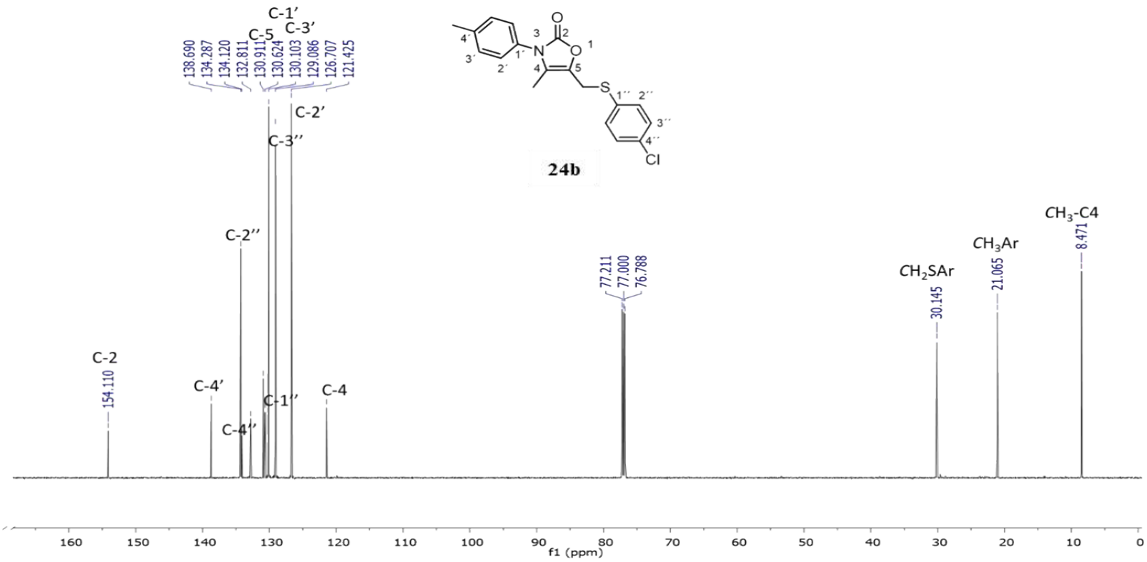

Fig. S16. ^{13}C NMR (150 MHz, CDCl3) spectrum of **24b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

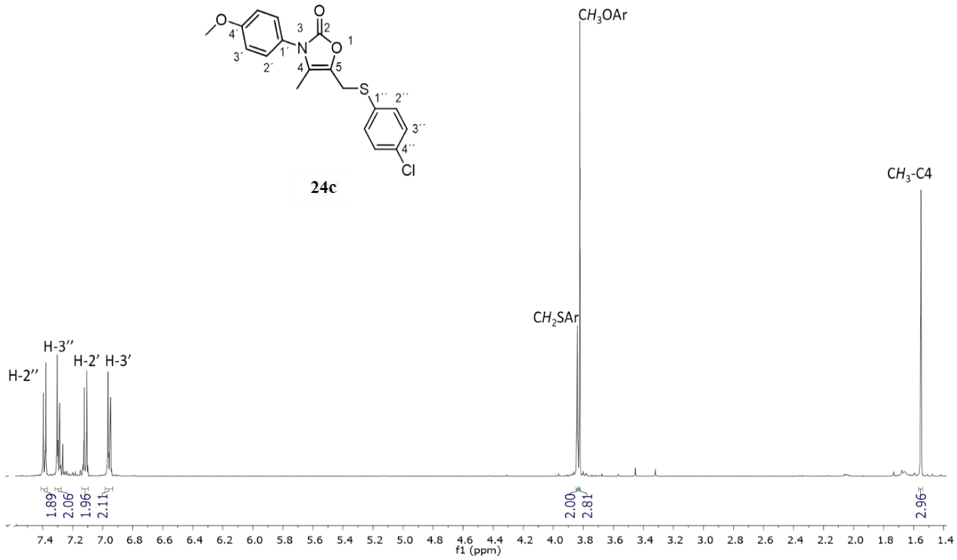

Fig. S17.[1]H NMR (500 MHz, CDCl3) spectrum of **24c**.

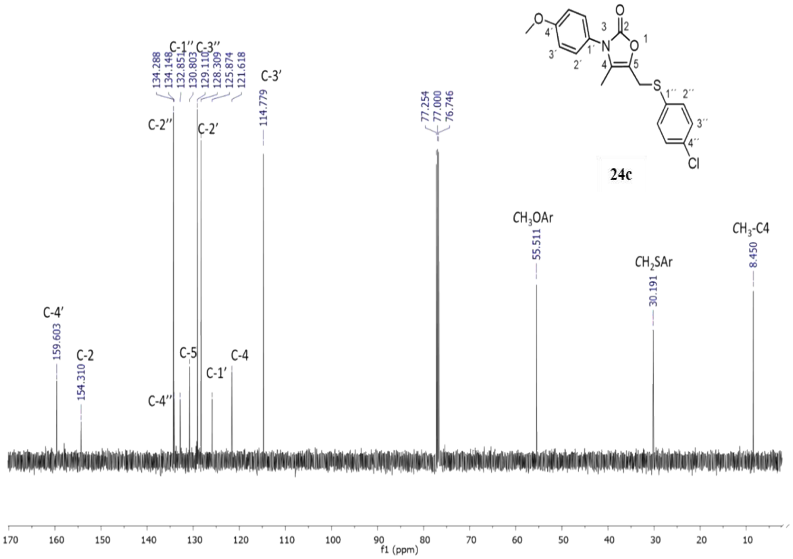

Fig. S18.[13]C NMR (125 MHz, CDCl3) spectrum of **24c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

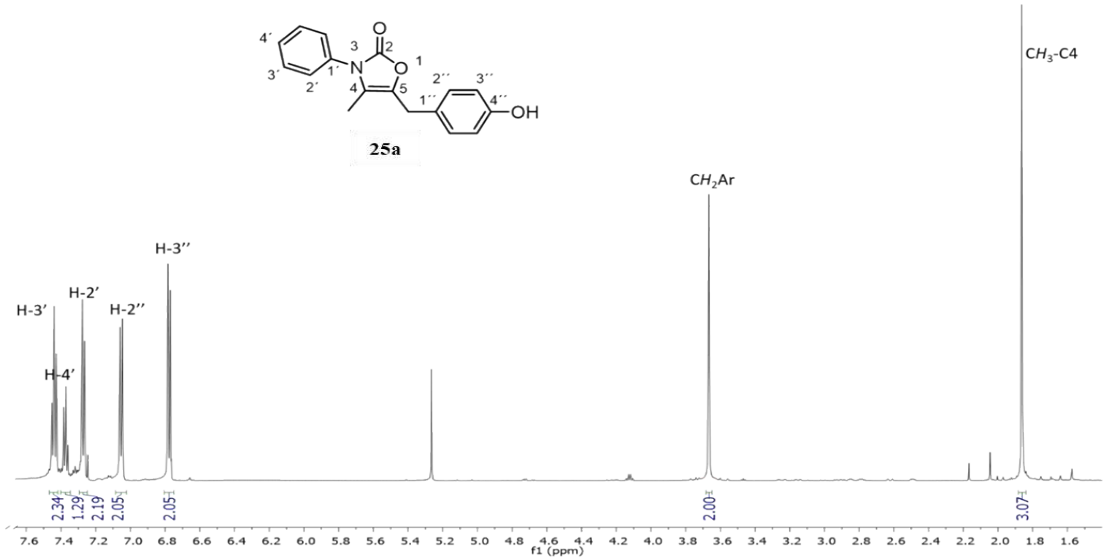

Fig. S19.[1]H NMR (600 MHz, CDCl3) spectrum of **25a**.

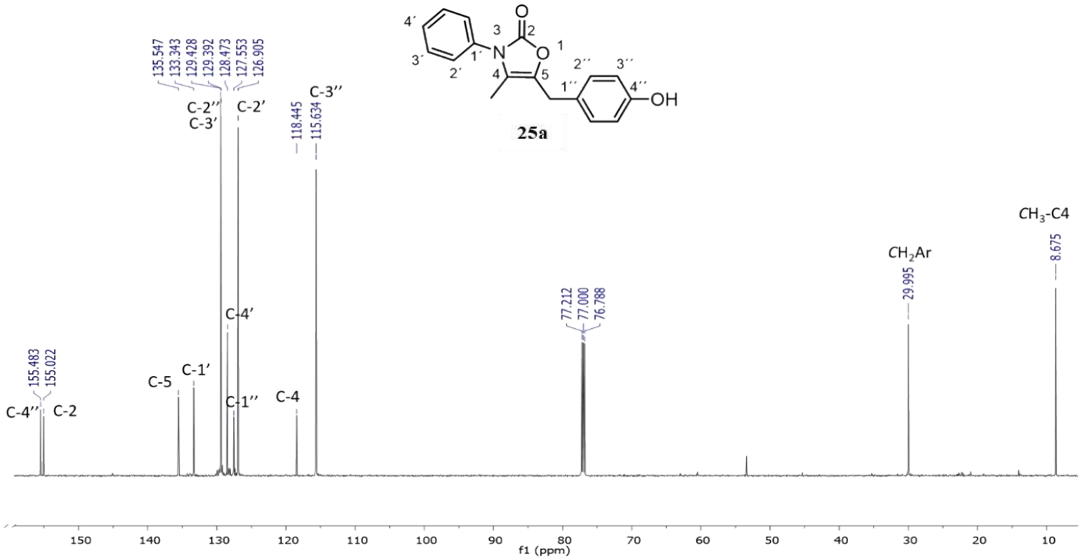

Fig. S20.[13]C NMR (150 MHz, CDCl3) spectrum of **25a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

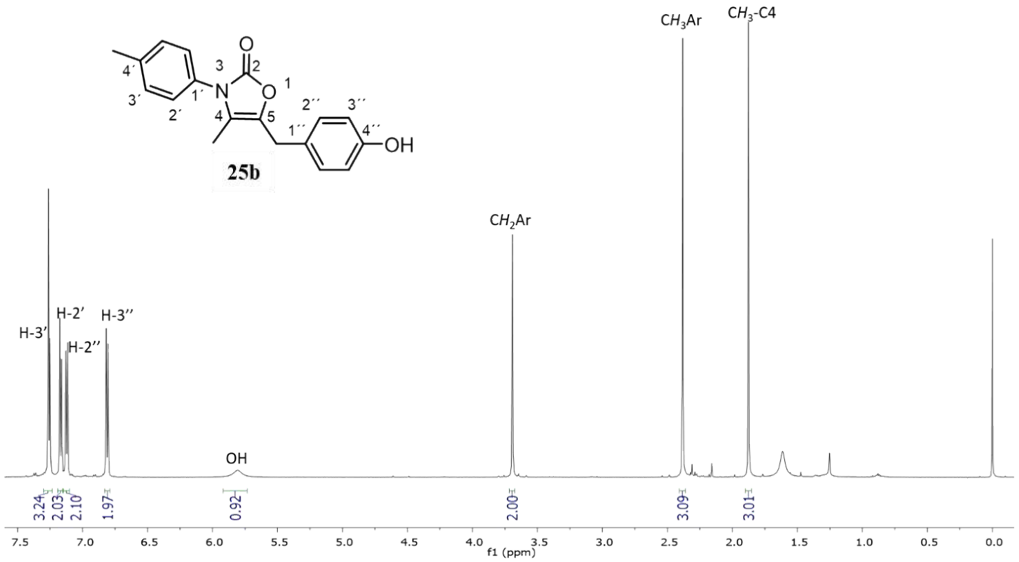

Fig. S21.[1]H NMR (600 MHz, CDCl3) spectrum of **25b**.

