

Supporting Information

Microwave-assisted one-pot efficient synthesis of functionalized 2-oxo-2-phenylethylenes-linked 2-oxobenzo[1,4]oxazines and 2-oxoquino[1,4]oxalines: Synthetic Applications, Antioxidant activity, SAR and Cytotoxic Studies

Vashundhra Sharma,^{a,‡} Pradeep K. Jaiswal,^{a,‡} Dharmendra K. Yadav,^{b,c} Mukesh Saran,^d Jaroslav Prikhodko,^e Manas Mathur,^d Ajit K. Swami,^d Irina V. Mashevskaya,^e and Sandeep Chaudhary,^{a,f,*}

^aDepartment of Chemistry, Malaviya National Institute of Technology, Jawaharlal Nehru Marg, Jaipur-302017, India.

^bDepartment of Biochemistry, All India Institute of Medical Sciences (AIIMS), Jodhpur, Rajasthan-342005, India.

^cCollege of Pharmacy, Gachon University of Medicine and Science, Room # 502, Hambakmoero 191, Yeonsu-gu, Incheon city, 406-799, Korea.

^dDepartment of Advance Molecular Microbiology, Seminal Applied Sciences Pvt. Ltd. Jaipur-302015, India.

^eDepartment of Organic Chemistry, Faculty of Chemistry, Perm State University, 15 Bukireva, Perm 614990, Russian Federation.

^fMaterials Research Centre, Malaviya National Institute of Technology, Jawaharlal Nehru Marg, Jaipur-302017, India.

Fax: 911412529029; Tel: 911412713319; E-mail: schaudhary.chy@mnit.ac.in

[‡]Both authors have equal contribution.

Contents	Page No.
Plausible mechanism for the formation of (Z)-3-(2-oxo-2-phenylethylidene)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (11a)	S2
Copies of characterization spectra of ¹ H and ¹³ C NMR of 2-oxobenzo[1,4]oxazines 11a-n , 2-oxoquino[1,4]oxalines 14a-h and Cephalandole A 16 .	S3-S25

Plausible mechanism for the formation of (Z)-3-(2-oxo-2-phenylethylidene)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-one (11a)

A plausible mechanism for the formation of the desired 2-oxo-benzo[1,4]oxazine **11a**, which was formed by the reaction between **9a** and **10a** under the optimized conditions involves intermolecular condensation followed by an intramolecular condensation and we obtained (Z)-isomer (*cis*) as the only product. We speculate that the probable reason could be the existence of H-bonding between proton on ring B nitrogen atom and oxygen of α, β -unsaturated carbonyl group which stabilizes the Z-isomer as the only product **11a**.

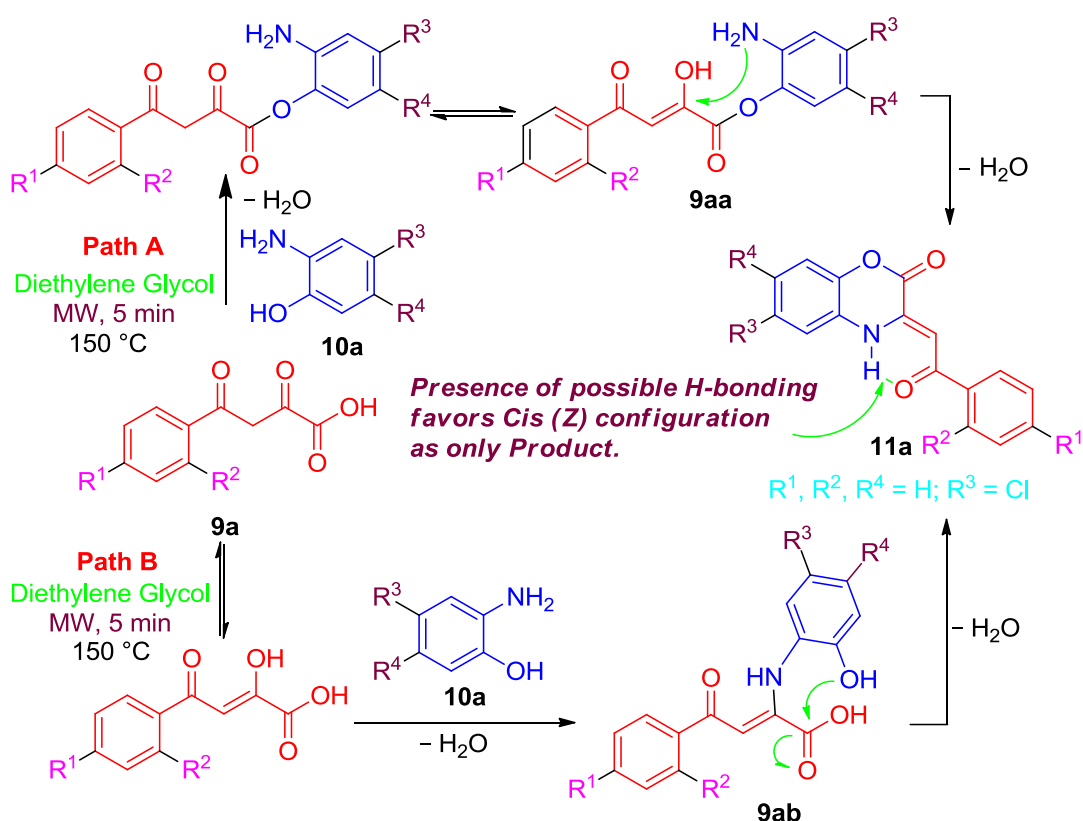


Figure 1. Possible pathway for the formation of 2-oxo-benzo[1, 4] oxazine **11a**.

Characterization spectra (^1H and ^{13}C NMR) of 2-oxobenzo[1,4]oxazines 11a-n, 2-oxoquino[1,4]oxalines 14a-h and Cephalandole A 16:

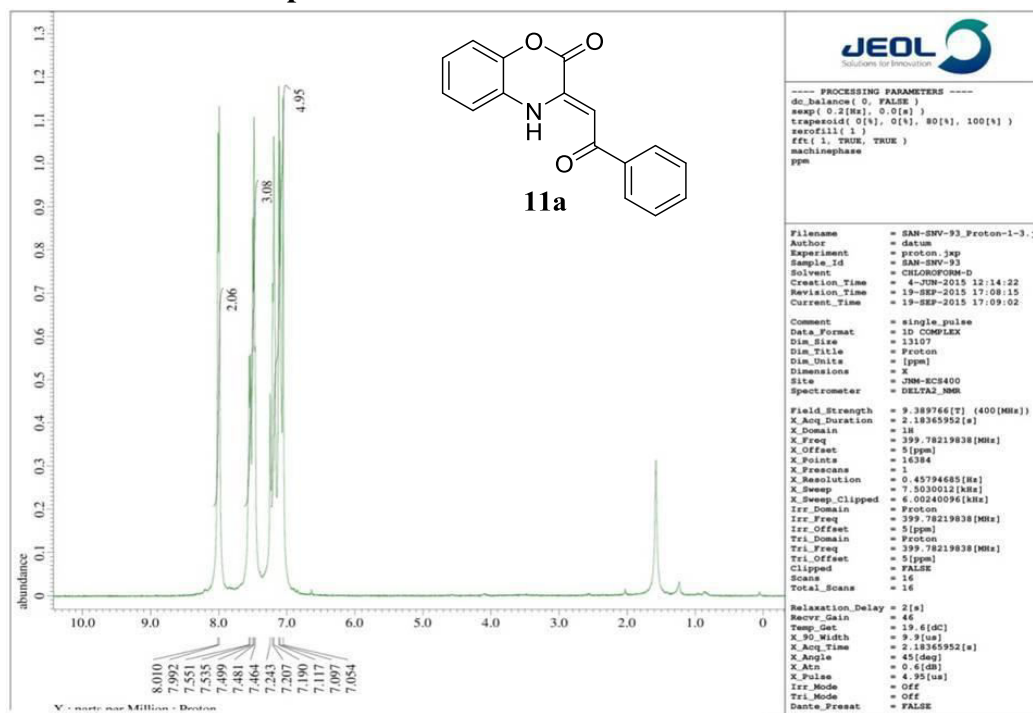


Figure 1. ^1H NMR Spectra of Compound 11a.

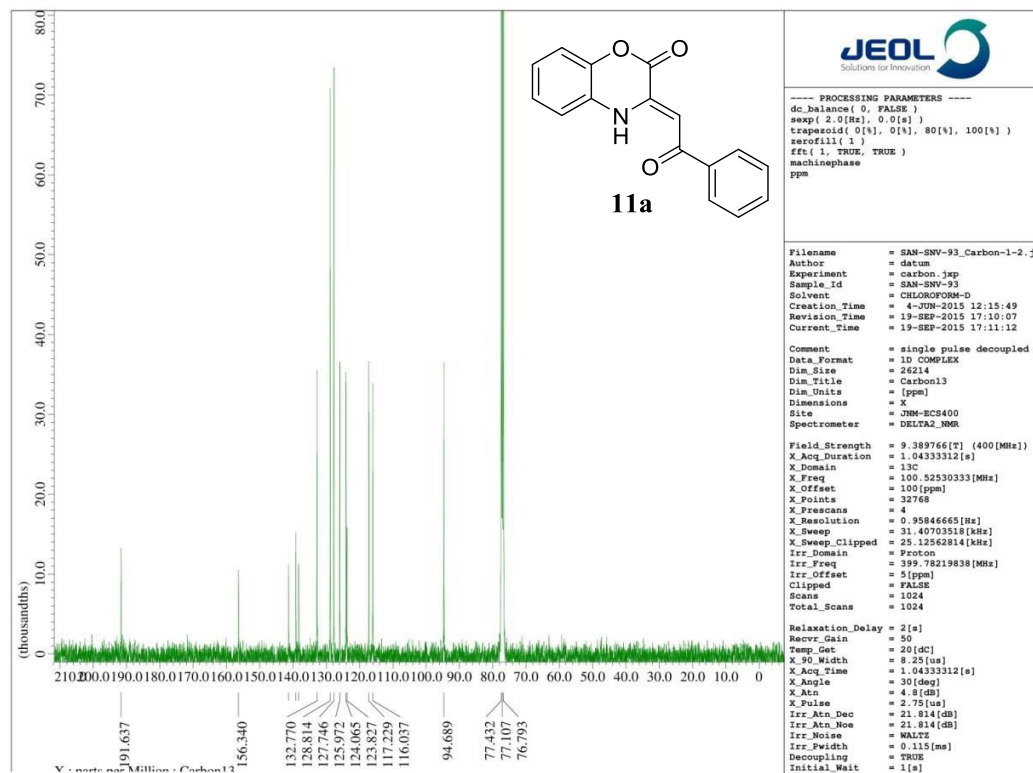


Figure 2. ^{13}C NMR Spectra of Compound 11a.

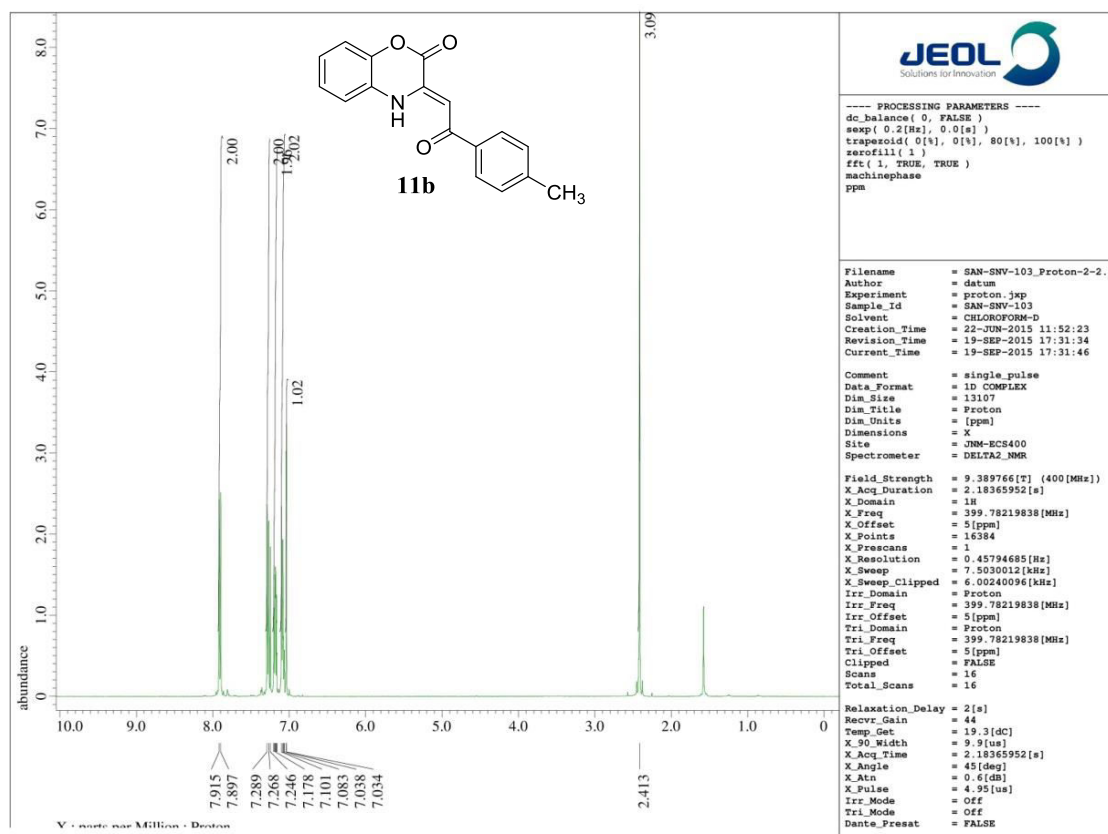


Figure 3. ¹H NMR Spectra of Compound 11b.

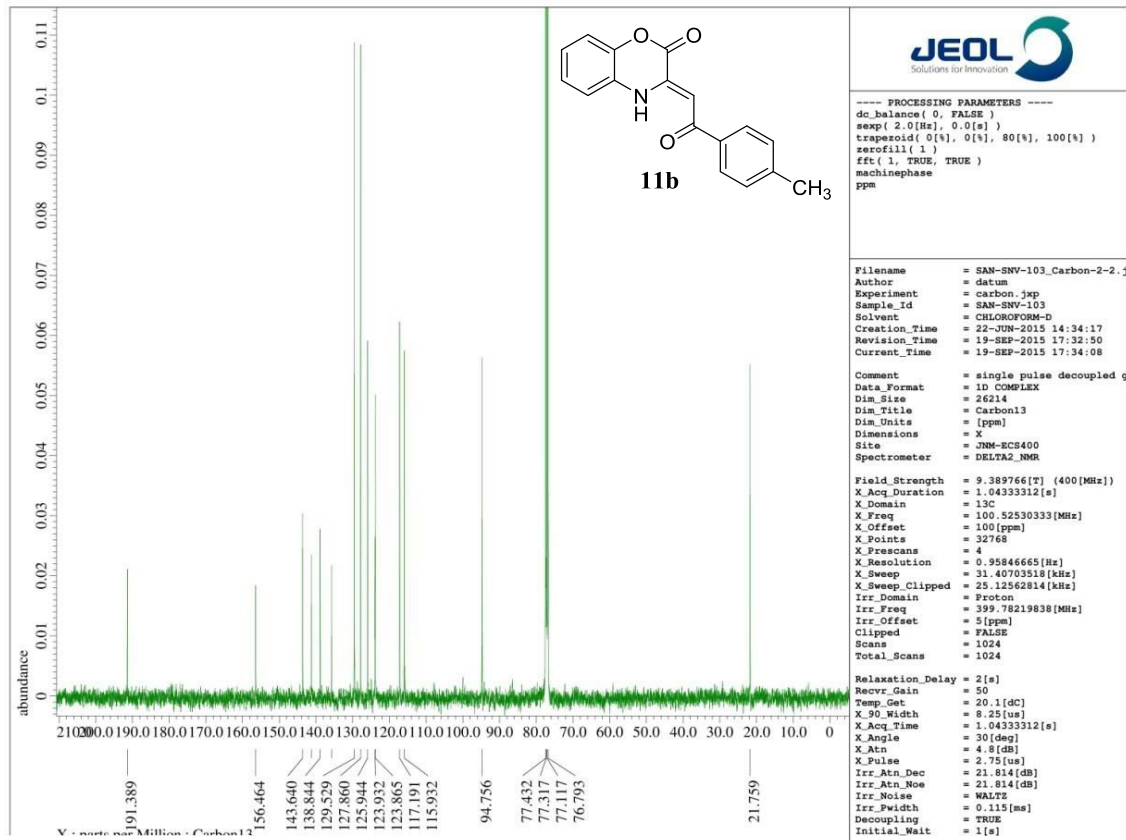


Figure 4. ¹³C NMR Spectra of Compound 11b.

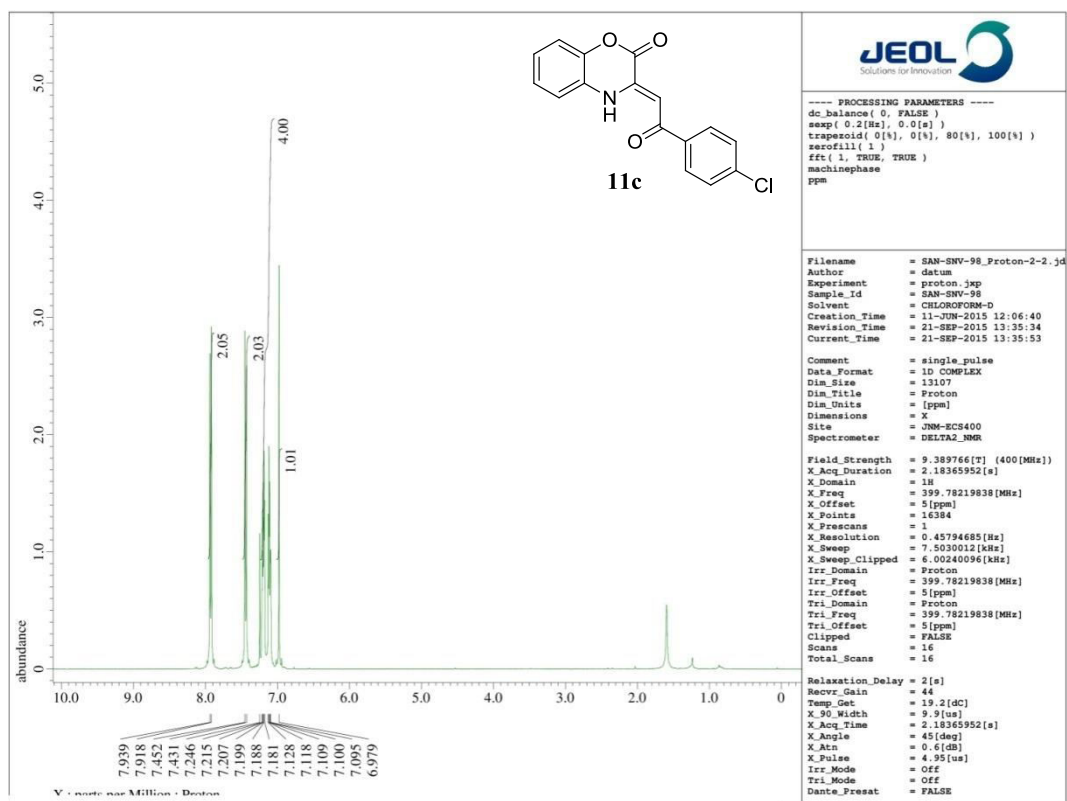


Figure 5. ¹H NMR Spectra of Compound 11c.

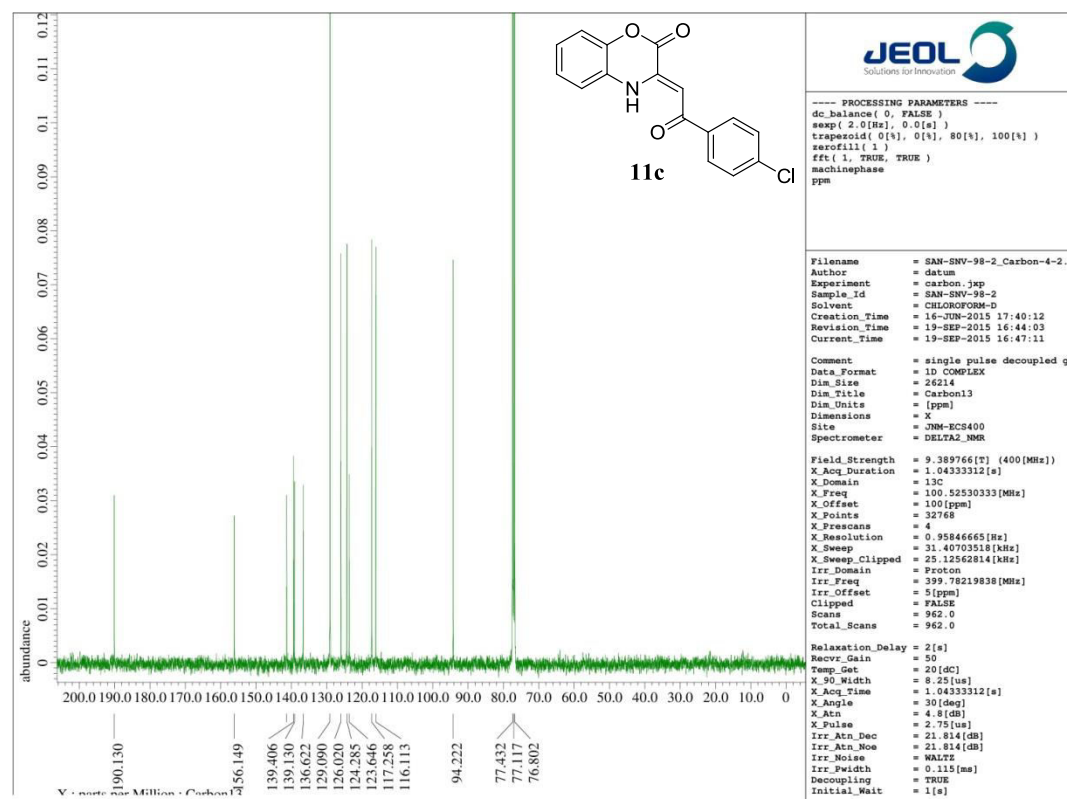


Figure 6. ¹³C NMR Spectra of Compound 11c.

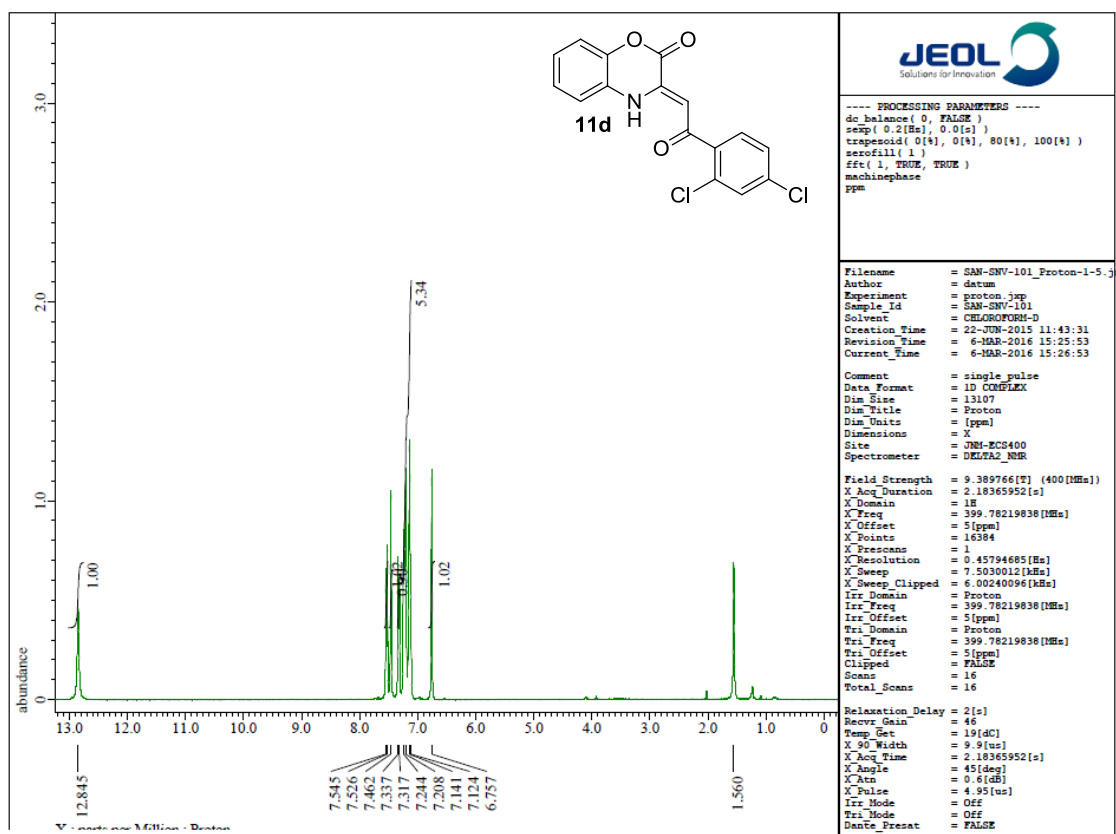


Figure 7. ¹H NMR Spectra of Compound 11d.

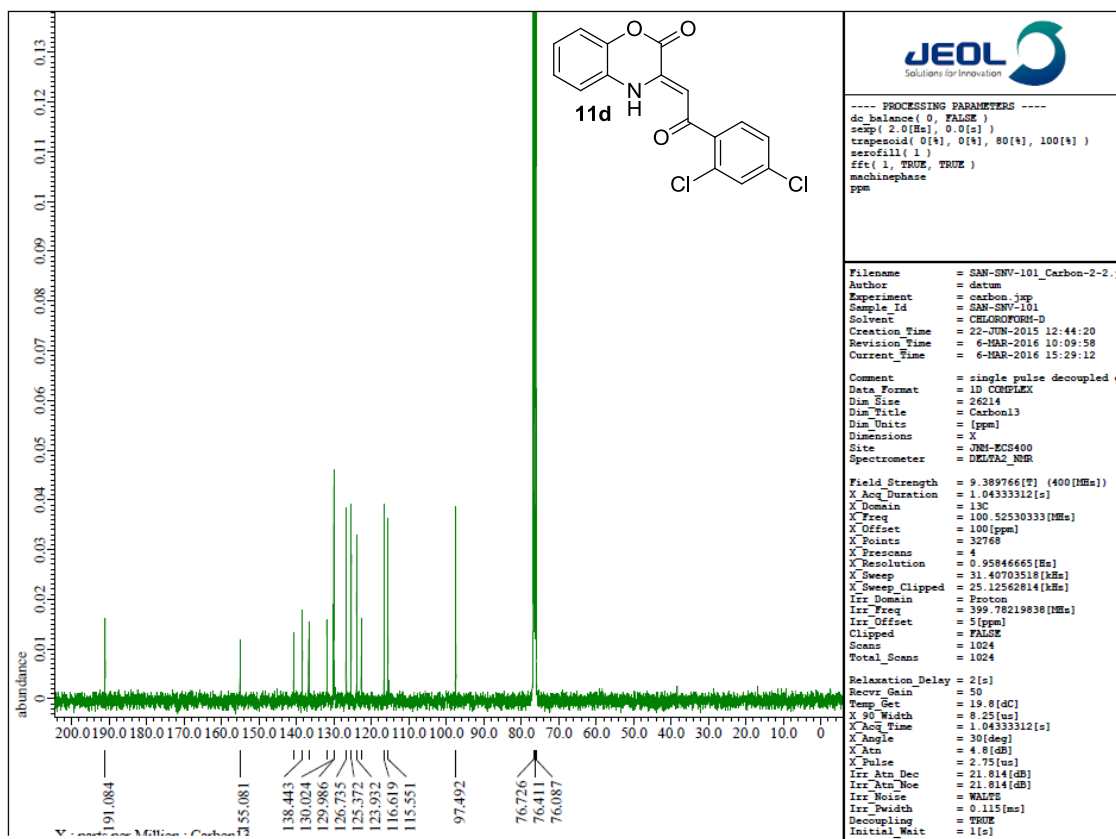


Figure 8. ¹³C NMR Spectra of Compound 11d.

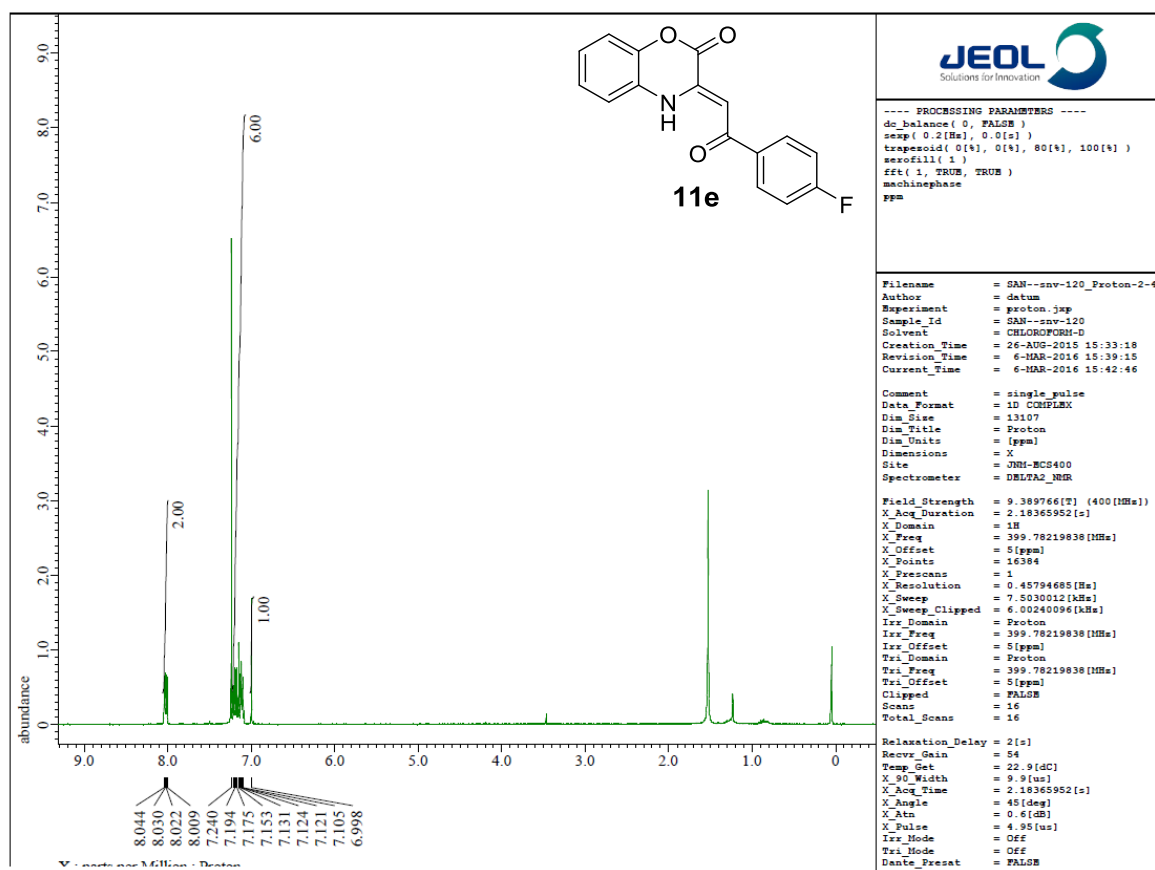


Figure 9. ¹H NMR Spectra of Compound 11e.

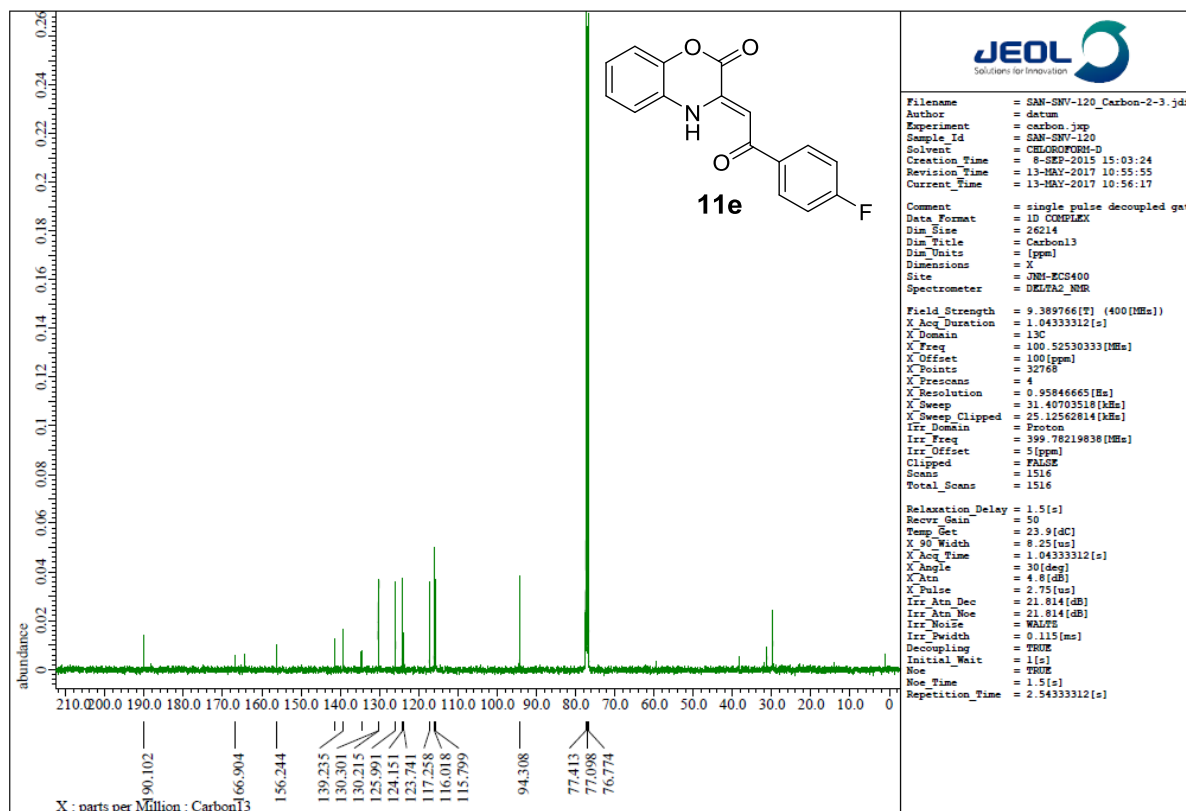


Figure 10. ¹³C NMR Spectra of Compound 11e.