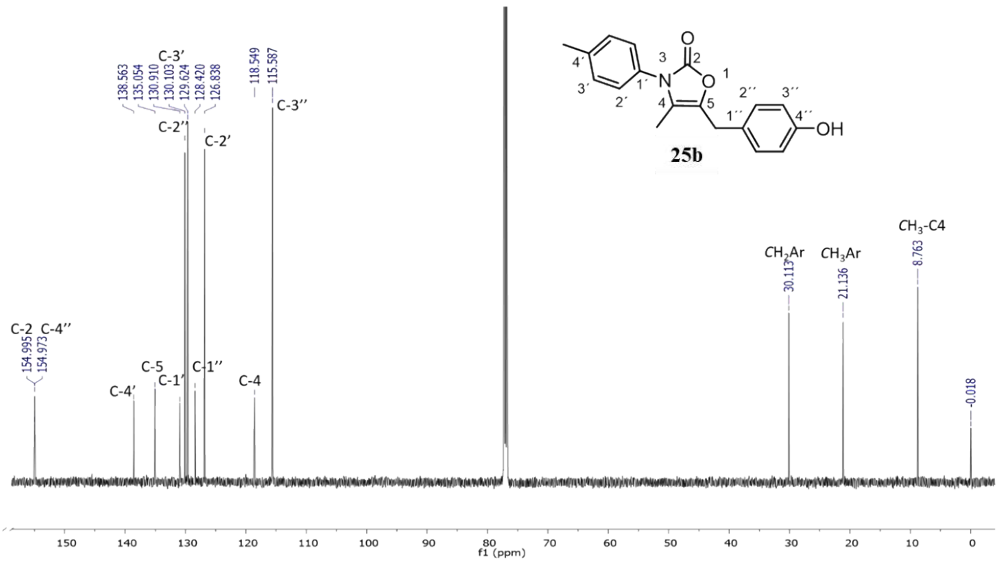

Fig. S22.[13]C NMR (150 MHz, CDCl3) spectrum of **25b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

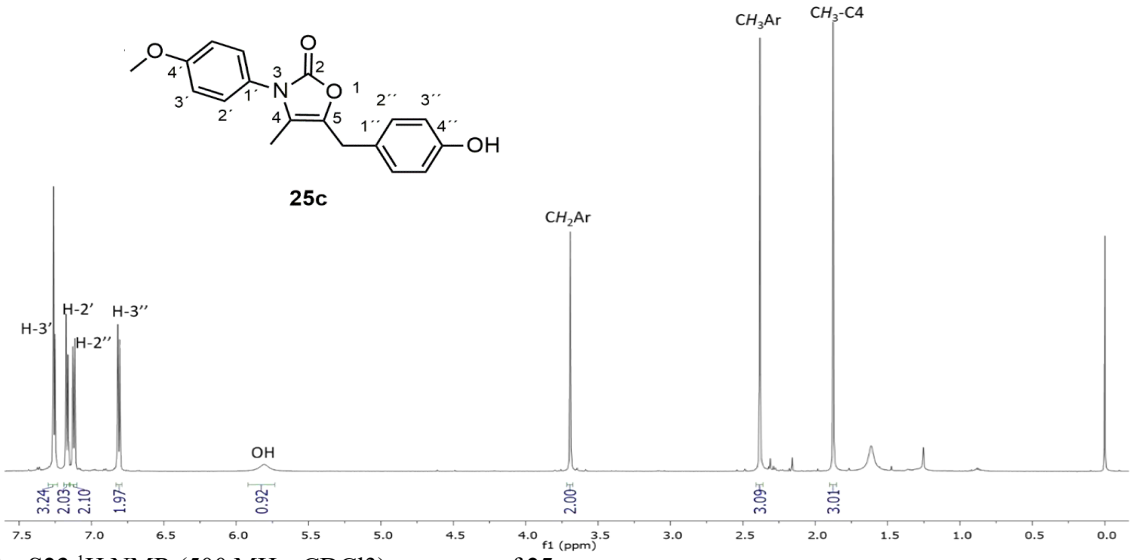

Fig. S23. ^{1}H NMR (500 MHz, CDCl3) spectrum of **25c**.

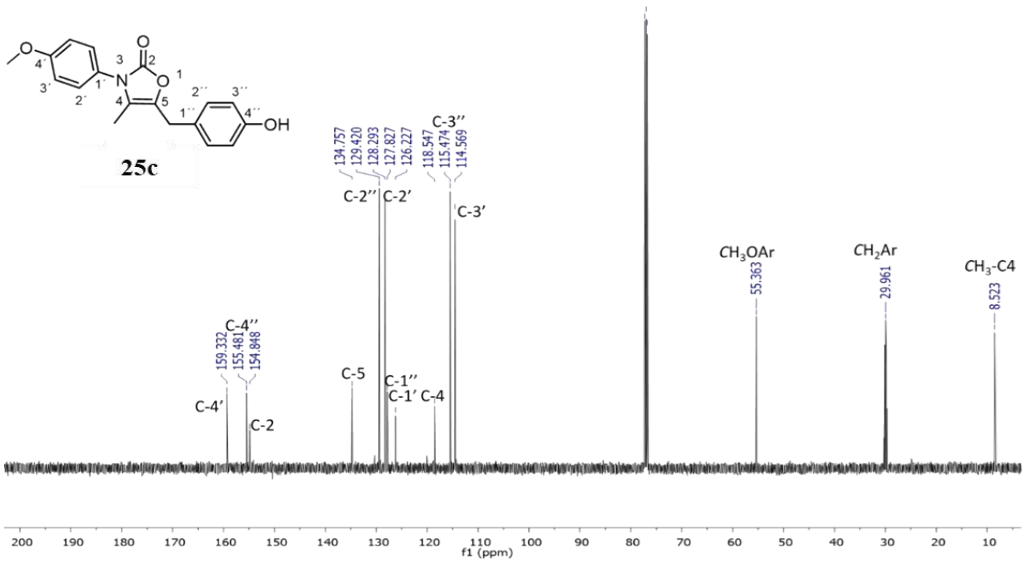

Fig. S24. ^{13}C NMR (125 MHz, CDCl3) spectrum of **25c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

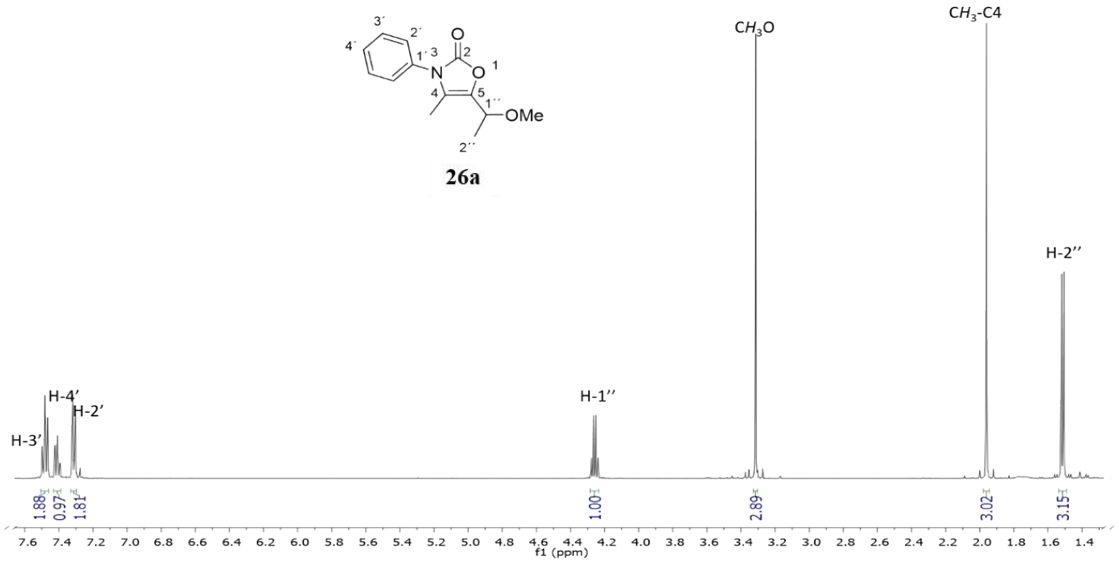

Fig. S25. ^{1}H NMR (500 MHz, CDCl3) spectrum of **26a**.

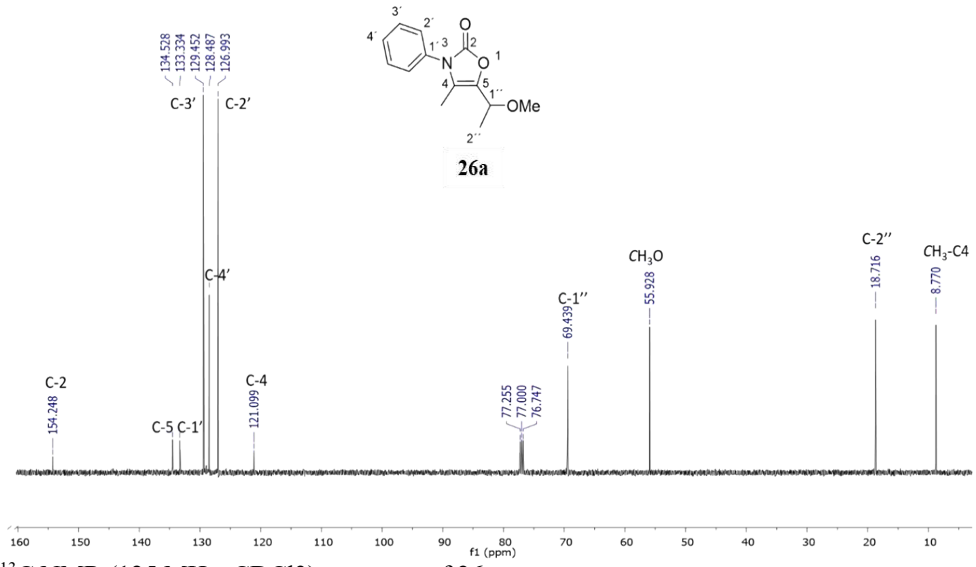

Fig. S26. ^{13}C NMR (125 MHz, CDCl3) spectrum of **26a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