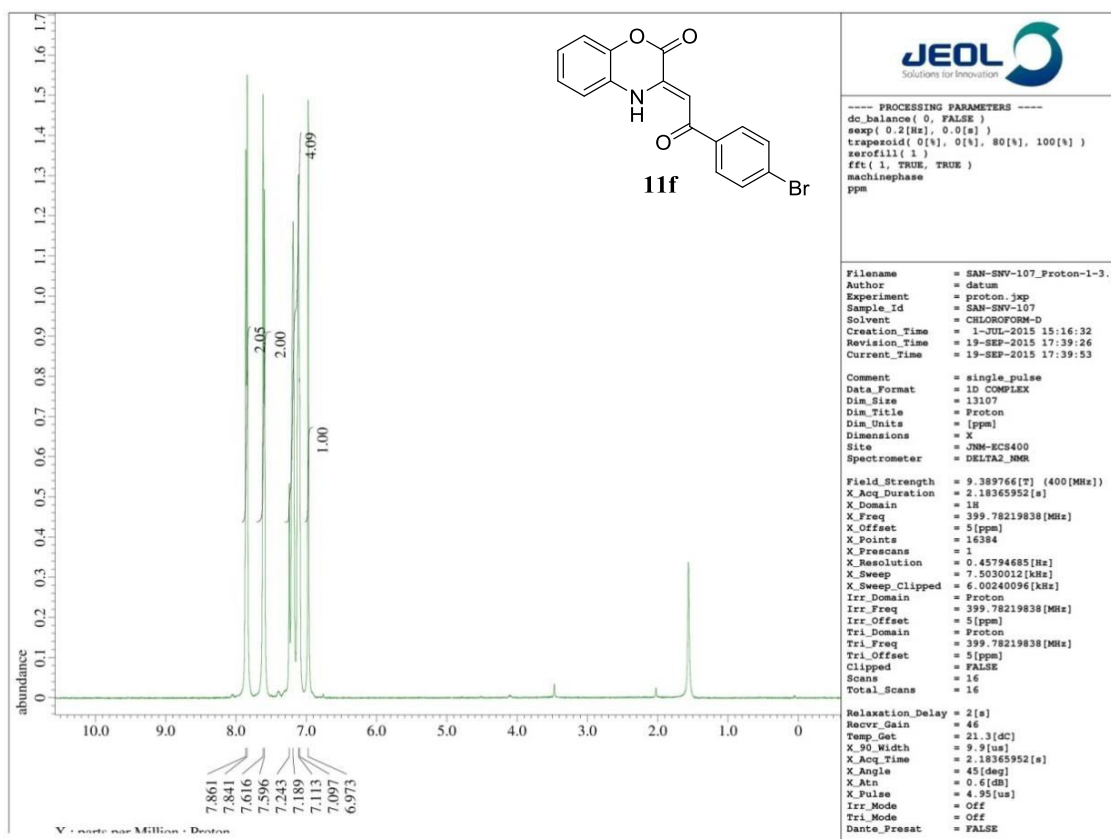


Figure 11. ¹H NMR Spectra of Compound 11f.

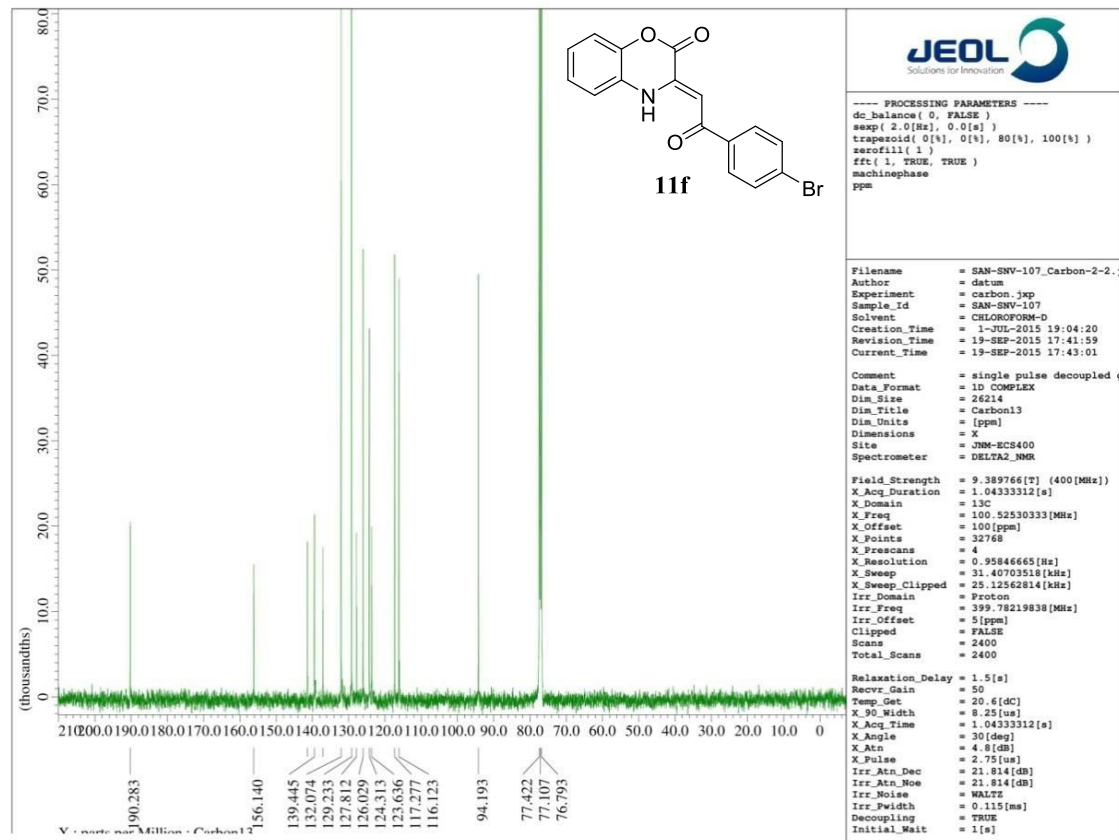


Figure 12. ¹³C NMR Spectra of Compound 11f.

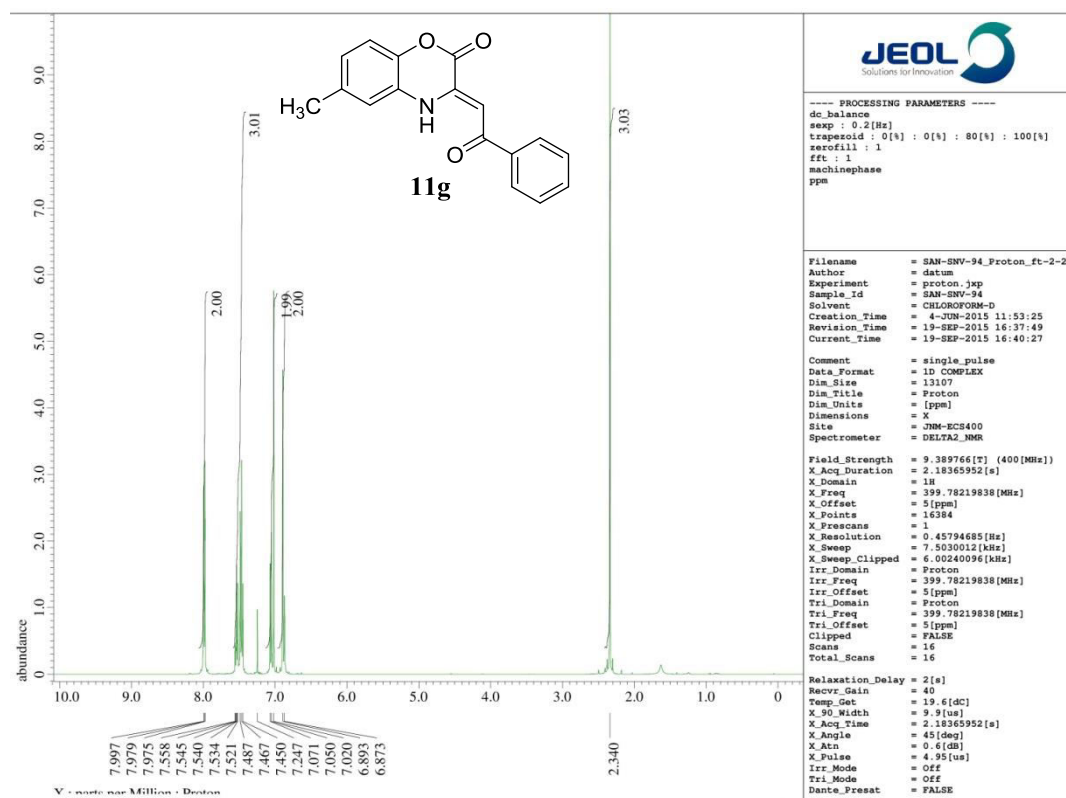


Figure 13. ¹H NMR Spectra of Compound 11g.

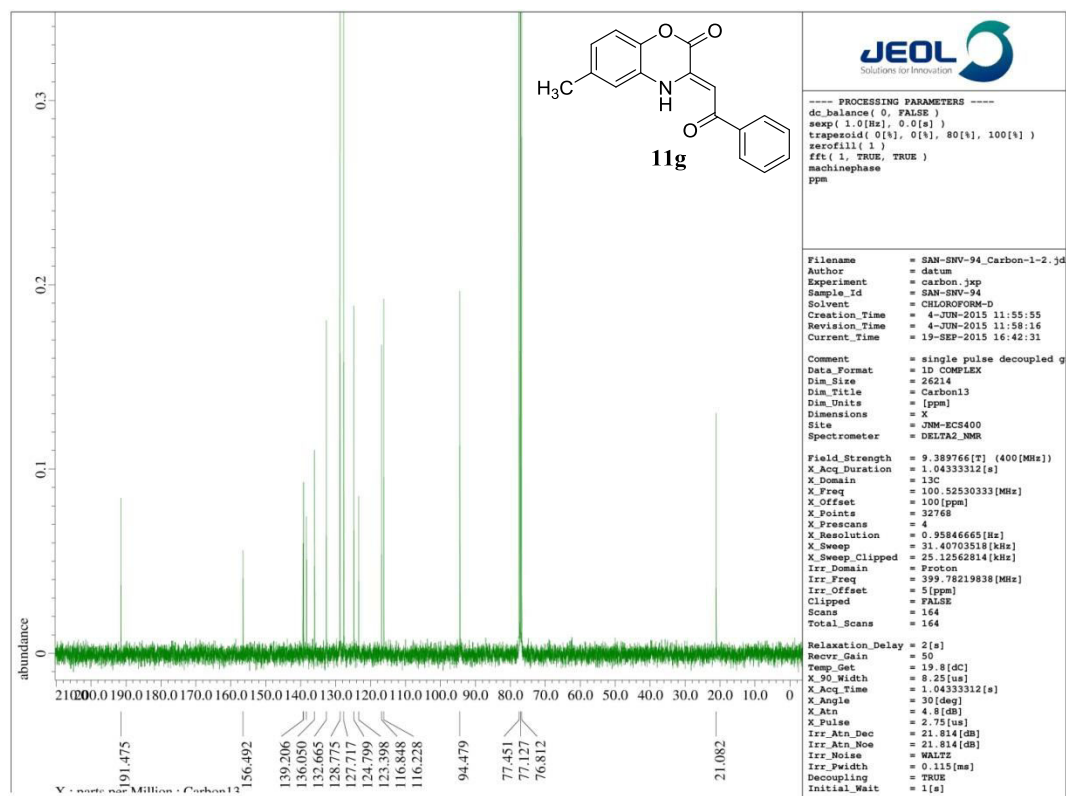


Figure 14. ¹³C NMR Spectra of Compound 11g.

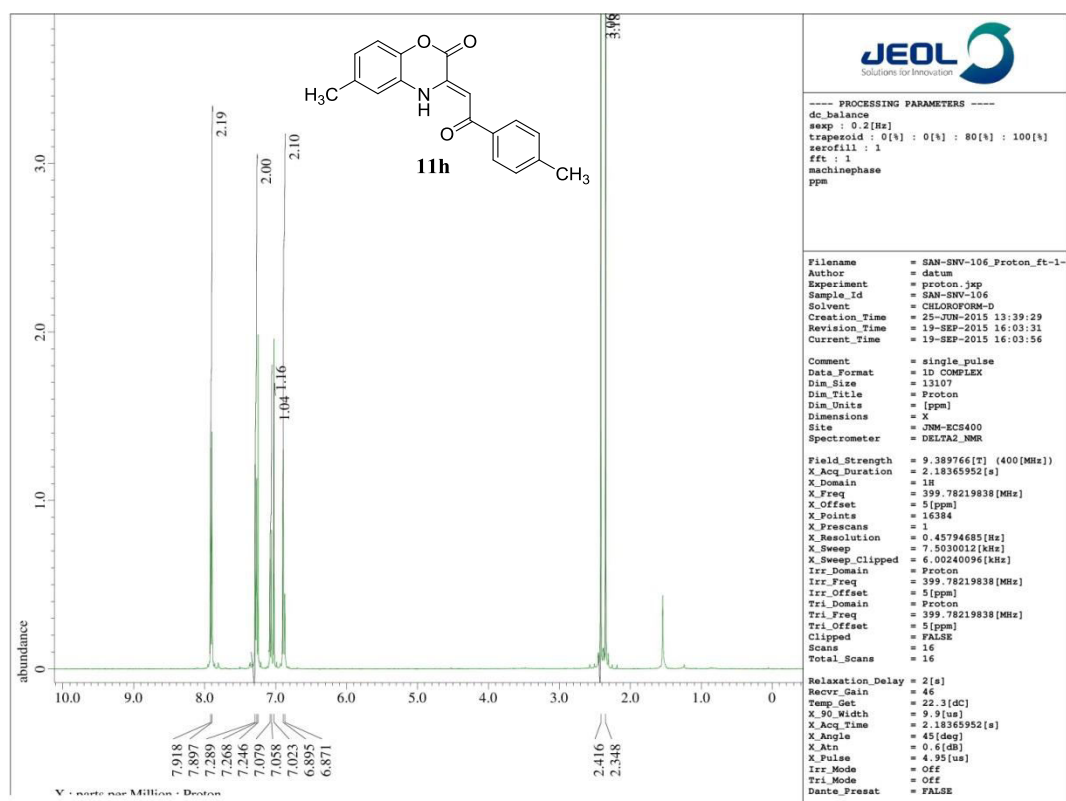


Figure 15. ¹H NMR Spectra of Compound 11h.

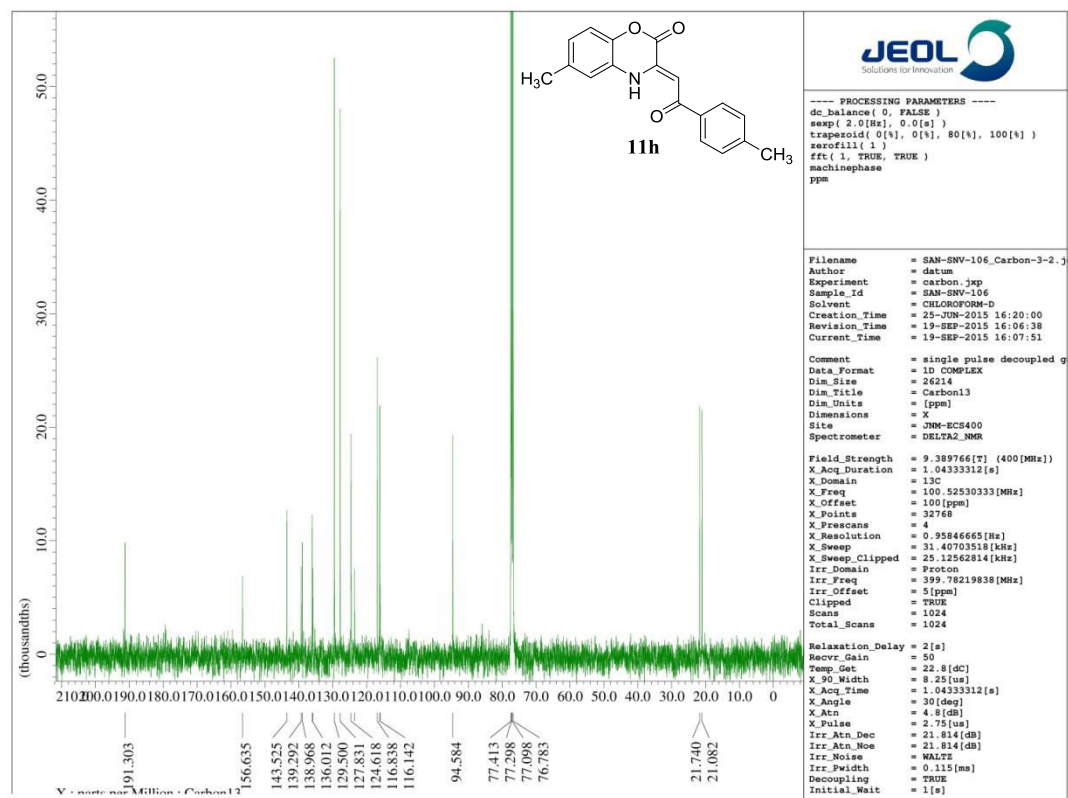


Figure 16. ¹³C NMR Spectra of Compound 11h.

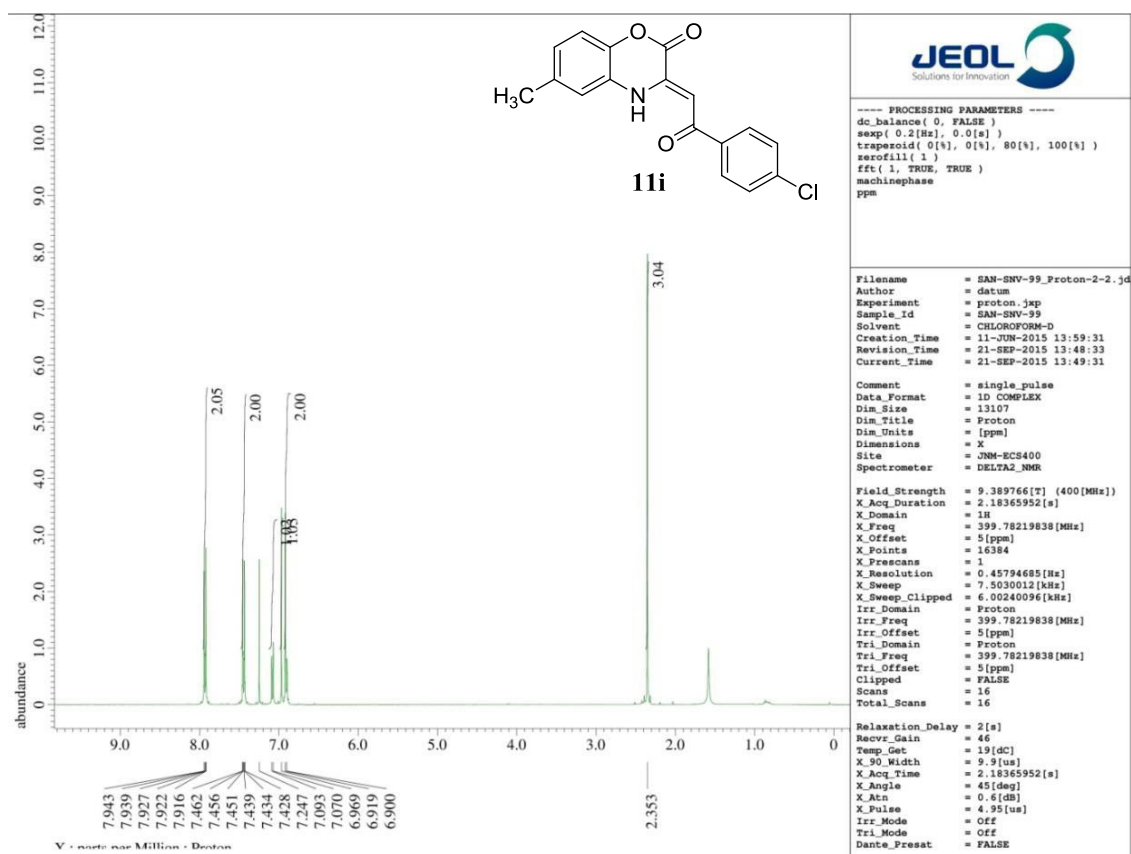


Figure 17. ^1H NMR Spectra of Compound 11i.

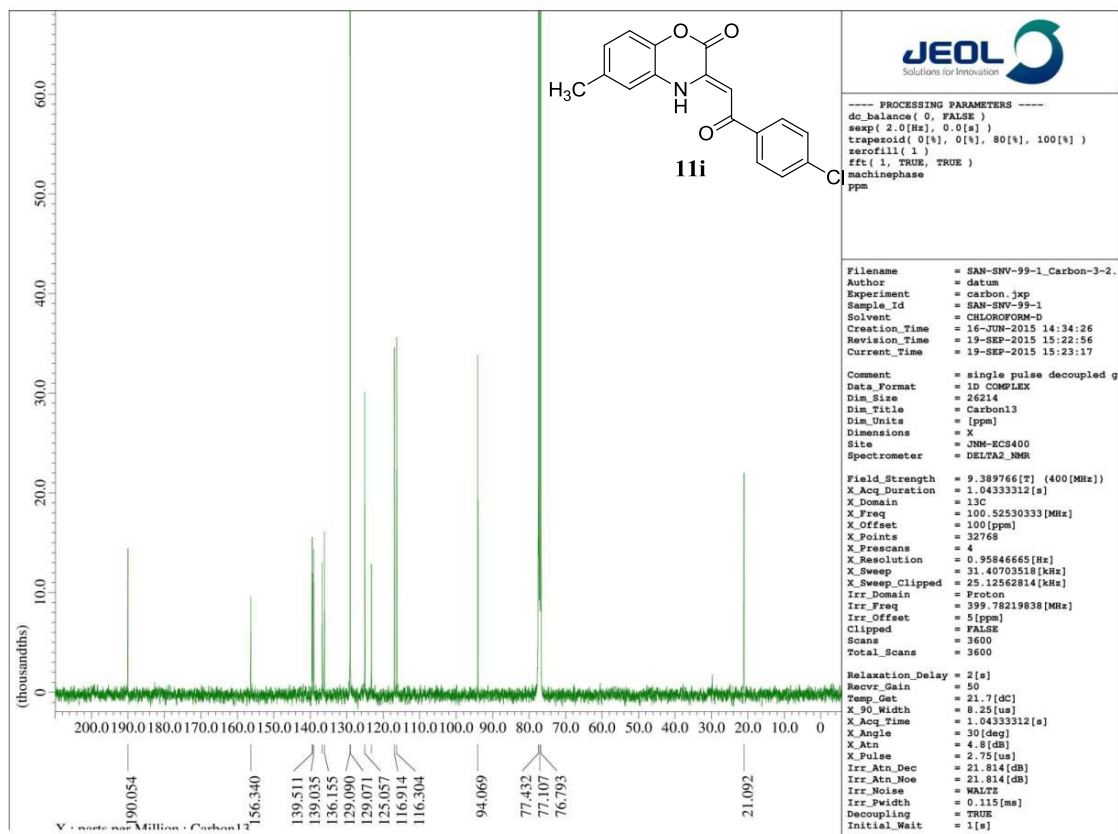


Figure 18. ^{13}C NMR Spectra of Compound 11i.

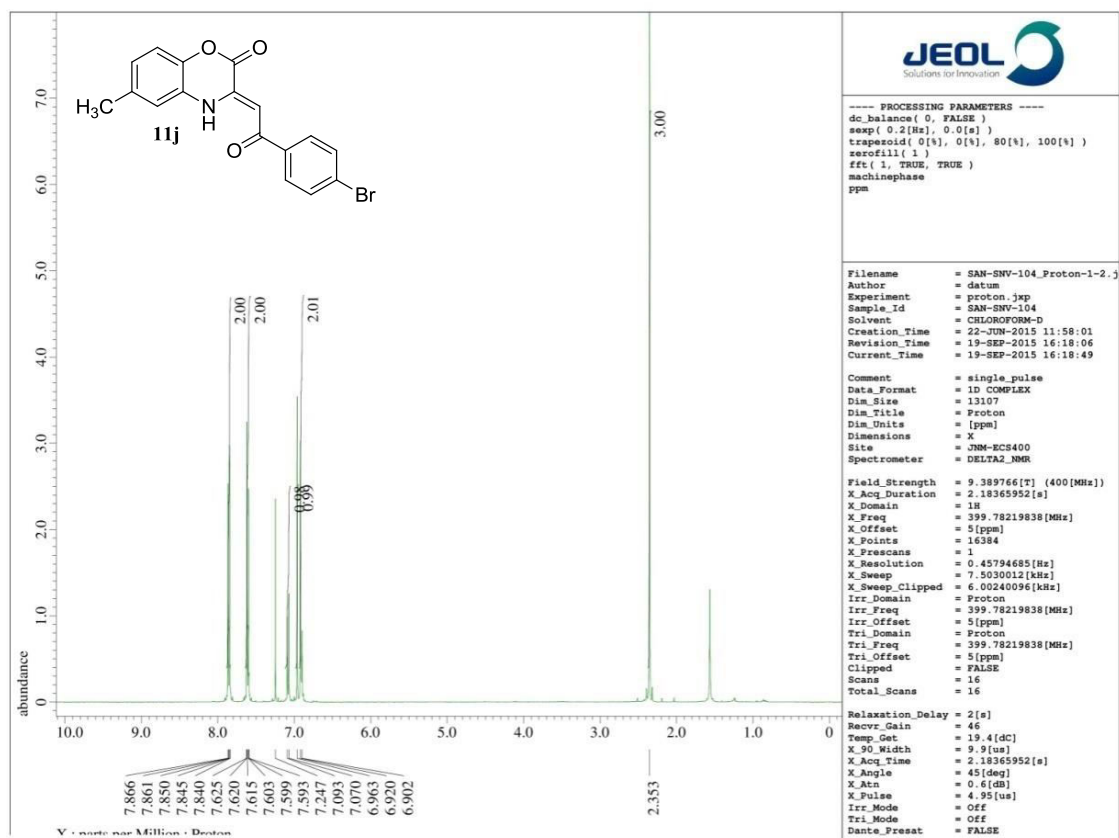


Figure 19. ¹H NMR Spectra of Compound 11j.

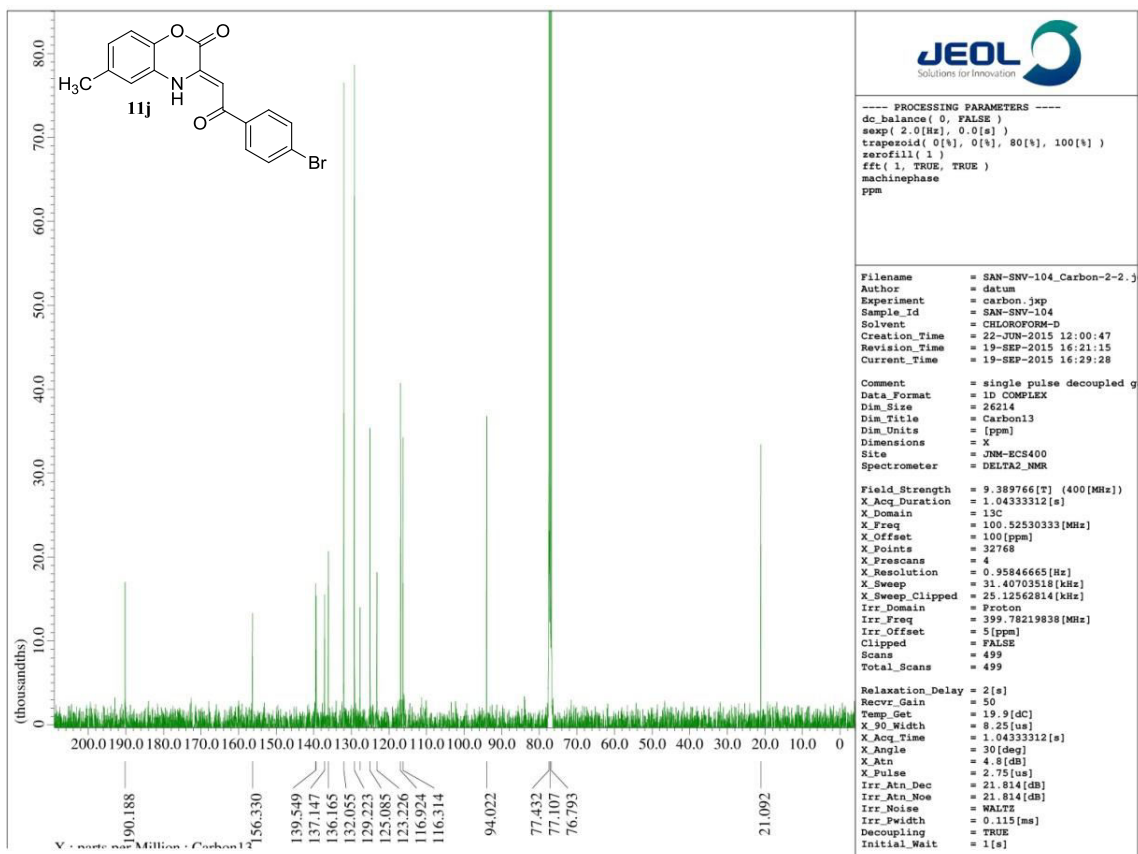


Figure 20. ¹³C NMR Spectra of Compound 11j.

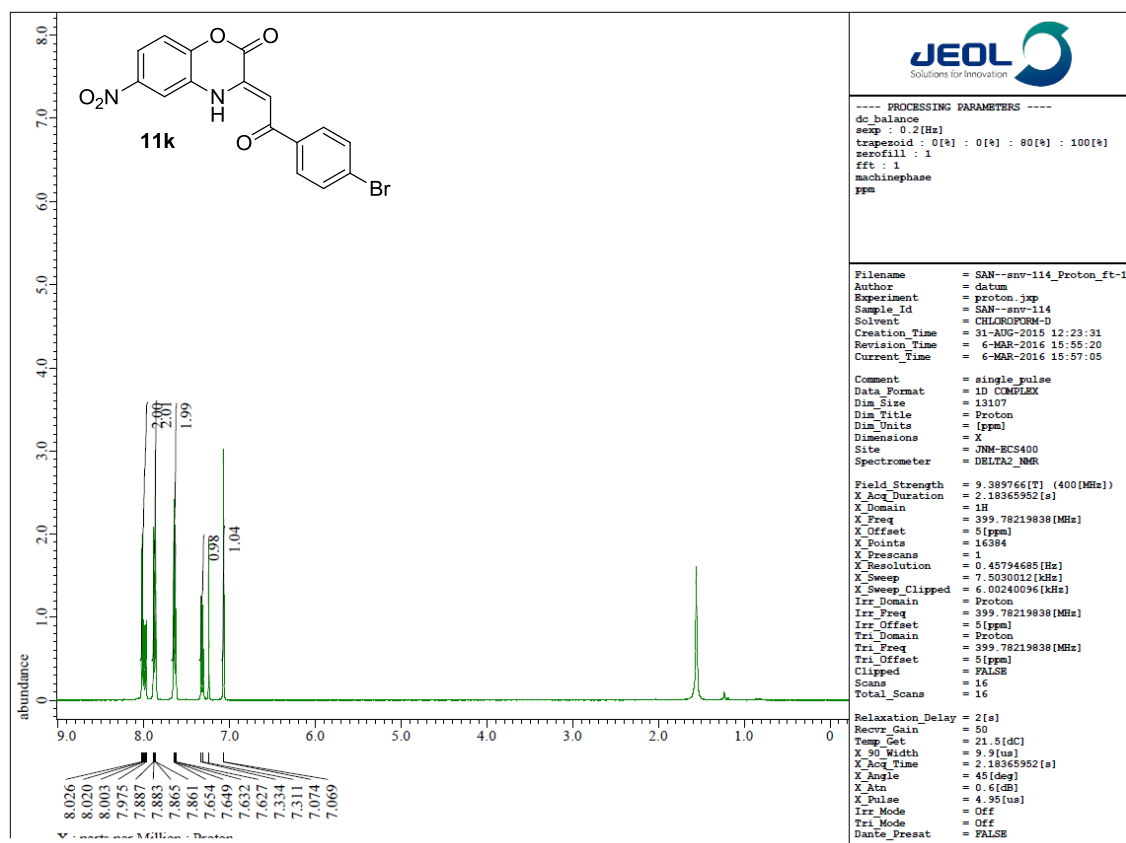


Figure 21. ¹H NMR Spectra of Compound 11k.