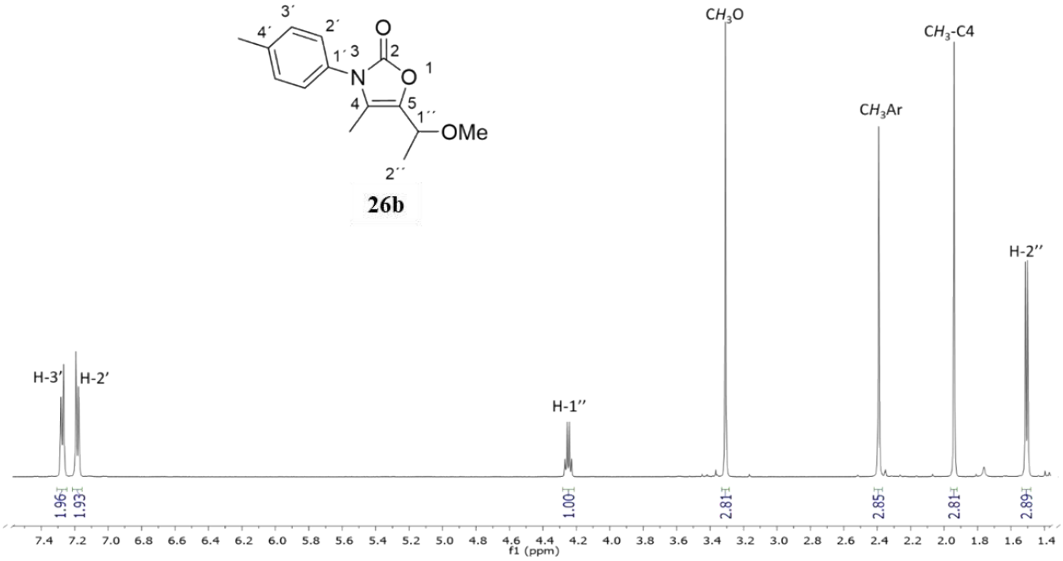

Fig. S27.[1]H NMR (500 MHz, CDCl3) spectrum of **26b**.

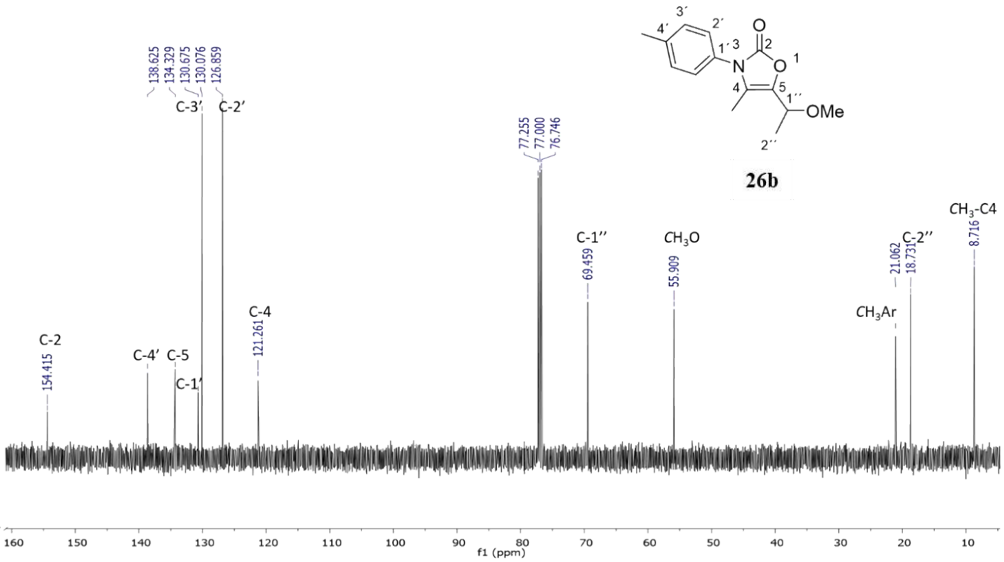

Fig. S28.[13]C NMR (125 MHz, CDCl3) spectrum of **26b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

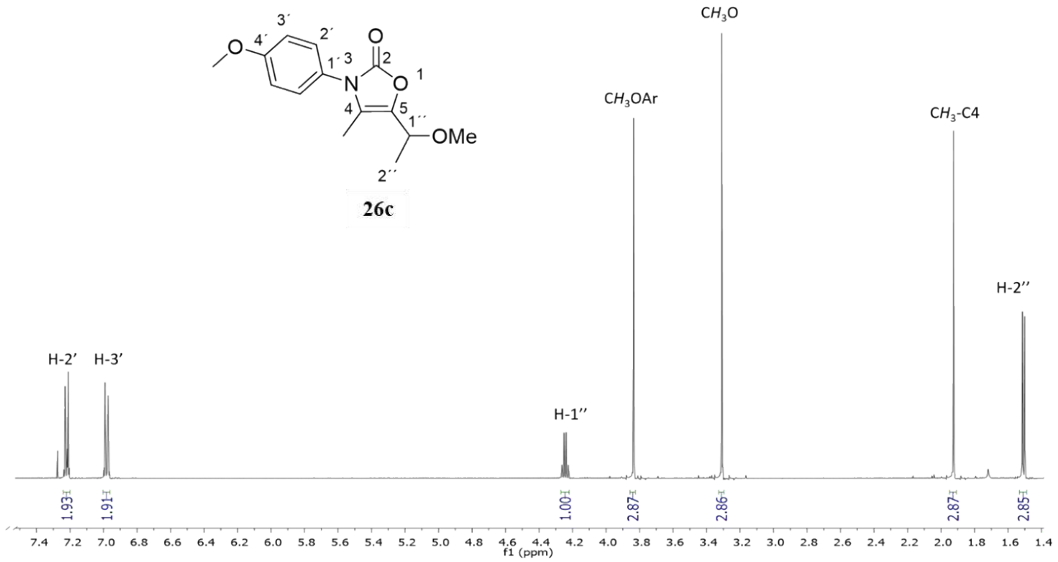

Fig. S29.[1]H NMR (500 MHz, CDCl3) spectrum of **26c**.

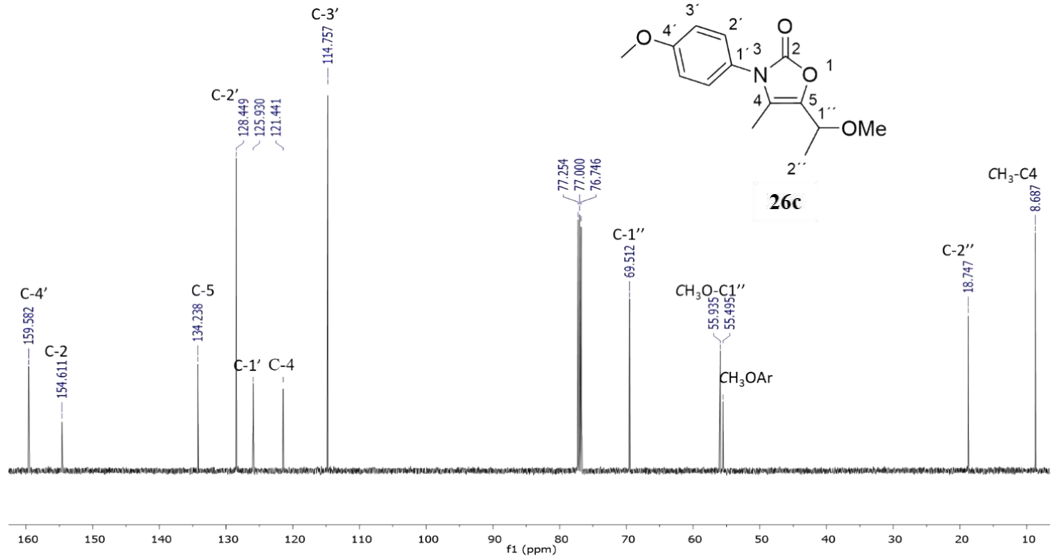

Fig. S30.[13]C NMR (125 MHz, CDCl3) spectrum of **26c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

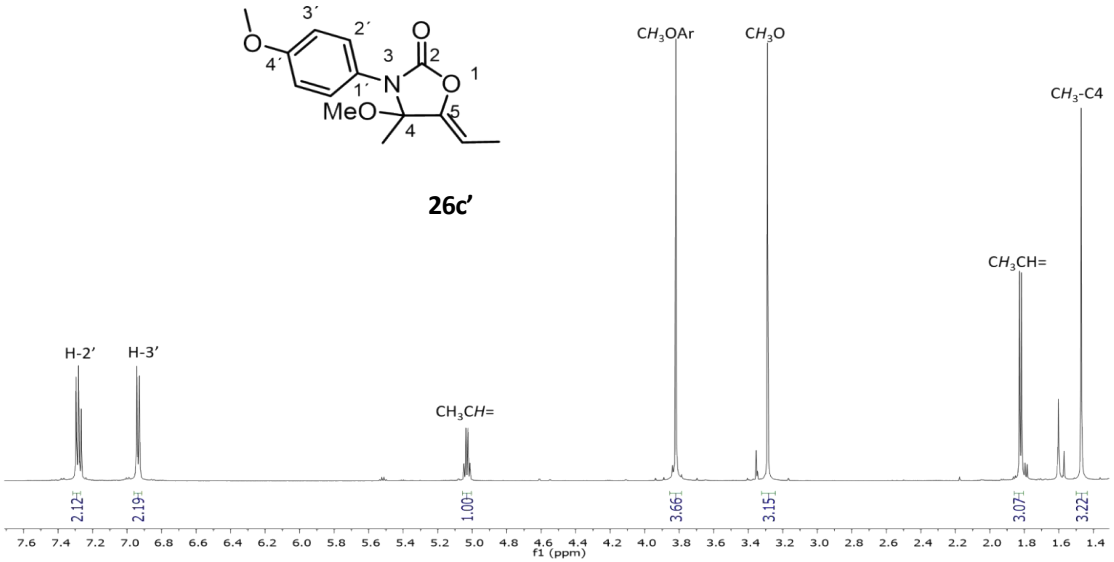

Fig. S31. ^{1}H NMR (600 MHz, CDCl3) spectrum of **26c'**.