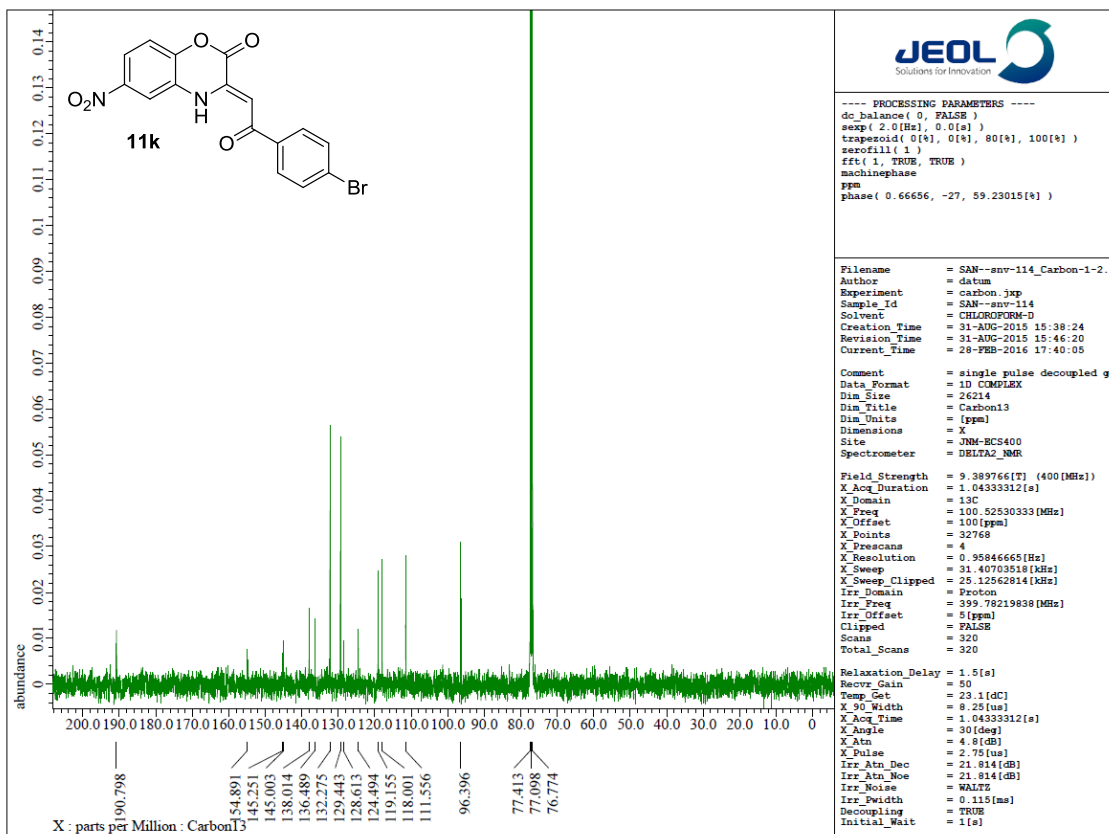


Figure 22. ¹³C NMR Spectra of Compound 11k.

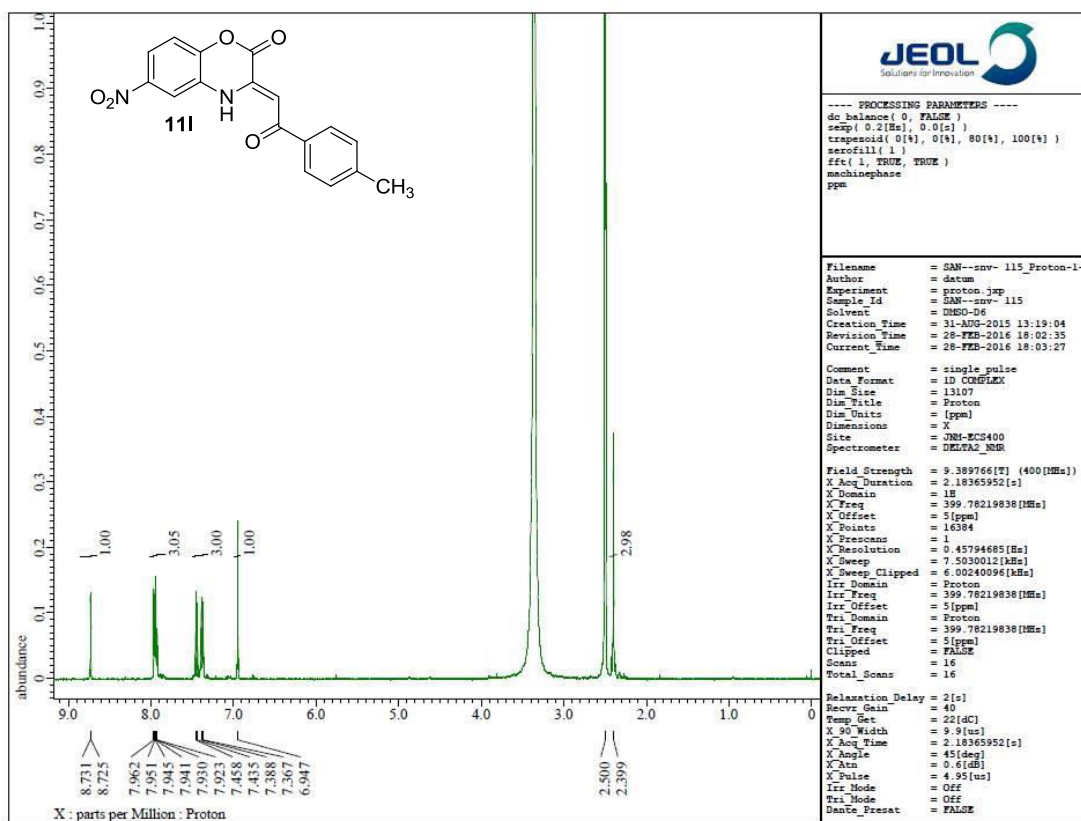


Figure 23. ¹H NMR Spectra of Compound 11l.

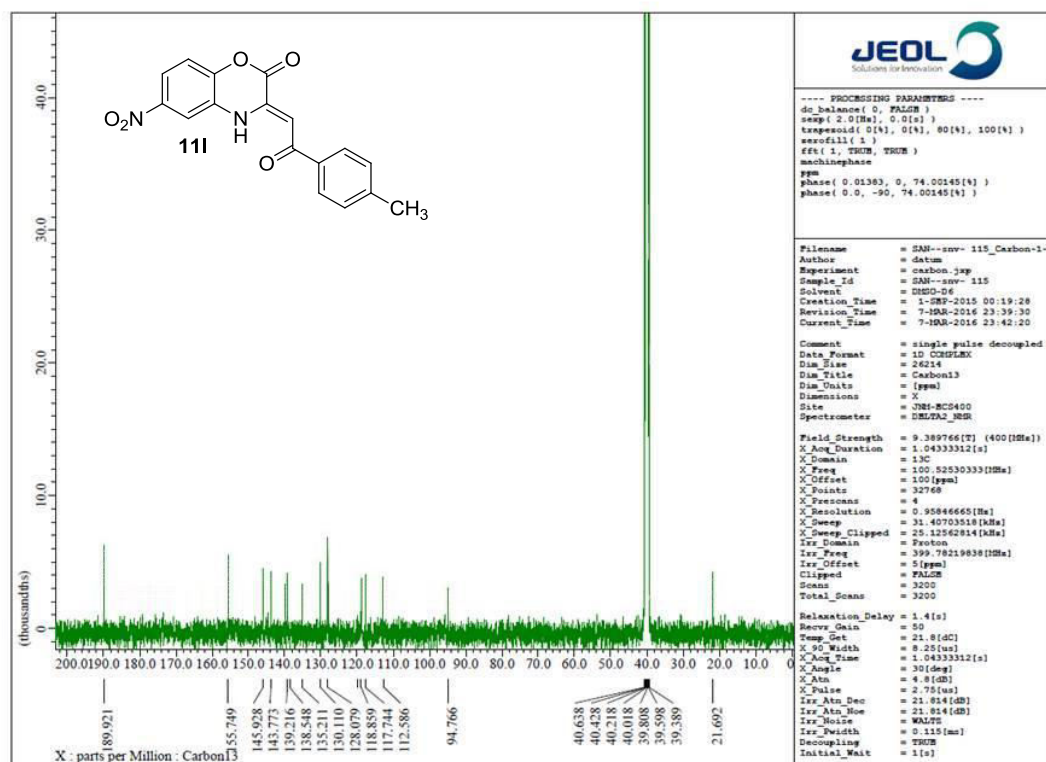


Figure 24. ¹³C NMR Spectra of Compound 11l.

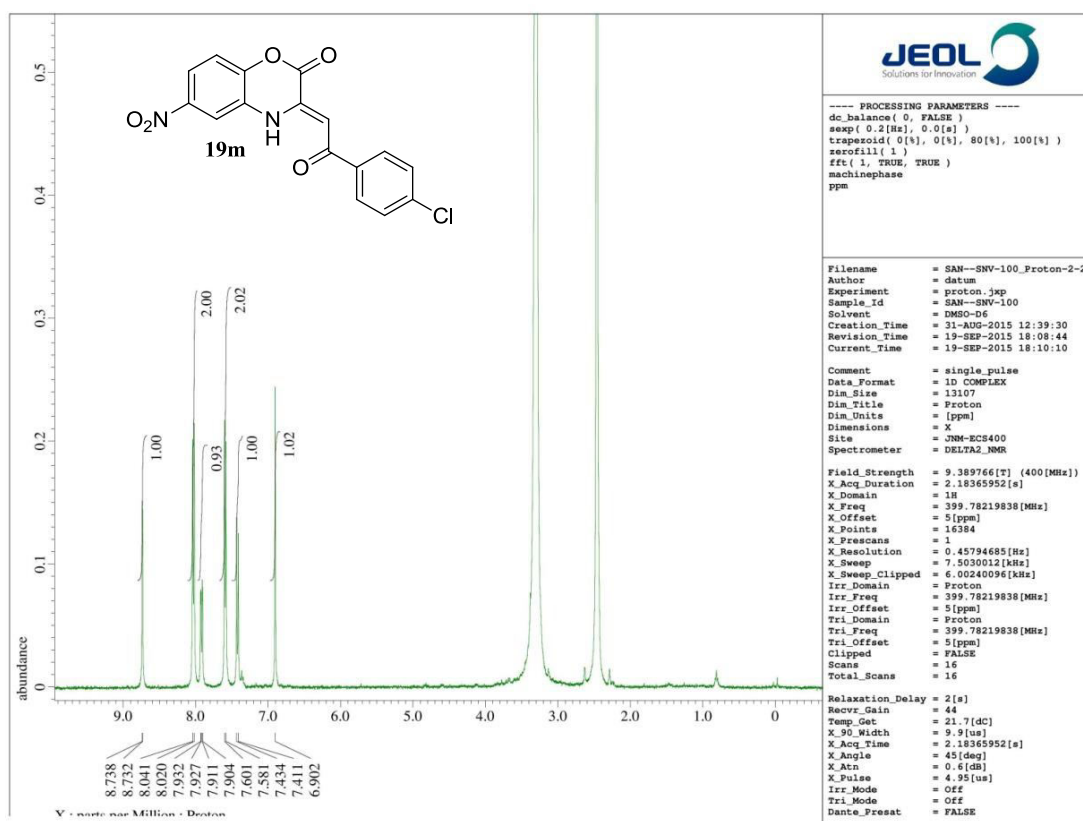


Figure 25. ¹H NMR Spectra of Compound 11m.

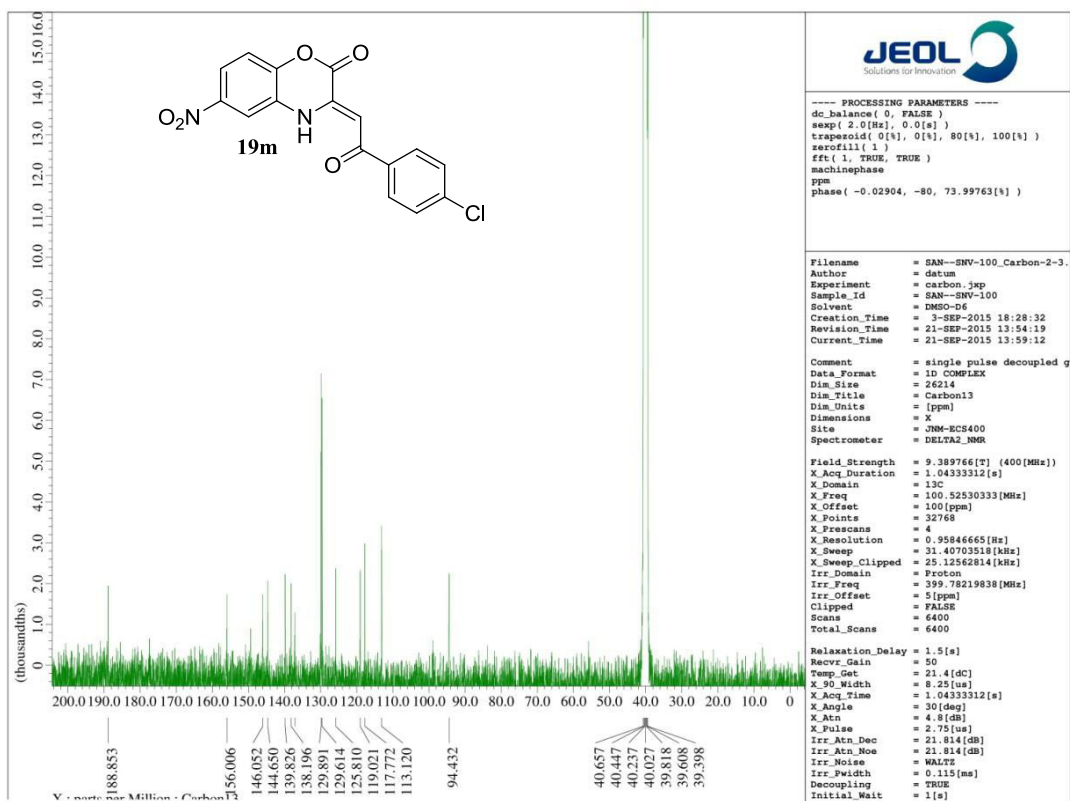


Figure 26. ¹³C NMR Spectra of Compound 11m.

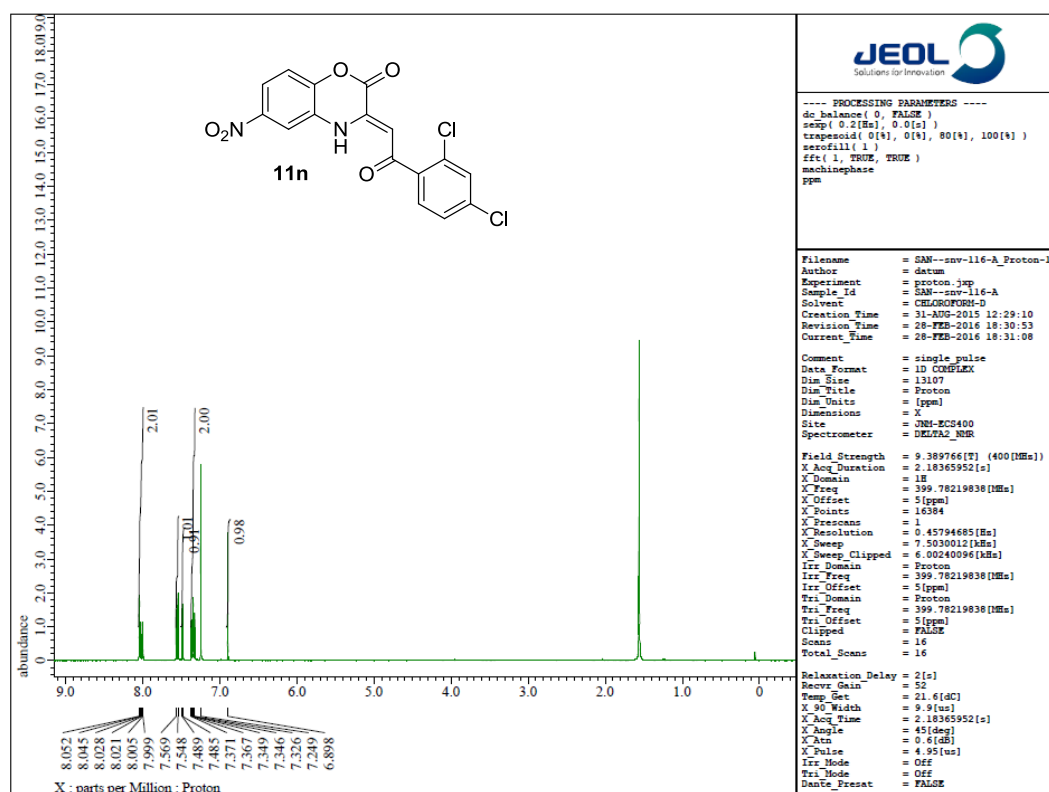


Figure 27. ¹H NMR Spectra of Compound 11n.