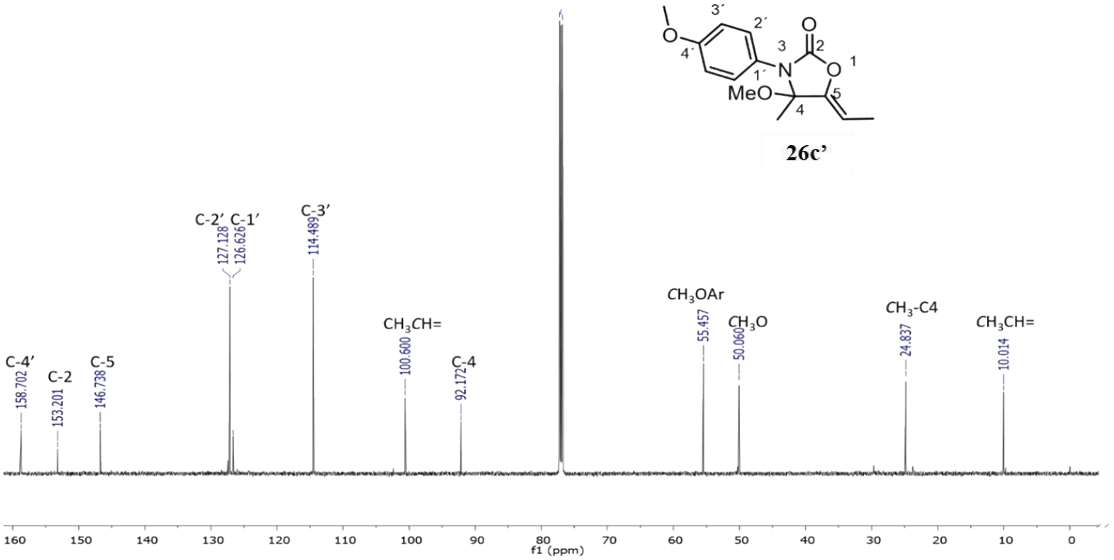

Fig. S32. ^{13}C NMR (150 MHz, CDCl3) spectrum of **26c'**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

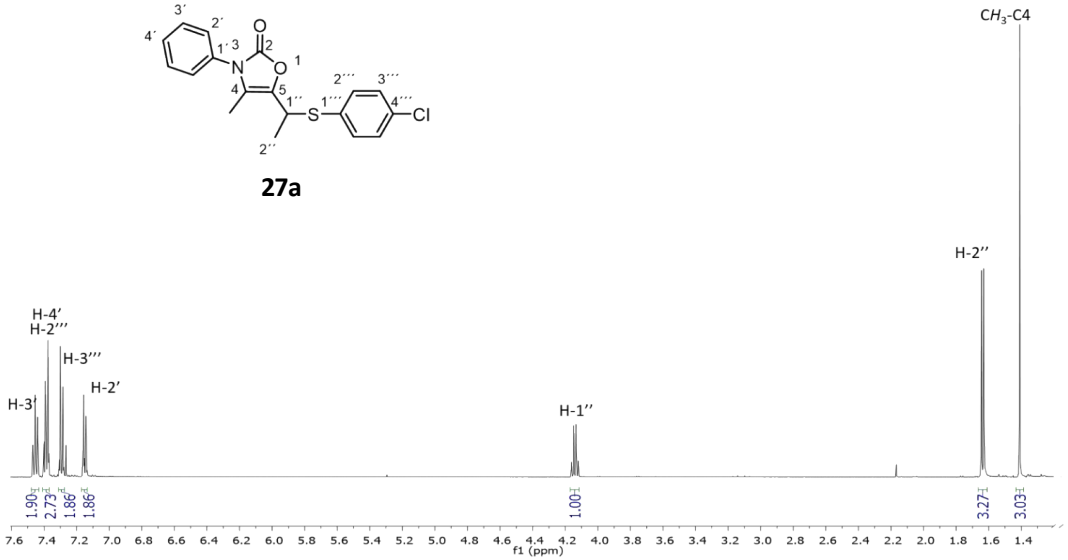

Fig. S33. ^{1}H NMR (500 MHz, CDCl3) spectrum of **27a**.

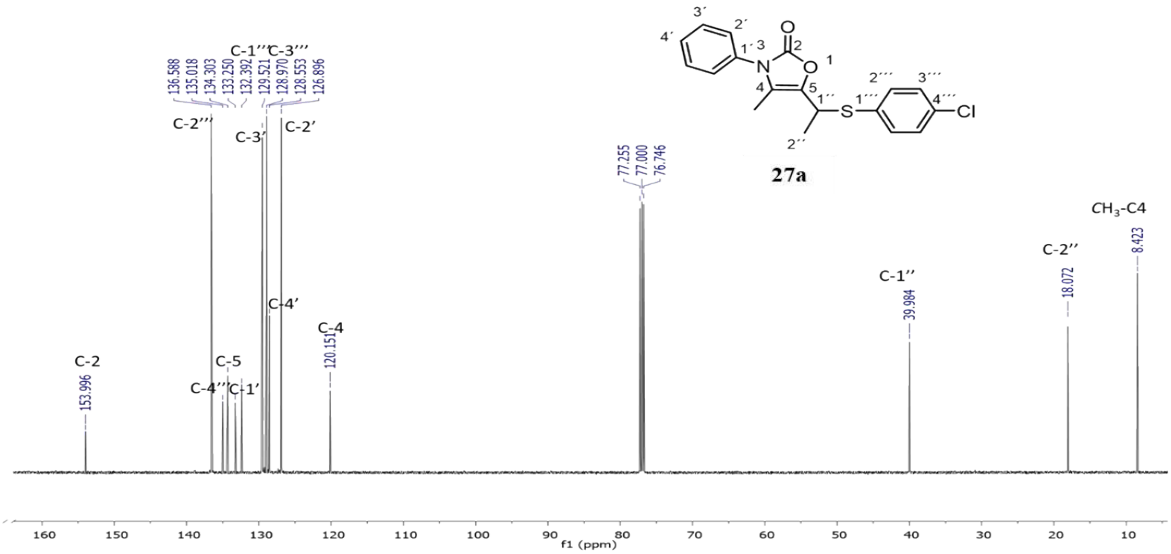

Fig. S34. ^{13}C NMR (125 MHz, CDCl3) spectrum of **27a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

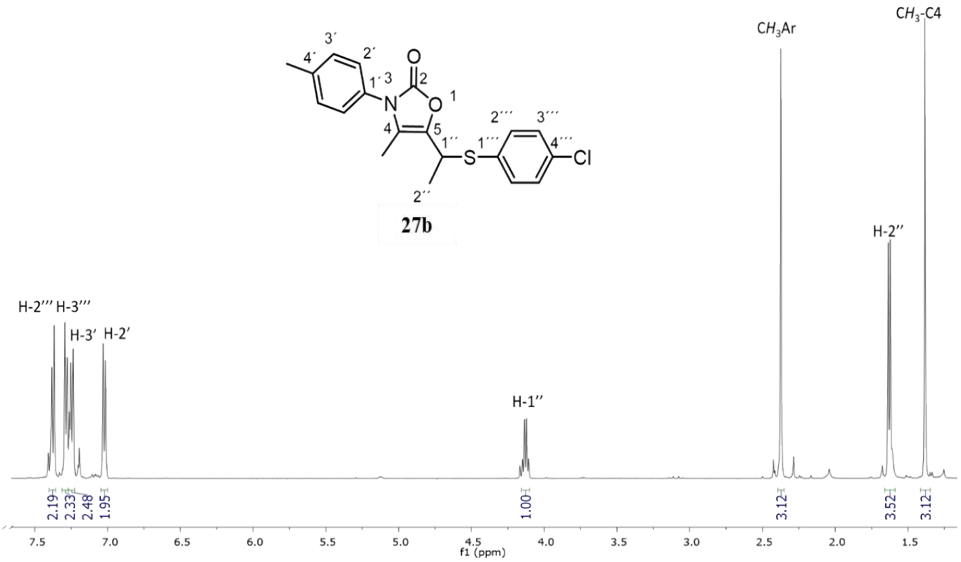

Fig. S35.[1]H NMR (500 MHz, CDCl3) spectrum of **27b**.

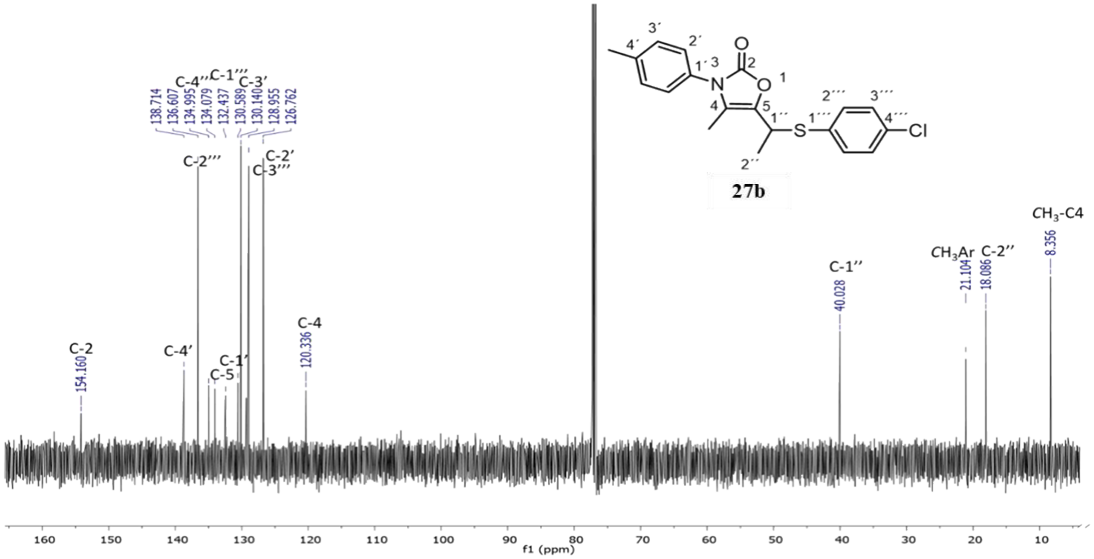

Fig. S36.[13]C NMR (125 MHz, CDCl3) spectrum of **27b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

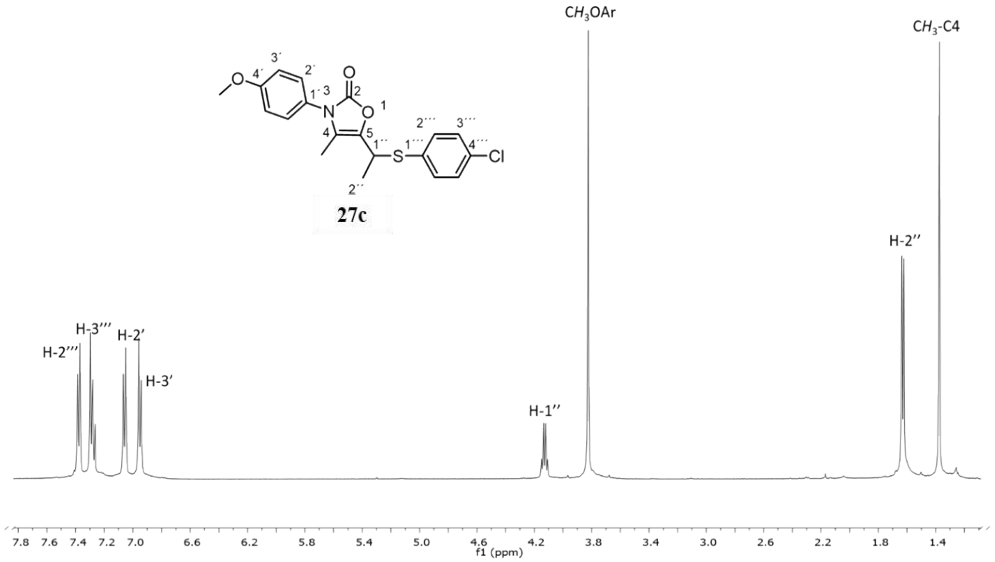

Fig. S37.[1]H NMR (500 MHz, CDCl3) spectrum of **27c**.