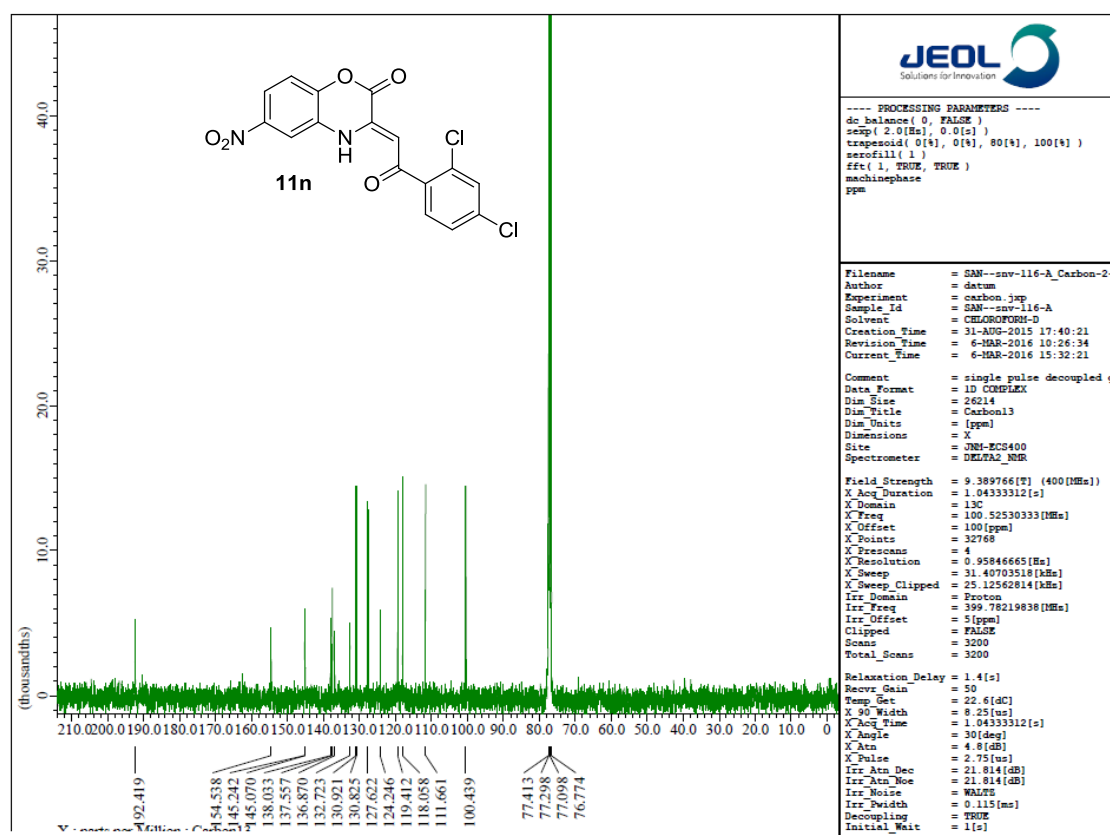
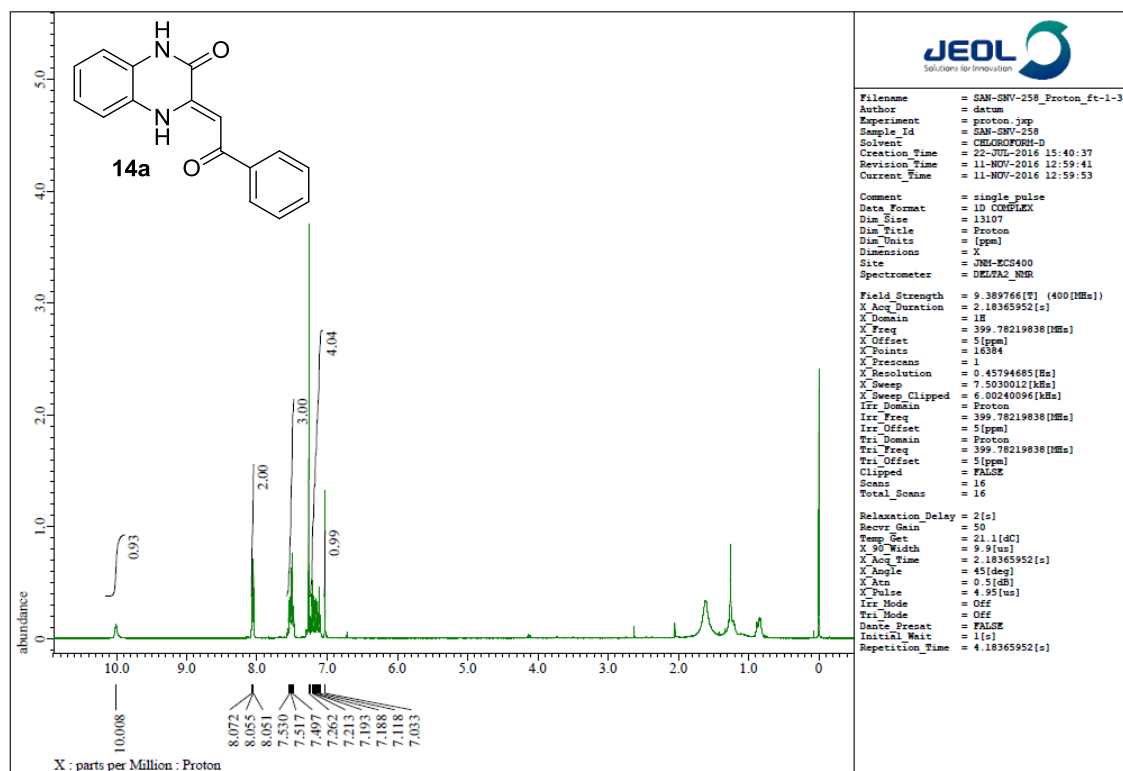
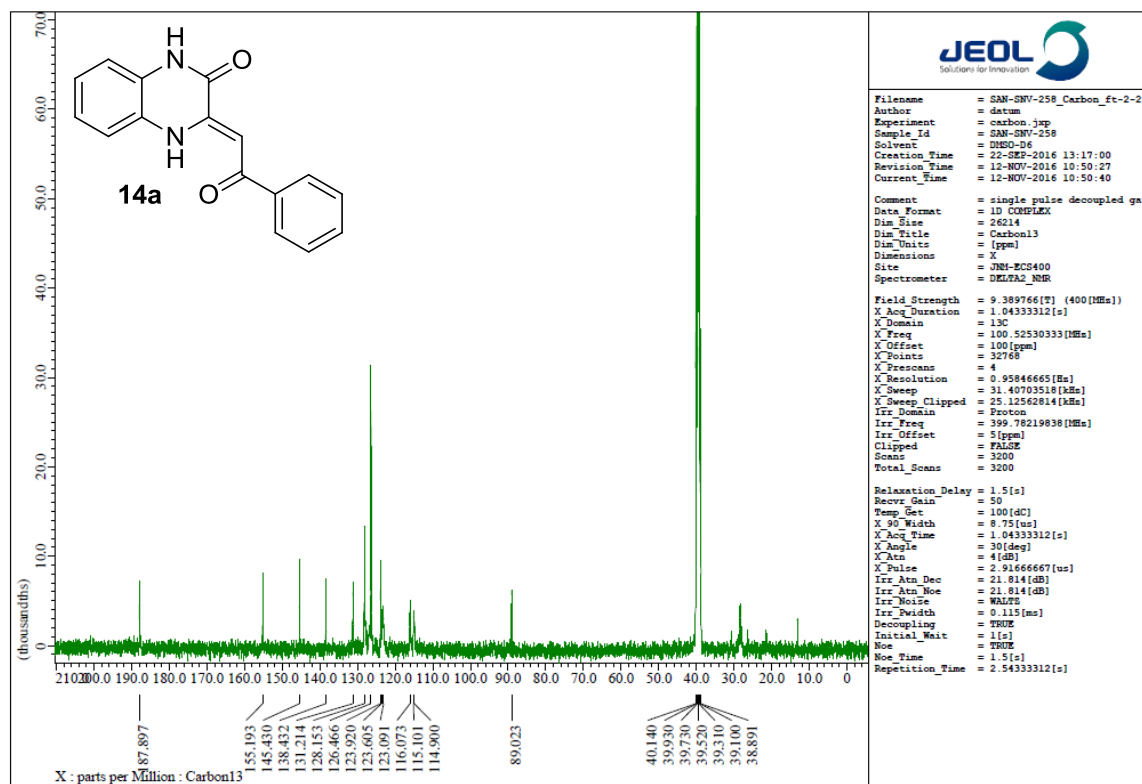


Figure 28. ¹³C NMR Spectra of Compound 11n.



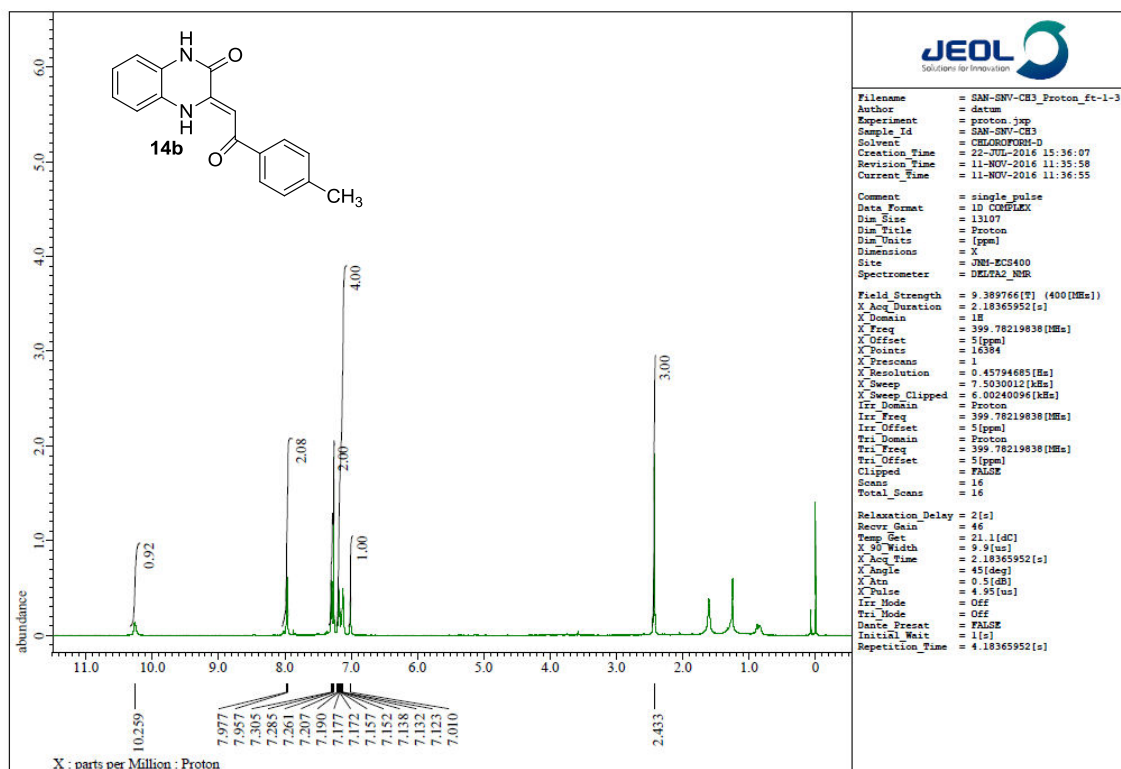
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Figure 29. ¹H NMR Spectra of Compound 14a.



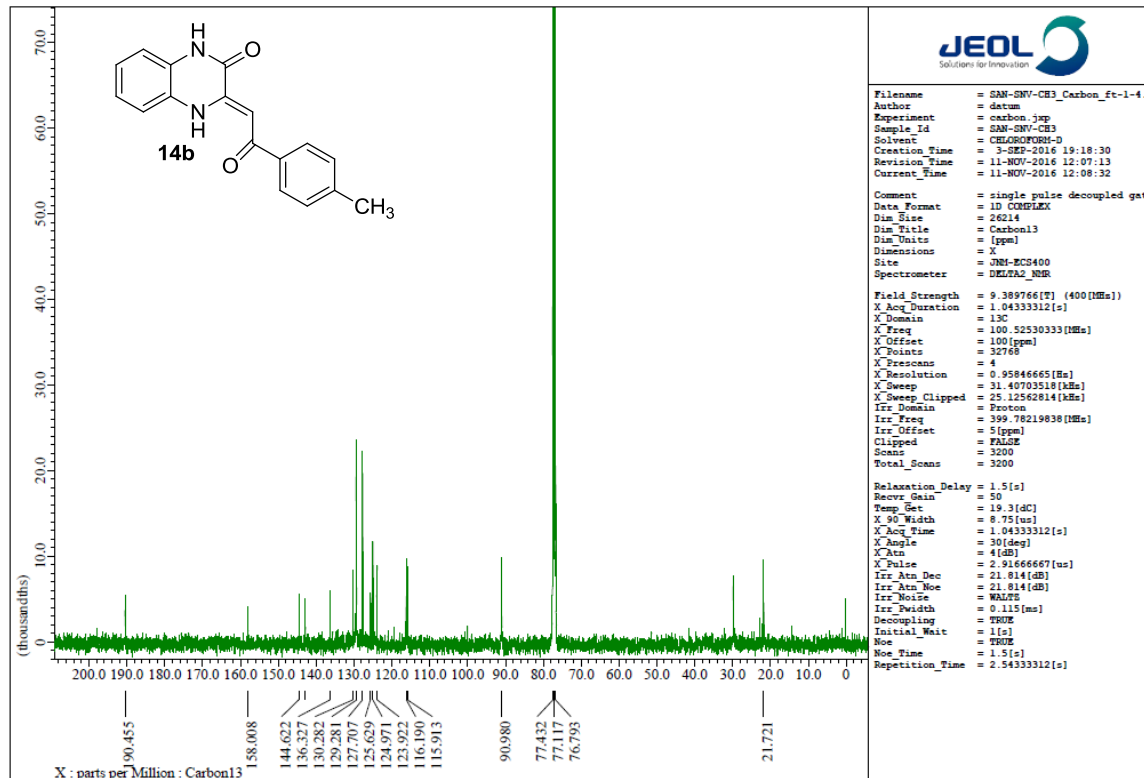
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Figure 30. ¹³C NMR Spectra of Compound 14a.



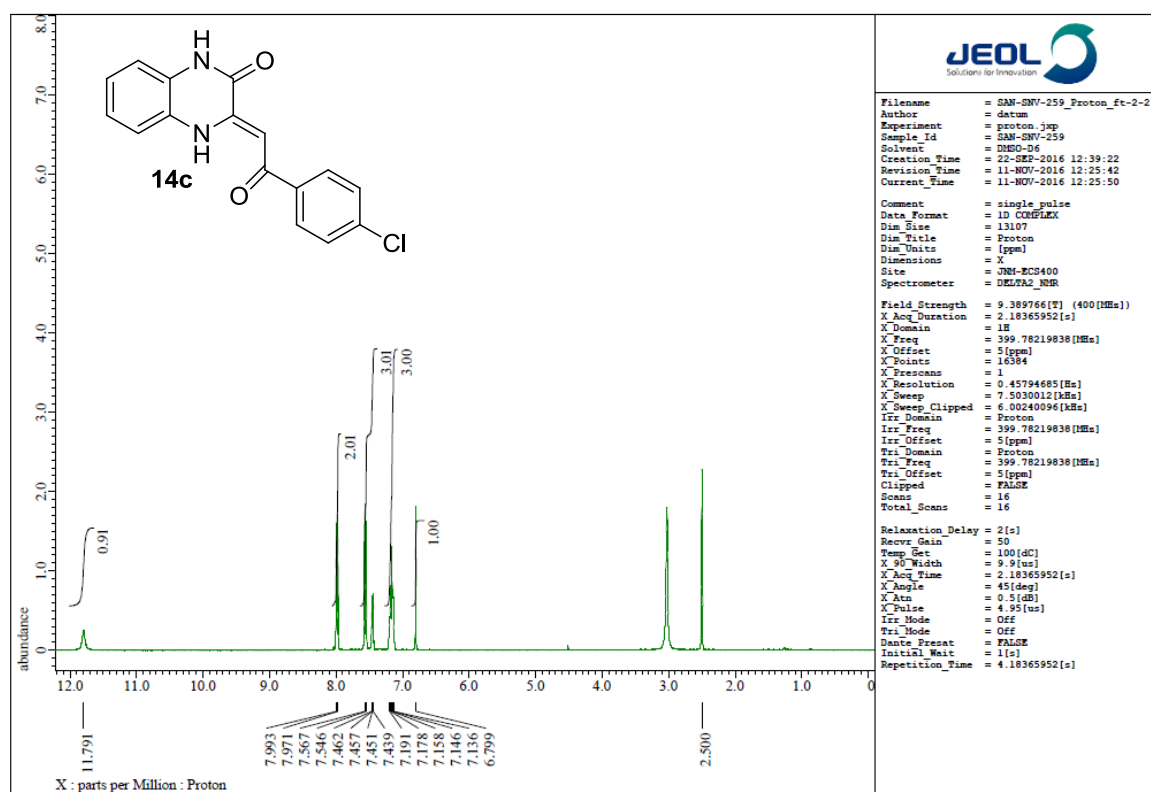
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Figure 31. ¹H NMR Spectra of Compound **14b**.



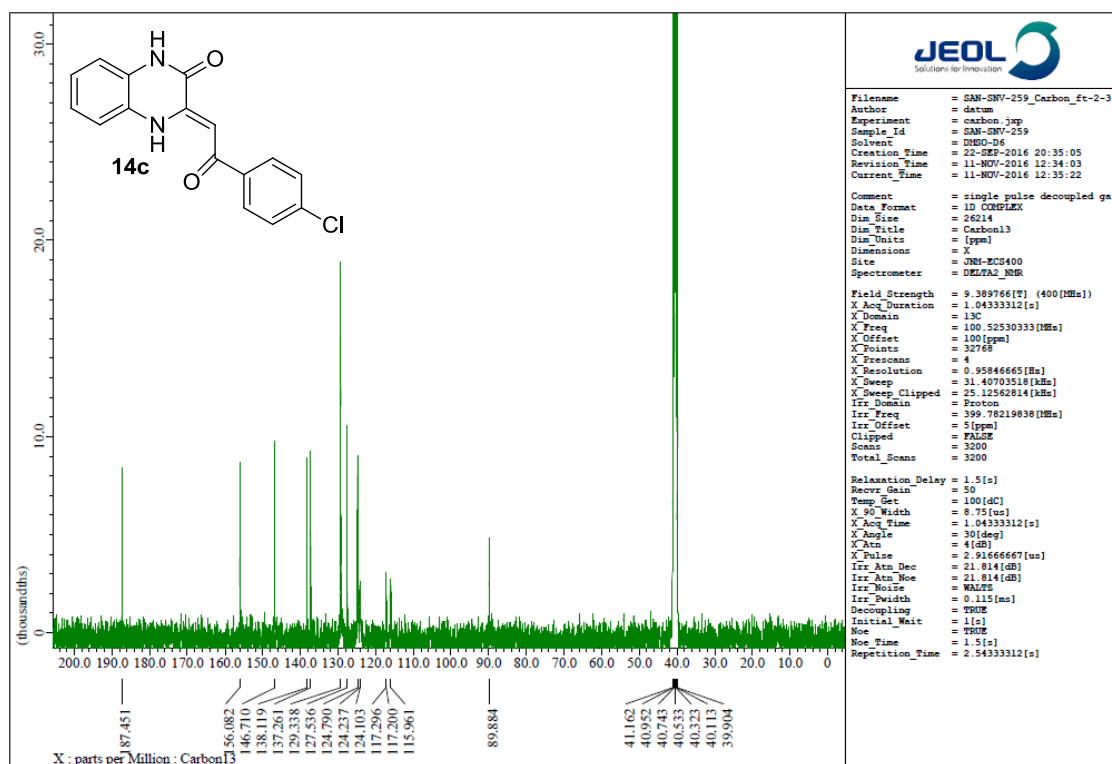
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Figure 32. ¹³C NMR Spectra of Compound **14b**.



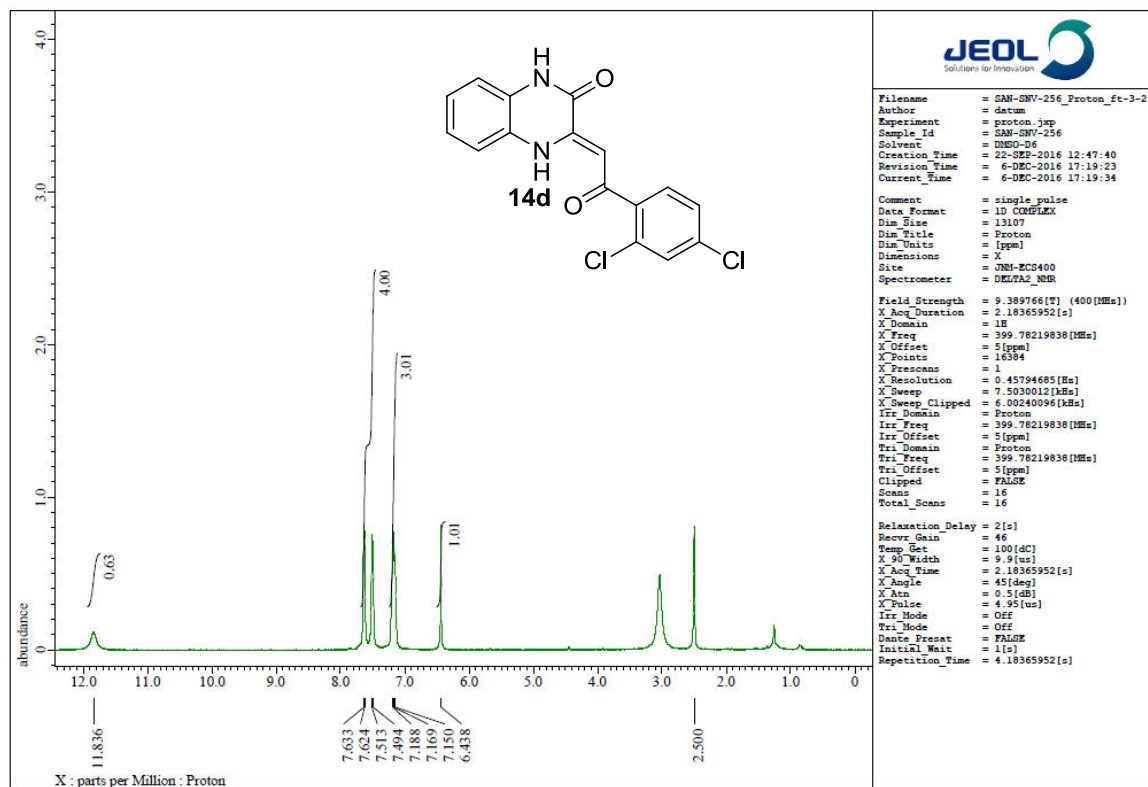
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Figure 33. ¹H NMR Spectra of Compound 14c.



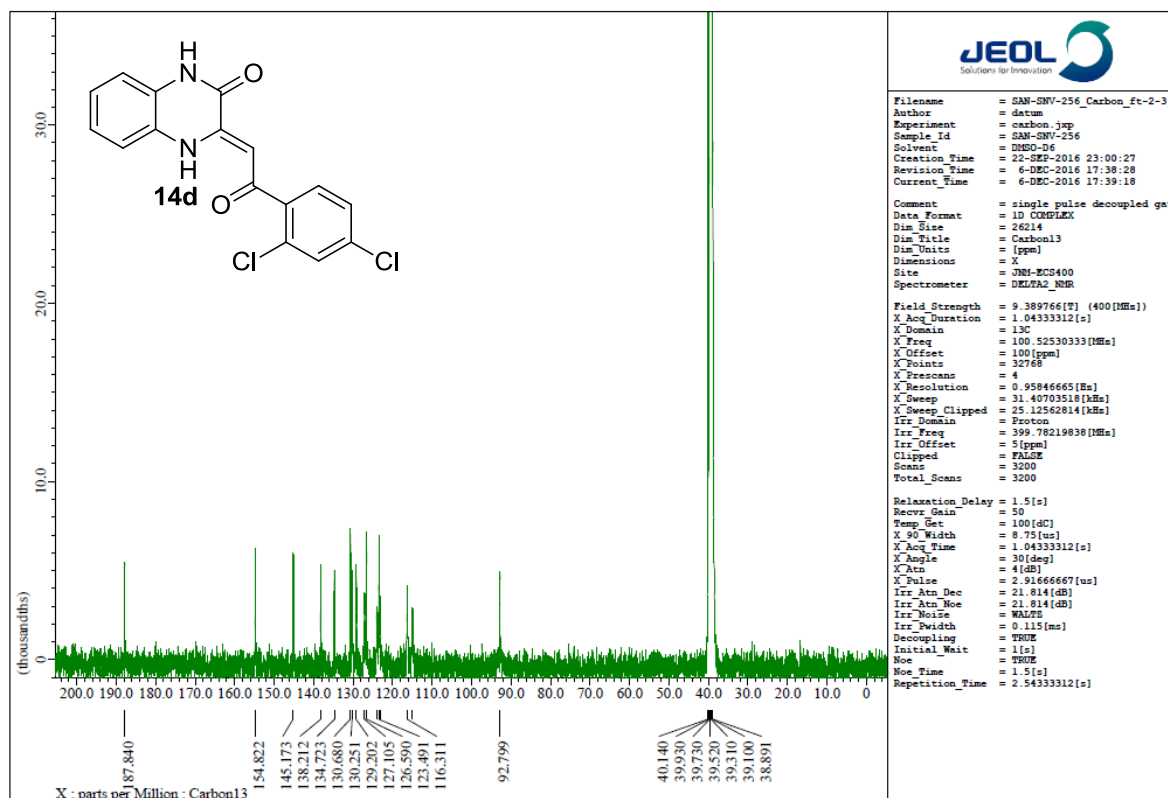
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Figure 34. ¹³C NMR Spectra of Compound 14c.



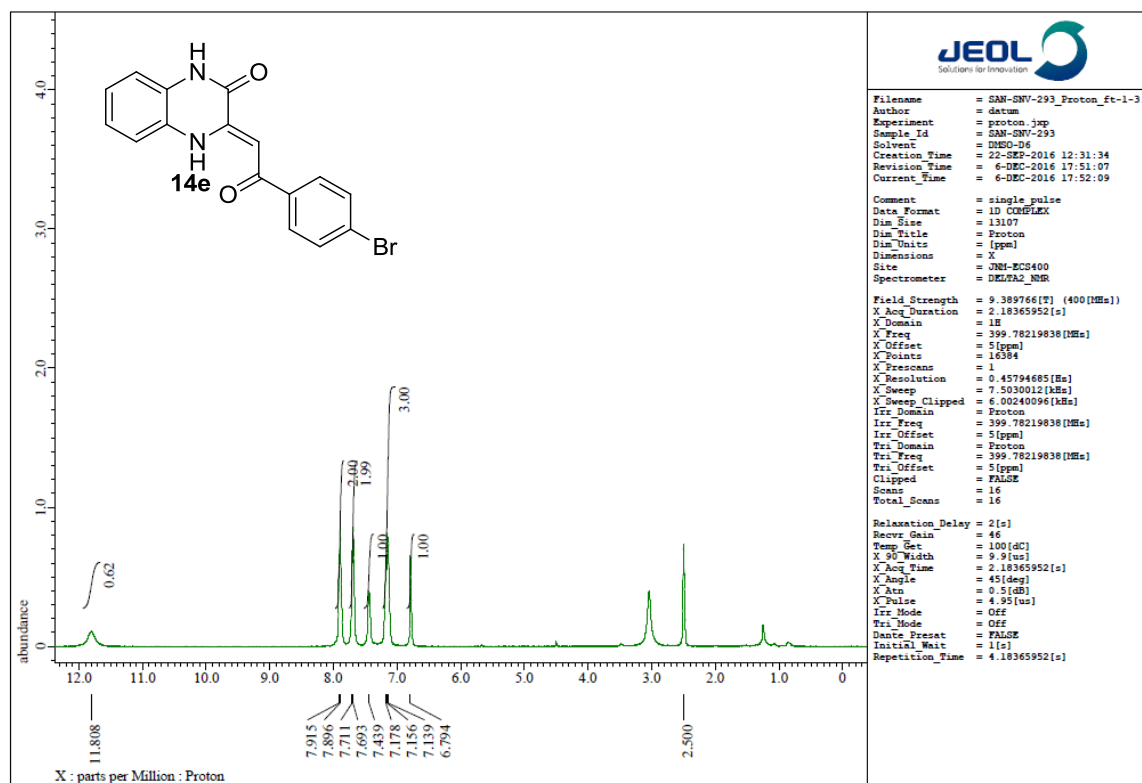
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Figure 35. ¹H NMR Spectra of Compound **14d**.



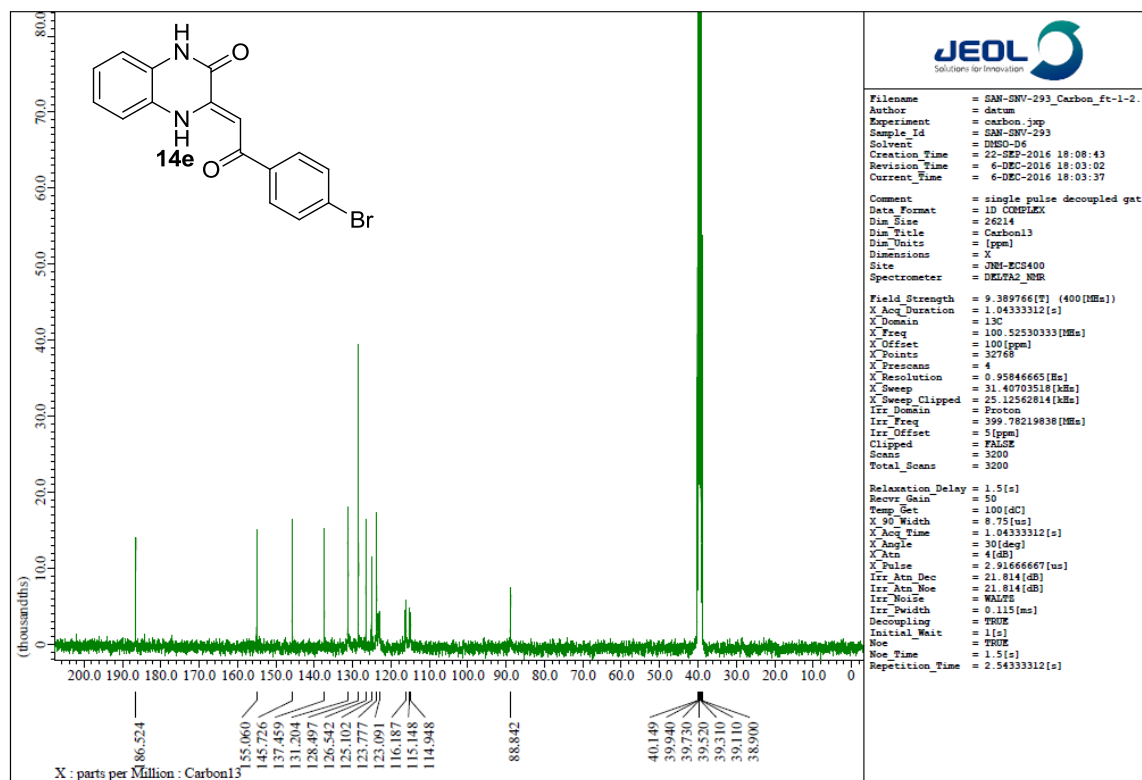
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Figure 36. ¹³C NMR Spectra of Compound **14d**.



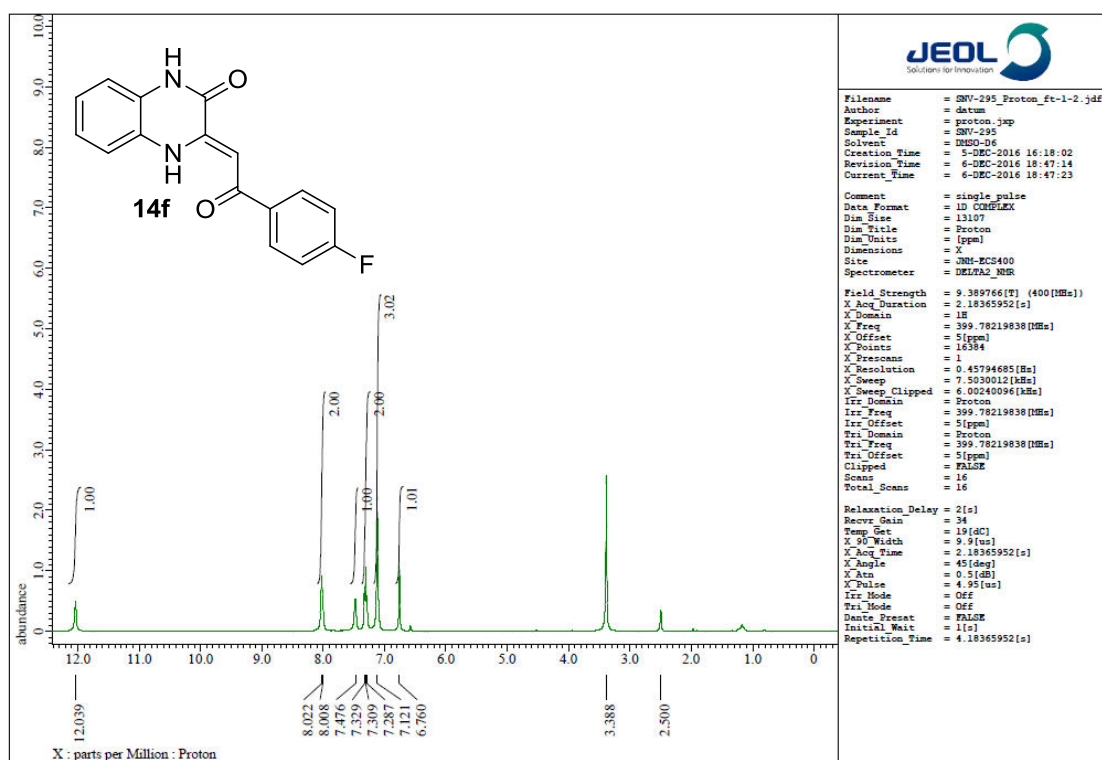
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Figure 37. ¹H NMR Spectra of Compound 14e.



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Figure 38. ¹³C NMR Spectra of Compound 14e.



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Figure 39. ¹H NMR Spectra of Compound **14f**.