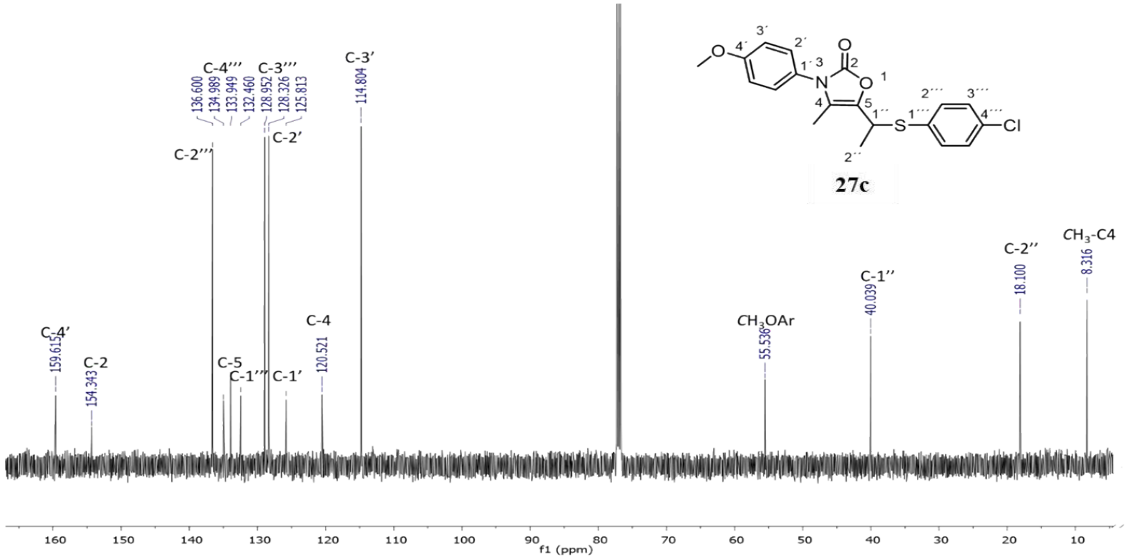

Fig. S38.[13]C NMR (125 MHz, CDCl3) spectrum of **27c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

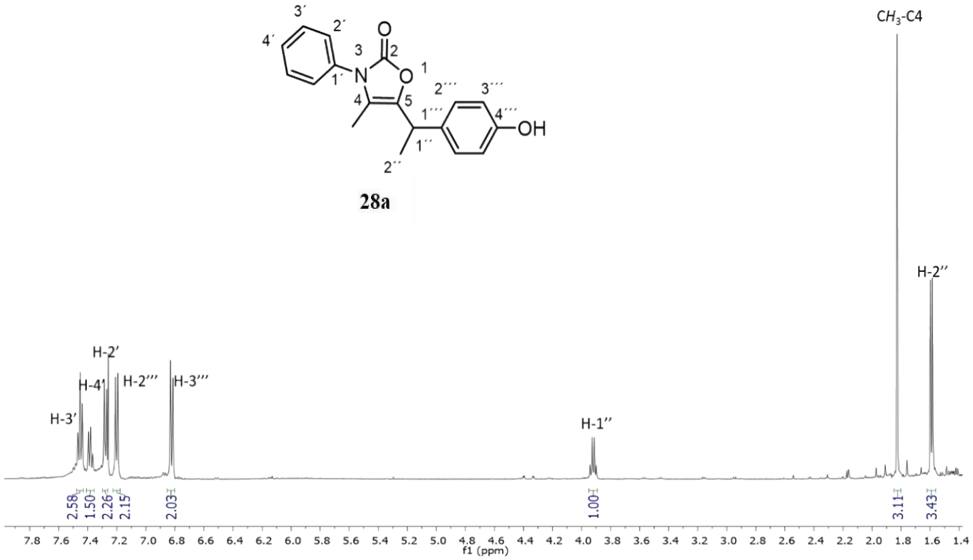

Fig. S39. ^{1}H NMR (500 MHz, CDCl3) spectrum of **28a**.

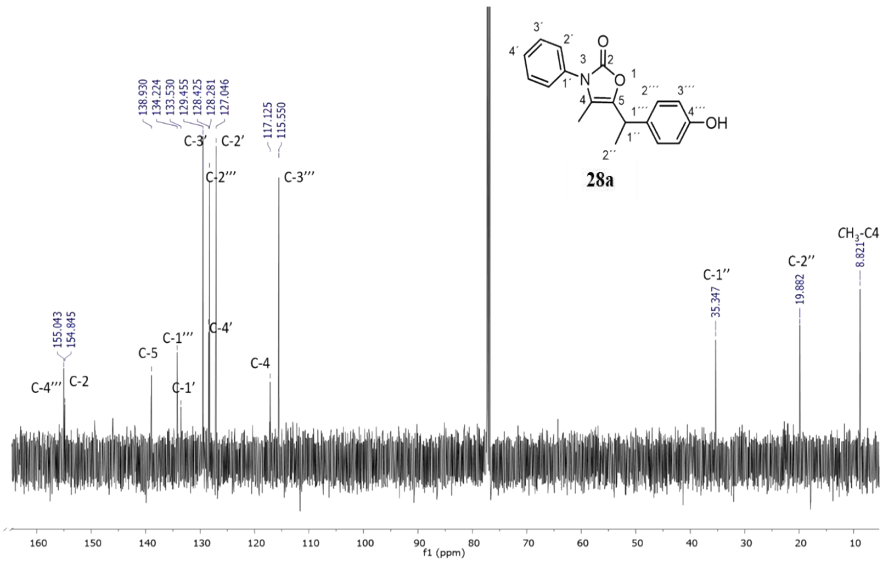

Fig. S40. ^{13}C NMR (125 MHz, CDCl3) spectrum.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

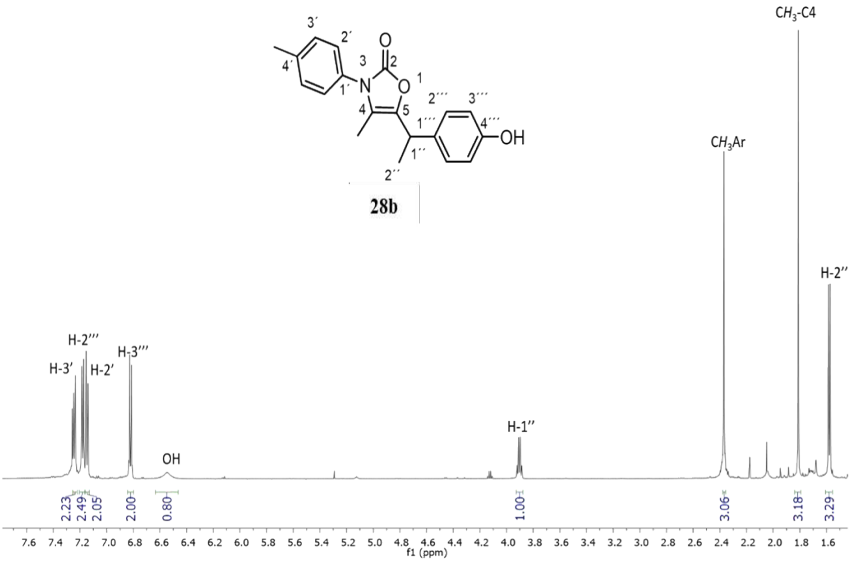

Fig. S41.[1]H NMR (600 MHz, CDCl3) spectrum of **28b**.

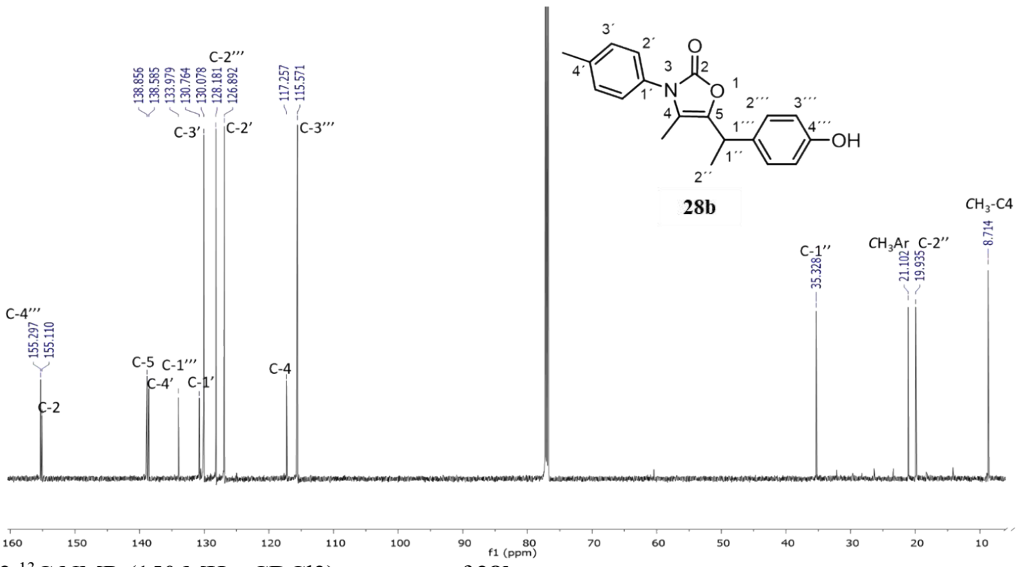

Fig. S42.[13]C NMR (150 MHz, CDCl3) spectrum of **28b.**

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

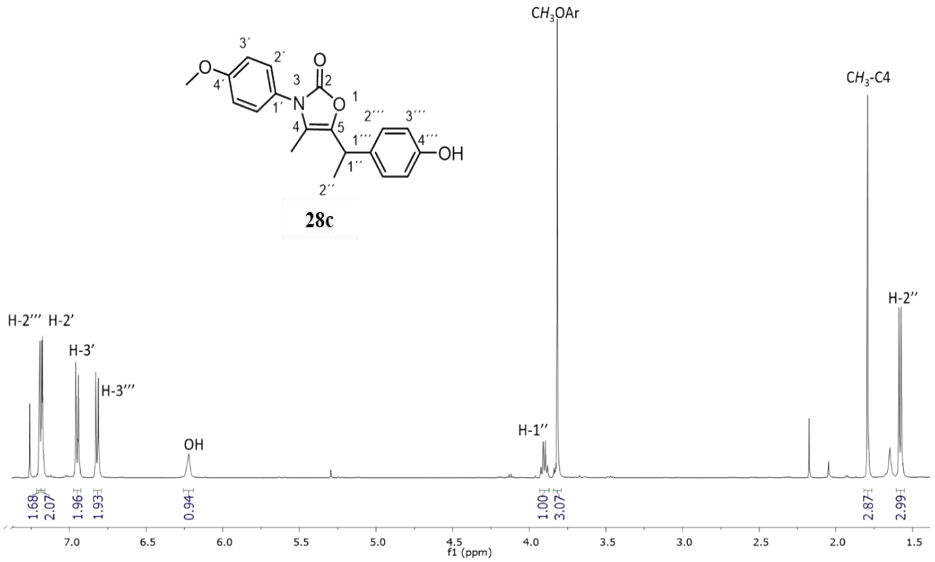

Fig. S43. ^{1}H NMR (500 MHz, CDCl3) spectrum of **28c**.