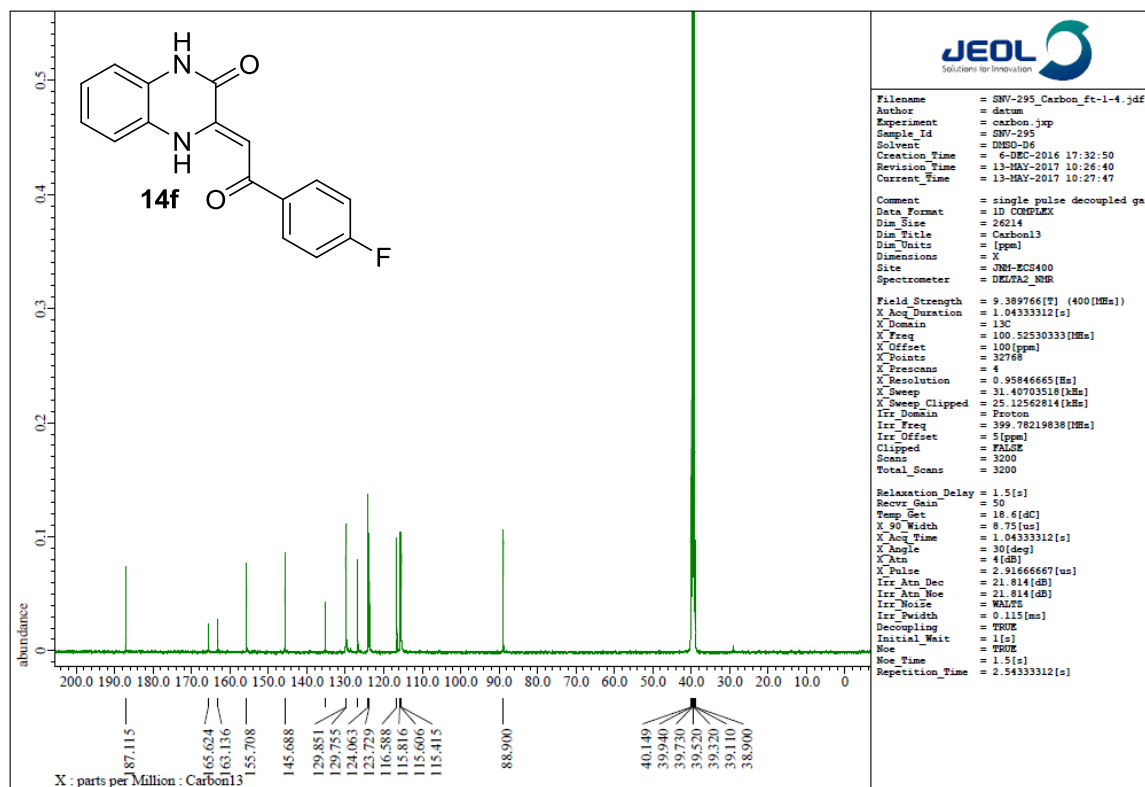
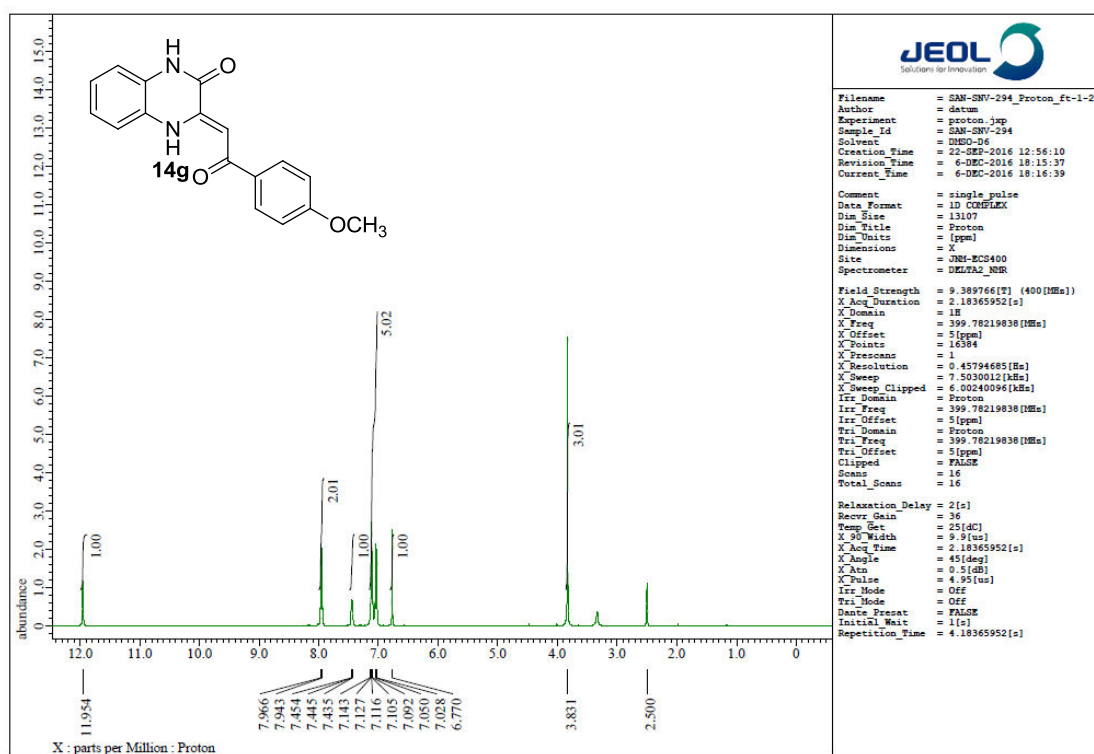
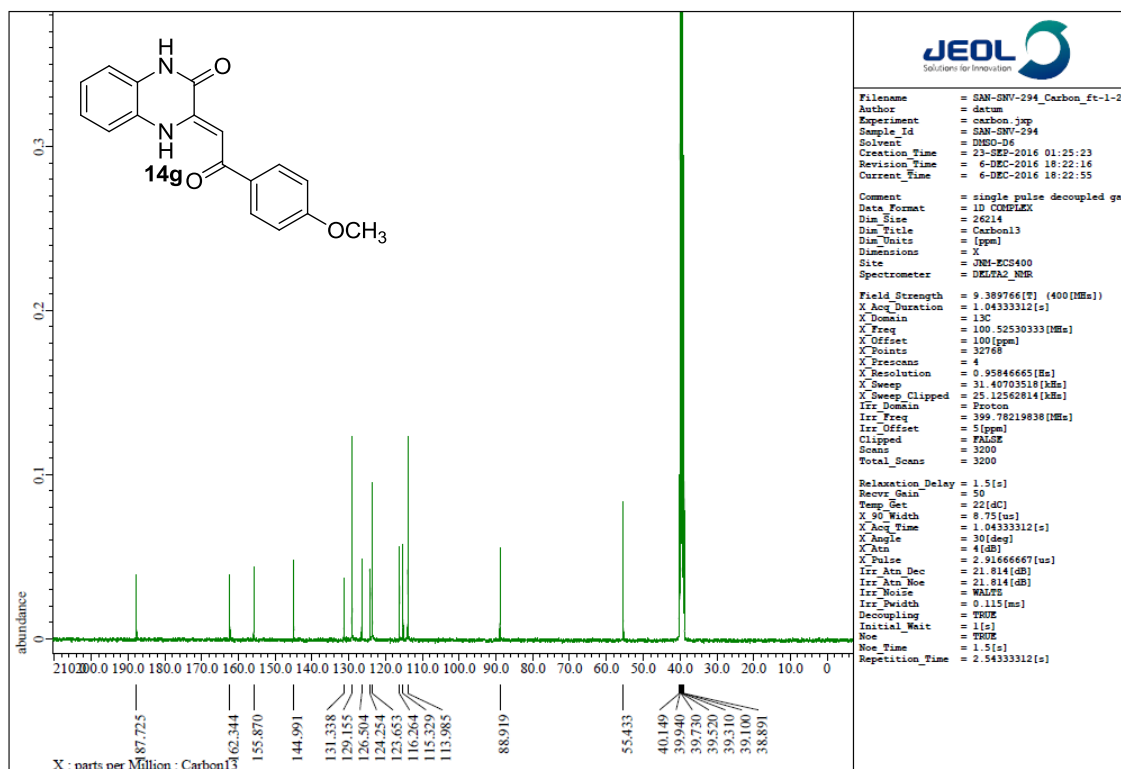


Figure 40. ¹³C NMR Spectra of Compound **14f**.



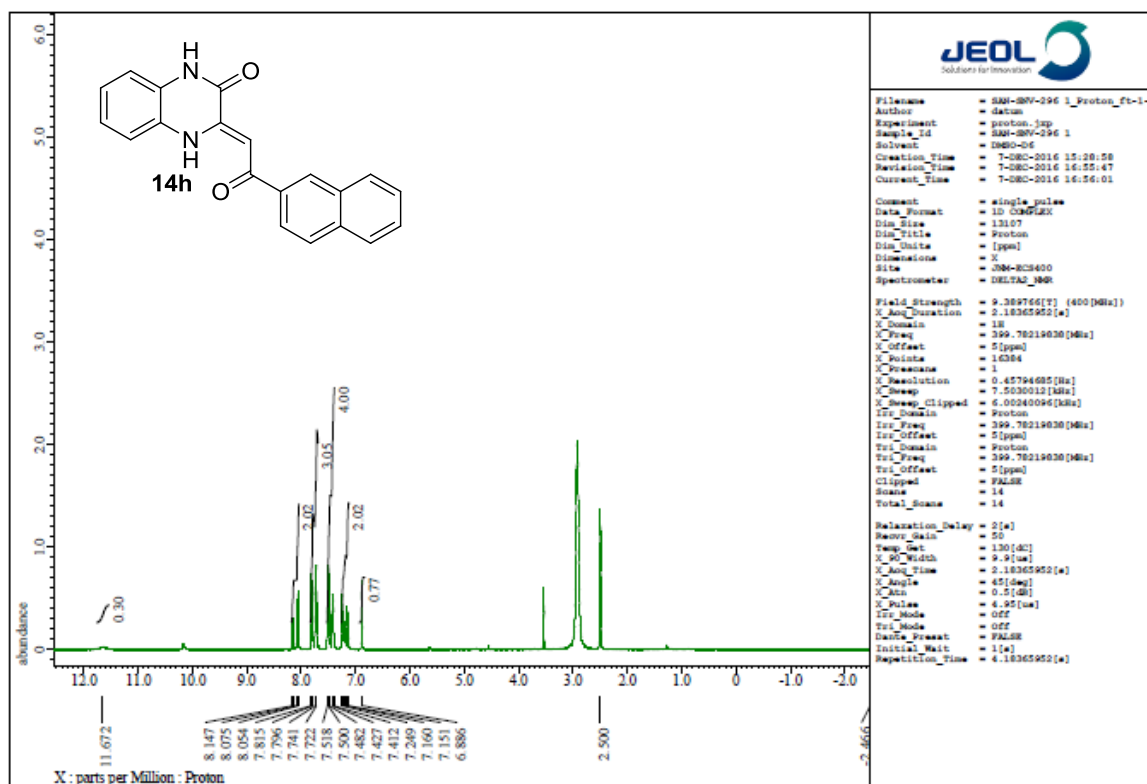
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Figure 41. ¹H NMR Spectra of Compound 14g.



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Figure 42. ¹³C NMR Spectra of Compound 14g.



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Figure 43. ¹H NMR Spectra of Compound 14h.

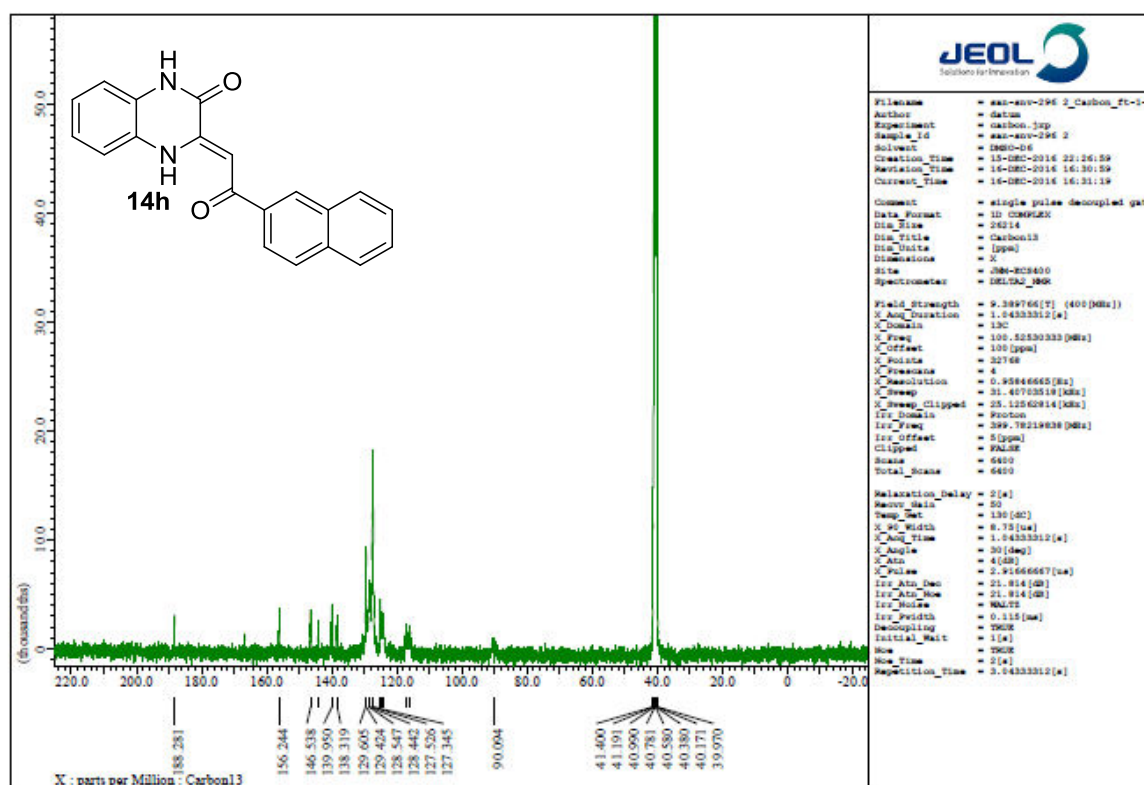


Figure 44. ¹³C NMR Spectra of Compound 14h.

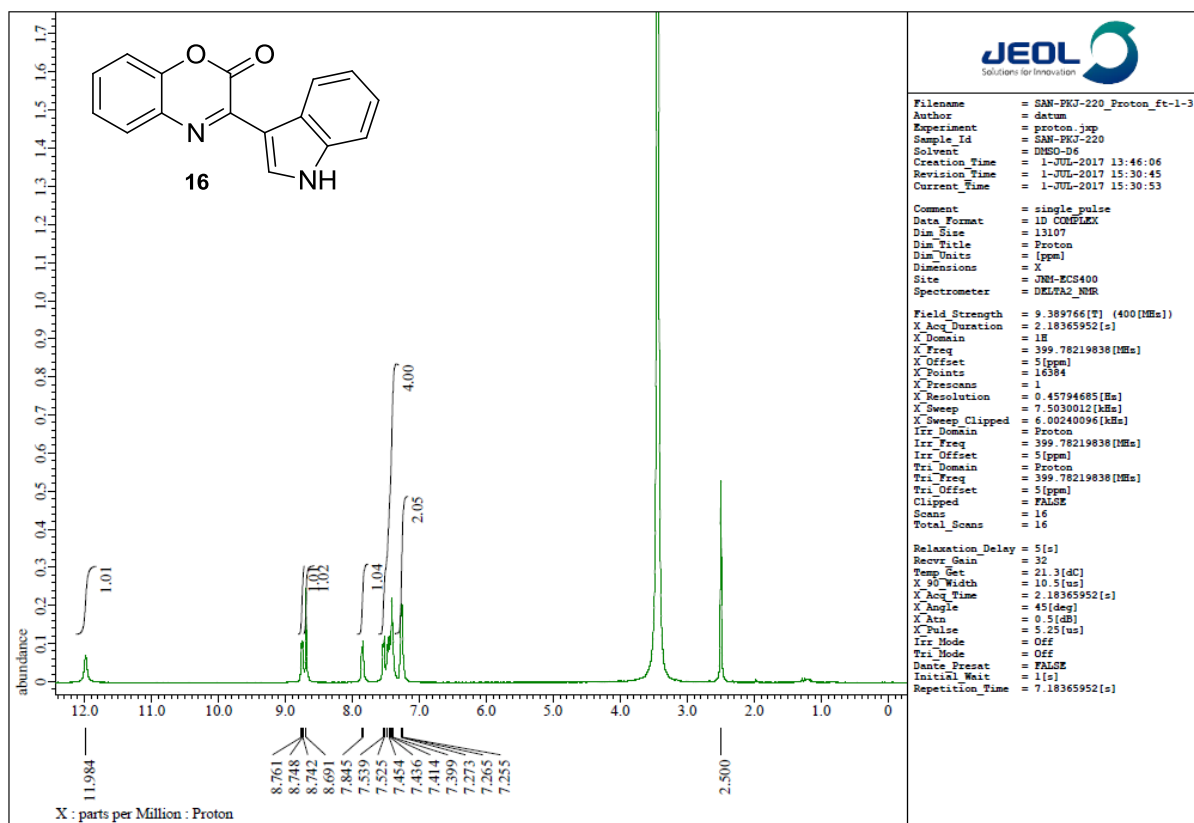


Figure 45. ^1H NMR Spectra of Compound 16.