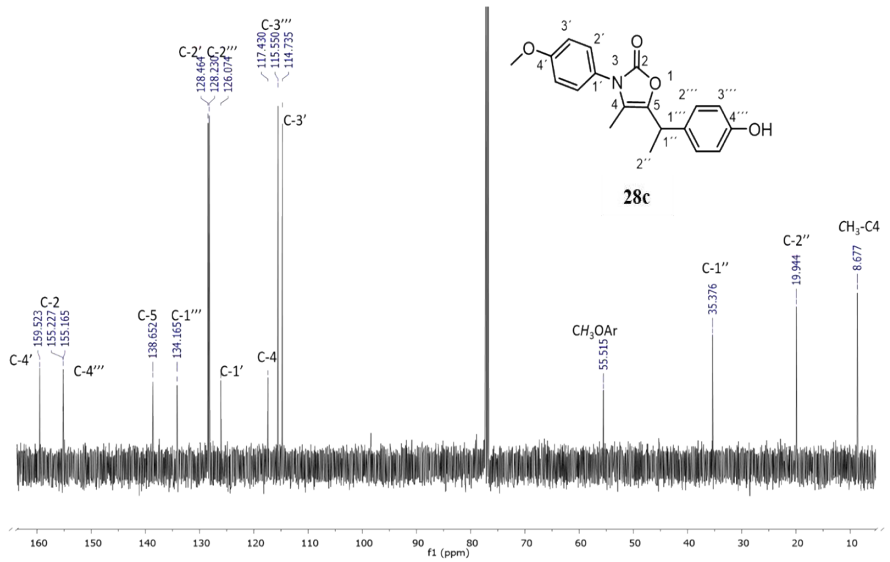

Fig. S44. ^{13}C NMR (125 MHz, CDCl3) spectrum of **28c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

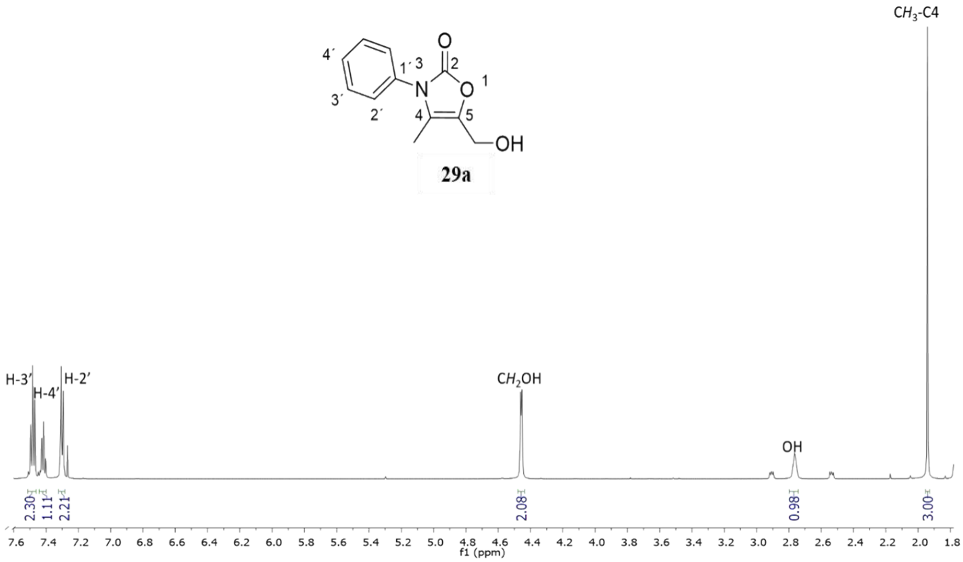

Fig. S45.[1]H NMR (600 MHz, CDCl3) spectrum of **29a**.

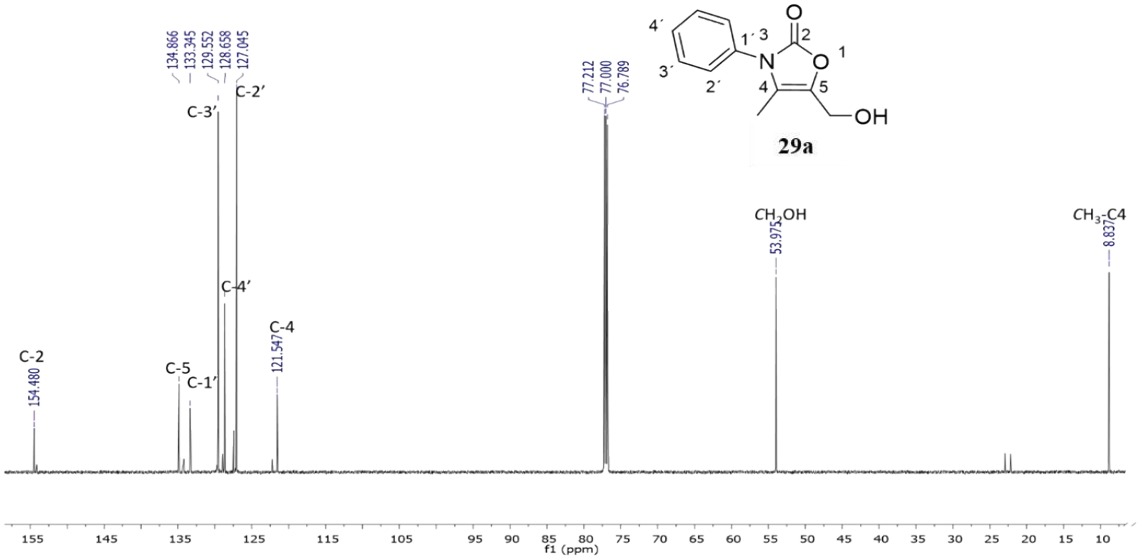

Fig. S46.[13]C NMR (150 MHz, CDCl3) spectrum of **29a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

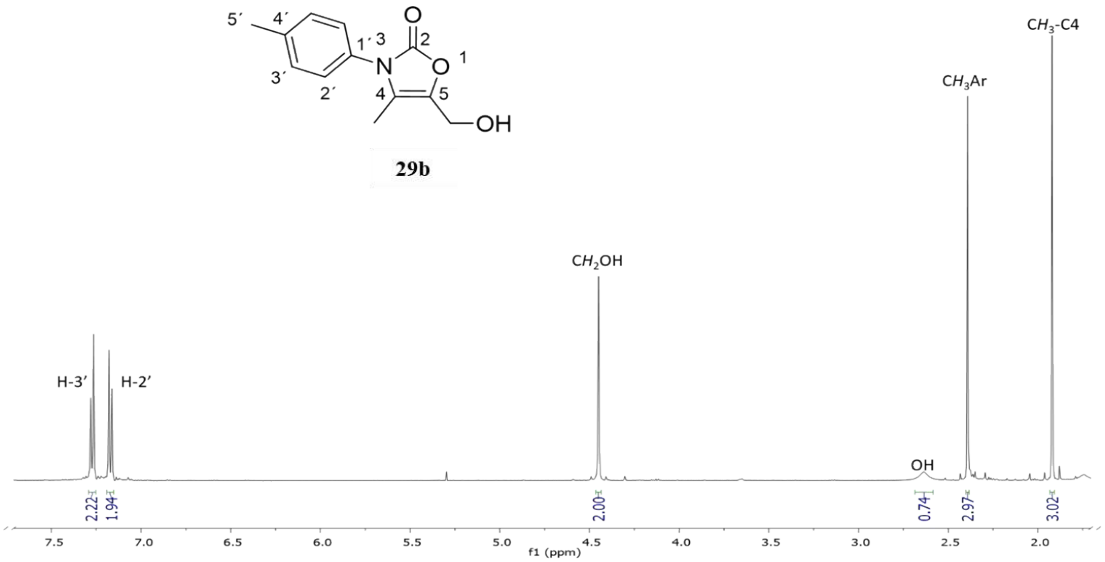

Fig. S47.[1]H NMR (500 MHz, CDCl3) spectrum of **29b**.

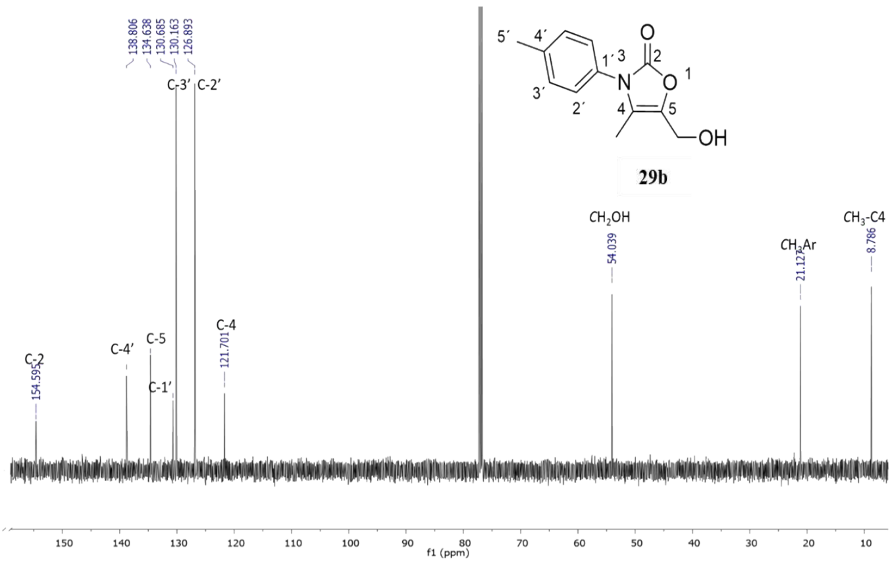

Fig. S48.[13]C NMR (125 MHz, CDCl3) spectrum of **29b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

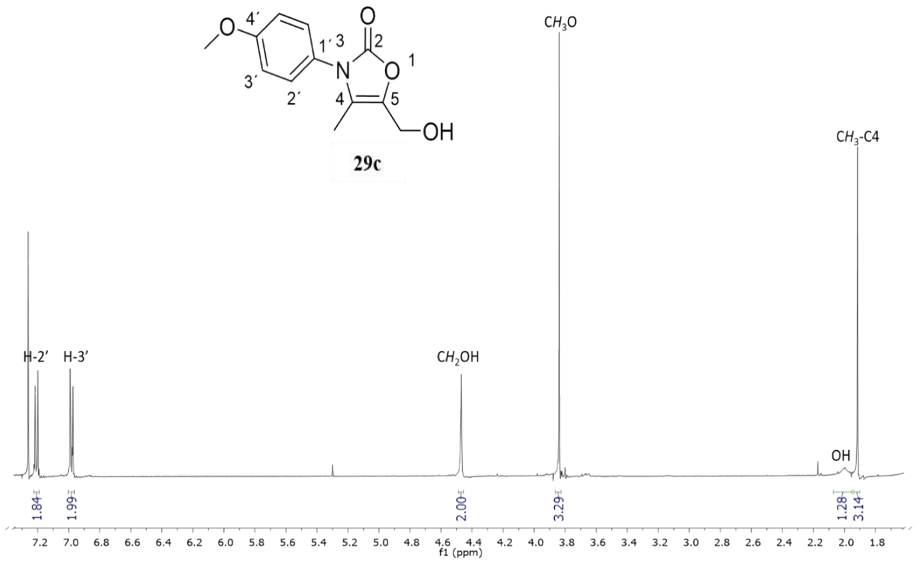

Fig. S49. ^{1}H NMR (500 MHz, CDCl3) spectrum of **29c**.

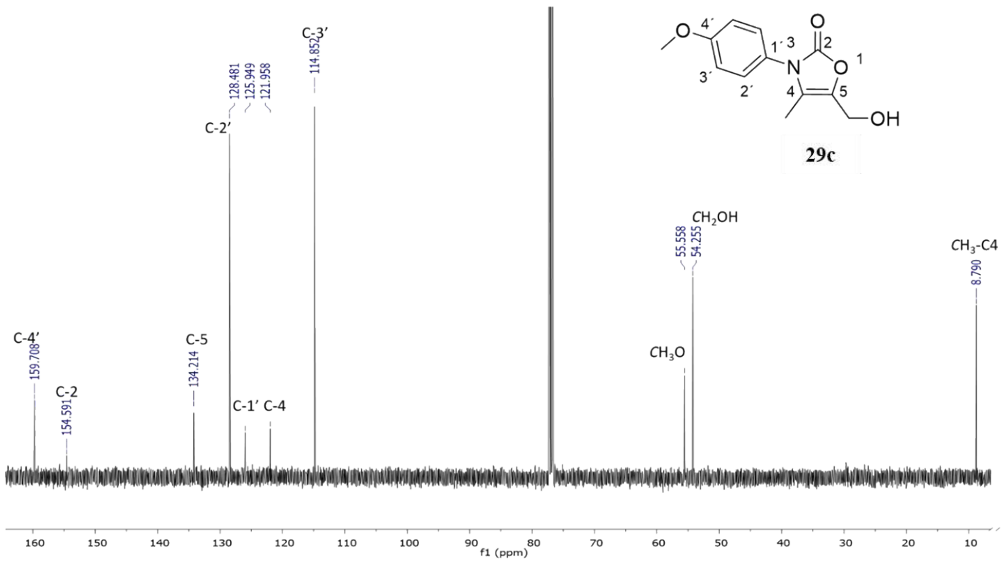

Fig. S50. ^{13}C NMR (125 MHz, CDCl3) spectrum of **29c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

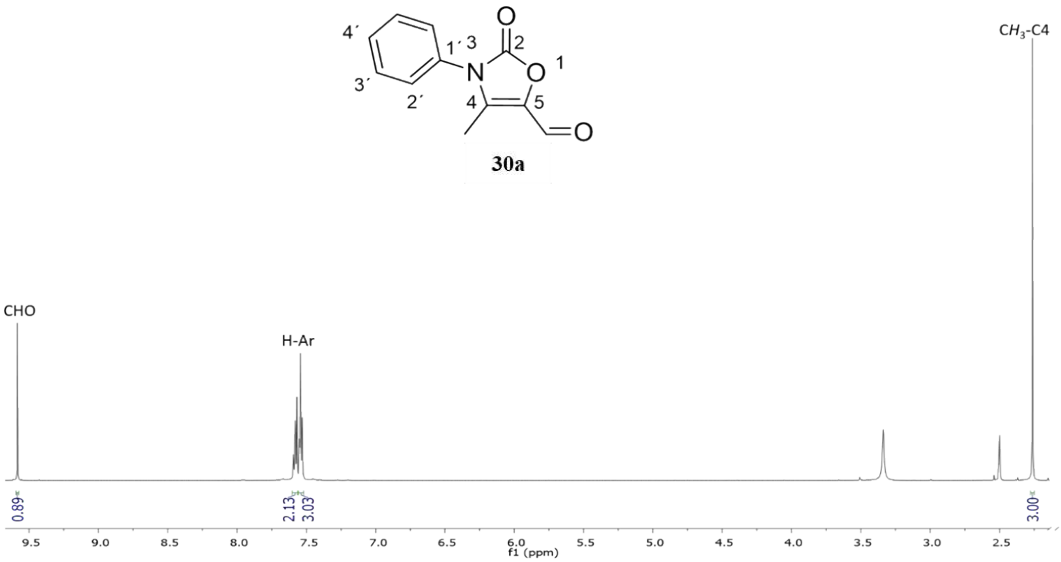

Fig. S51. ^{1}H NMR (600 MHz, DMSO-*d*6) spectrum of **30a**.

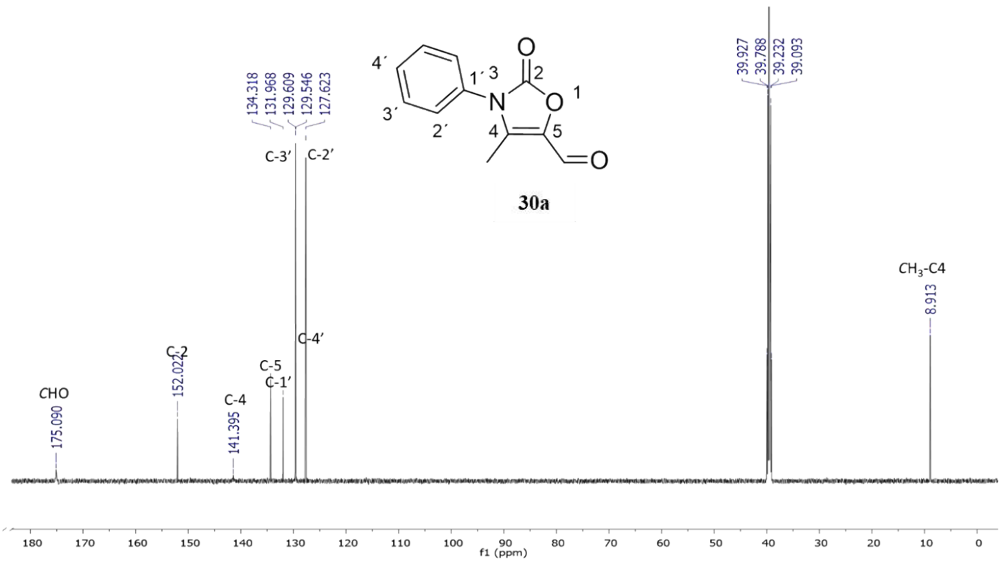

Fig. S52. ^{13}C NMR (150 MHz, DMSO-*d*6) spectrum of **30a**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

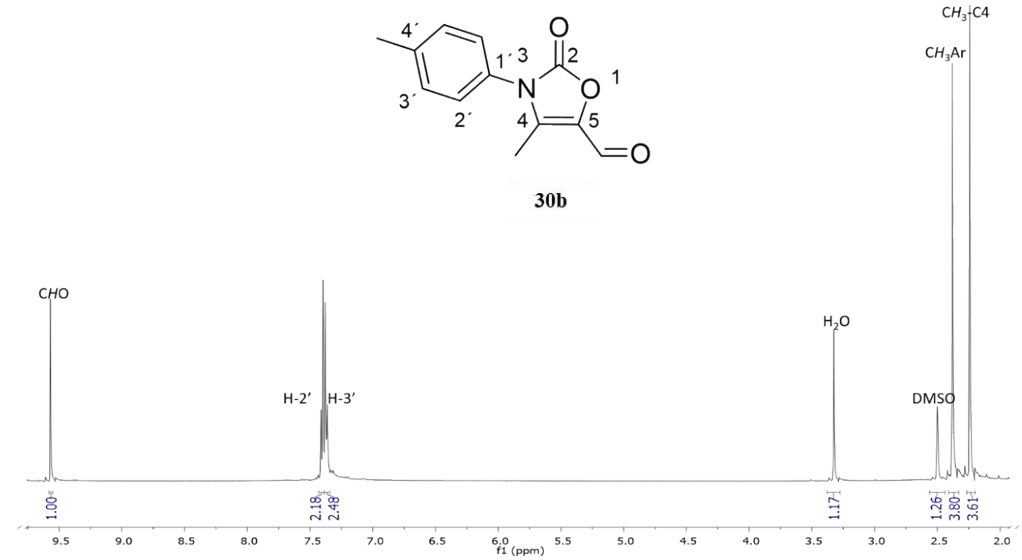

Fig. S53. ^{1}H NMR (500 MHz, DMSO-*d*6) spectrum of **30b**.

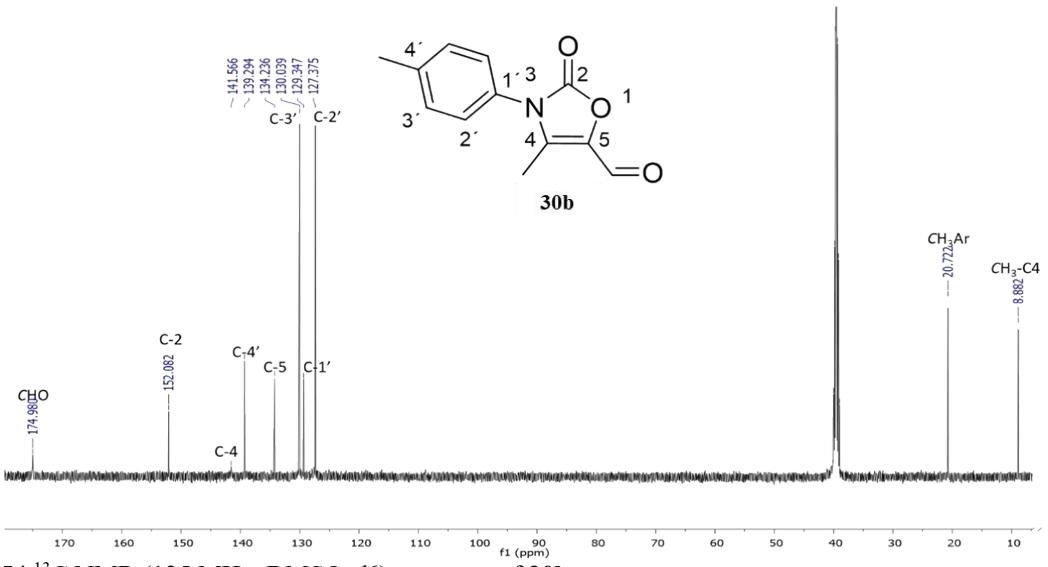

Fig. S54. ^{13}C NMR (125 MHz, DMSO-*d*6) spectrum of **30b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

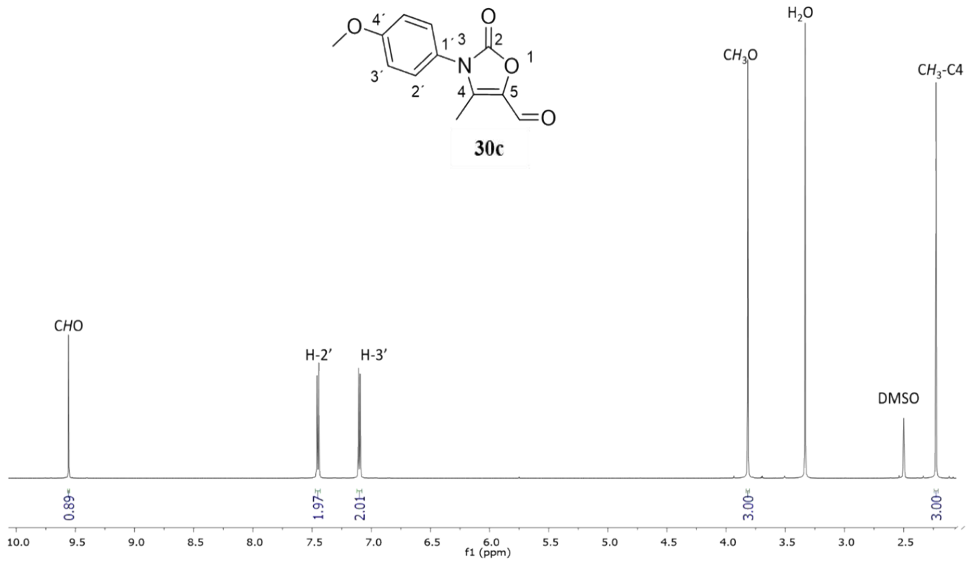

Fig. S55. ^{1}H NMR (600 MHz, DMSO-*d*6) spectrum of **30c**.

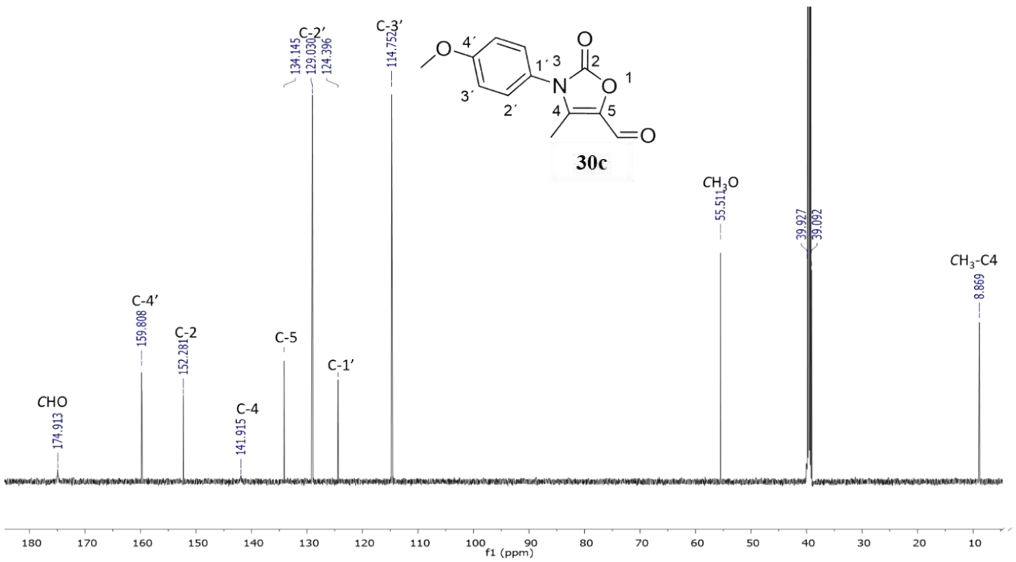

Fig. S56. ^{13}C NMR (150 MHz, DMSO-*d*6) spectrum of **30c**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

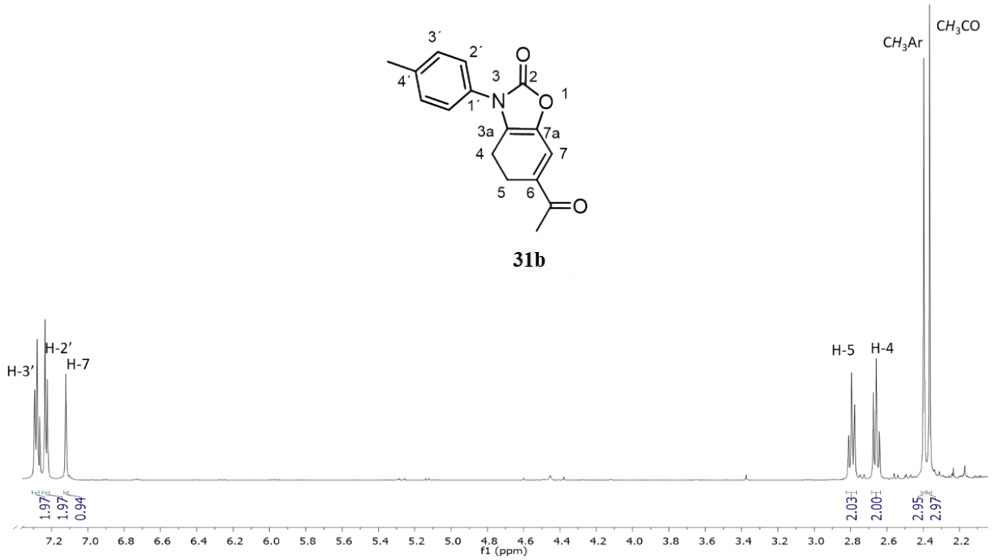

Fig. S57.[1]H NMR (600 MHz, CDCl3) spectrum of **31b**.

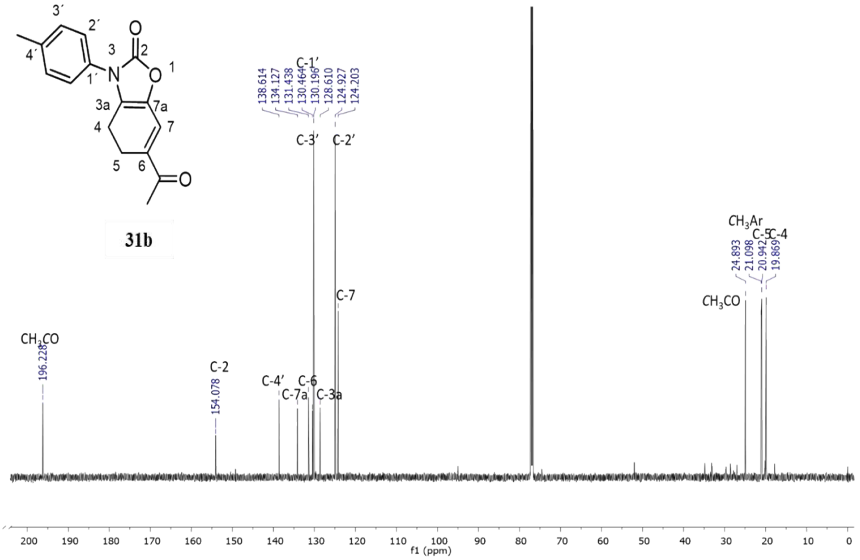

Fig. S58.[13]C NMR (150 MHz, CDCl3) spectrum of **31b**.

J. Mex. Chem. Soc. **2025**, *69*(4)
Regular Issue

ISSN-e 2594-0317

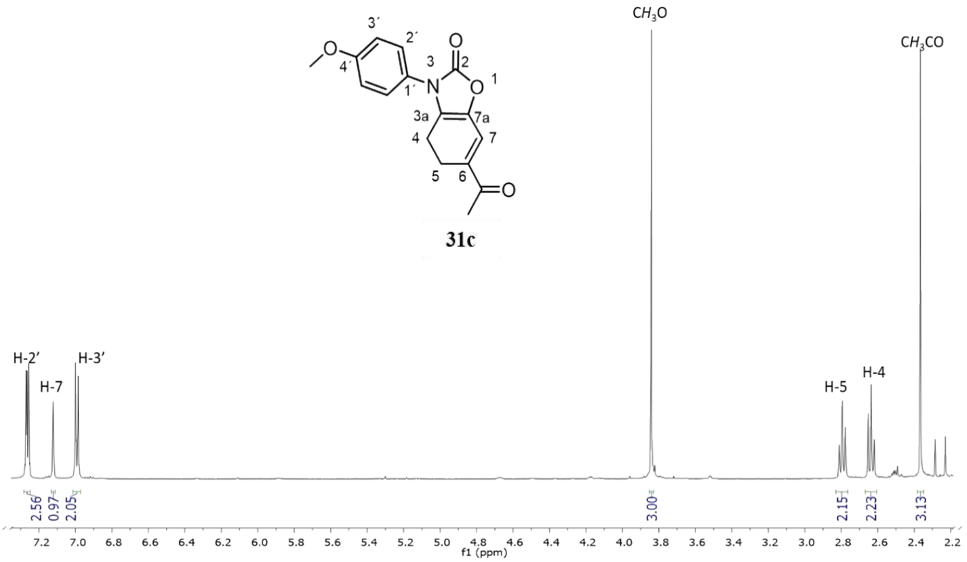

Fig. S59. ^{1}H NMR (600 MHz, CDCl3) spectrum of **31c**.

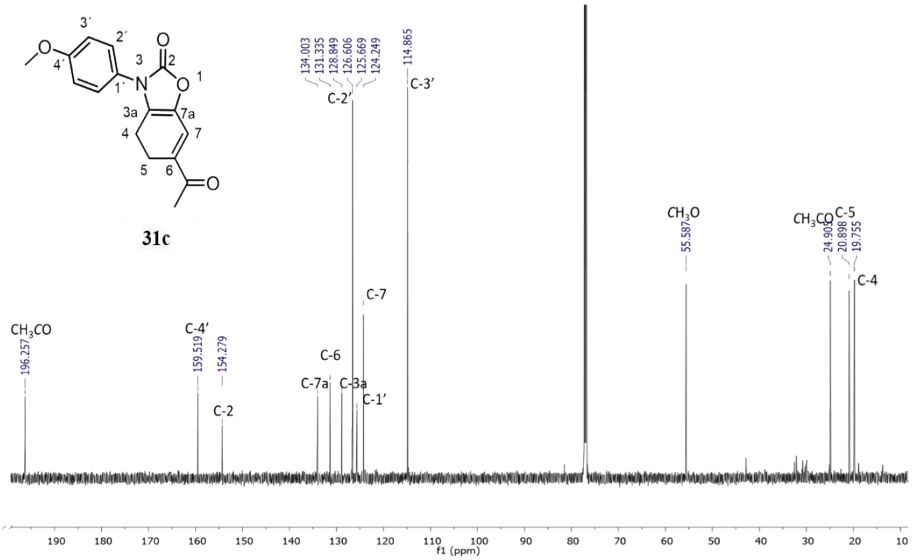

Fig. S60. ^{13}C NMR (150 MHz, CDCl3) spectrum of **31c**