

Supporting information

Solid-Phase Synthesis of Aryl Squaramides Using Liebeskind-Srogl Cross-Coupling

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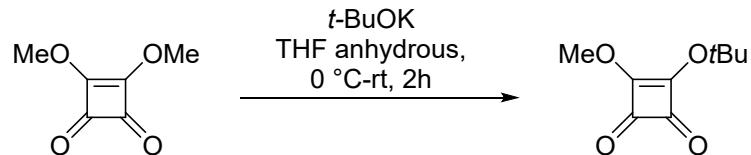
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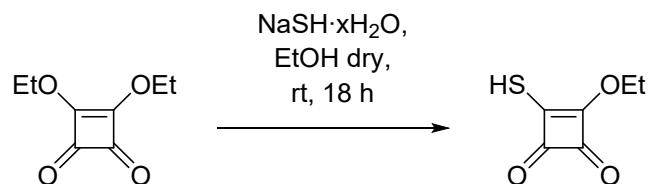
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Scheme S1. Synthesis of 3-(tert-butoxy)-4-methoxycyclobut-3-ene-1,2-dione



3,4-dimethoxy-3-cyclobutene-1,2-dione (2 g, 14.1 mmol) was placed in annealed Schlenk flasks and dissolved in THF dry (50 mL) under argon at 0 °C. Then, *t*BuOK (1.57 g, 14.1 mmol) was added portion wisely. The mixture was stirred for 2 h at 0 °C and another 2 h at rt. Then, the reaction mixture was quenched with saturated NH₄Cl (30 mL) and extracted with Et₂O (3x 30 mL). The combined organic phases were washed with brine (30 mL), dried over MgSO₄ and evaporated under reduced pressure. The product was purified by LC using DCM/MeOH 9:0.15 as mobile phase. The product was obtained as a white solid. Yield: 1.5g (56%). ¹H NMR (400 MHz, Chloroform-*d*) δ 4.38 (s, 3H), 1.57 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 189.63, 188.64, 185.80, 184.79, 87.54, 60.94, 28.71. HRMS: m/z: calcd. for C₉H₁₃O₄⁺: 185.0808 [M+H]⁺; found: 185.0812.

Scheme S2. Synthesis of 3-ethoxy-4-mercaptocyclobut-3-ene-1,2-dione



3,4-diethoxy-3-cyclobutene-1,2-dione (340 mg, 2 mmol) was placed in annealed Schlenk flasks and dissolved in EtOH dry (5 mL) under argon atmosphere. Then NaSH · xH₂O was added portion wisely. The mixture was stirred for 18 h at rt. Solids from the reaction mixture were filtered and the filtrate was precipitated by the addition of Et₂O (30 mL). Formed precipitation was filtered and washed by Et₂O (20 mL). The product was obtained as yellow solid. Yield: 302.4mg (96%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 4.73 (q, *J* = 7.0 Hz, 2H), 1.32 (*t*, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 207.30, 203.92, 197.30, 192.29, 66.88, 15.97. HRMS: m/z: calcd. for C₆H₅O₃S⁻: 156.9953 [M-H]⁻; found: 156.9954.

Fig S1. ^1H NMR spectra of 3-(tert-butoxy)-4-methoxycyclobut-3-ene-1,2-dione

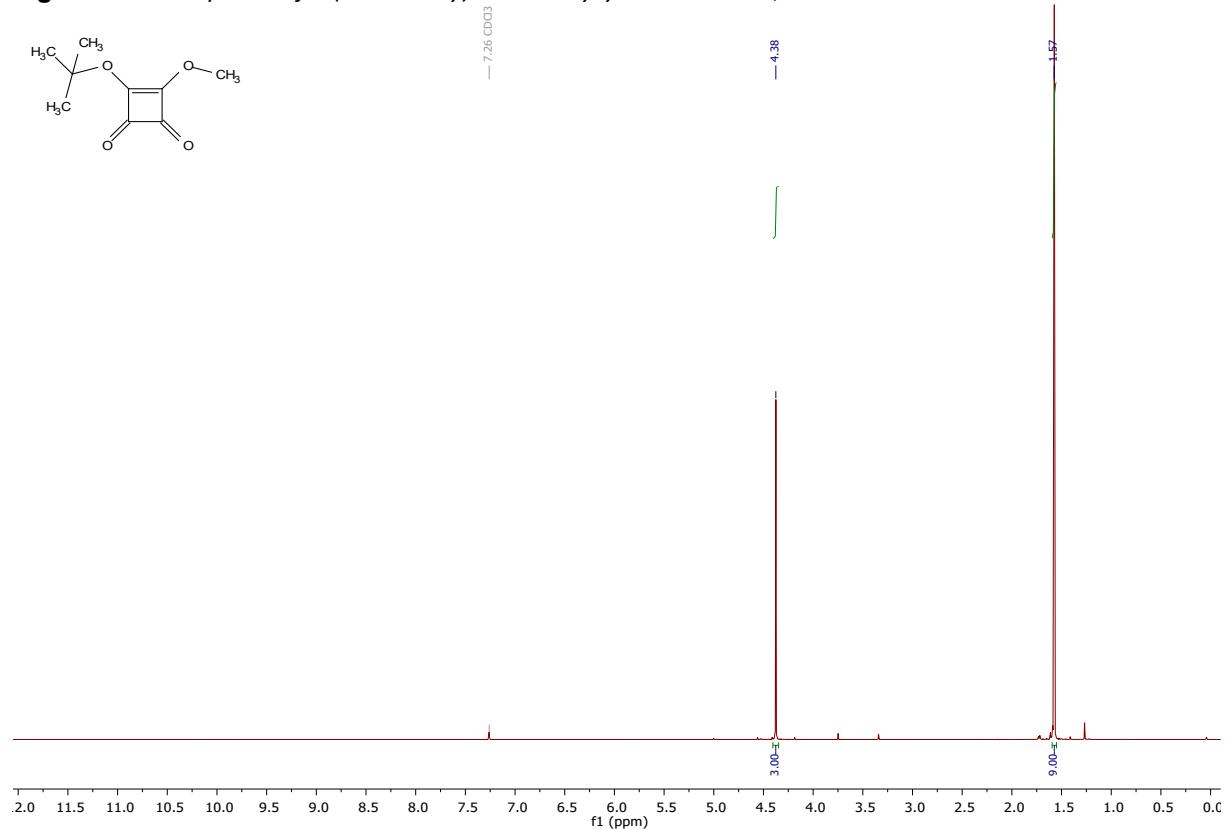


Fig S2. ^{13}C NMR spectra of 3-(tert-butoxy)-4-methoxycyclobut-3-ene-1,2-dione

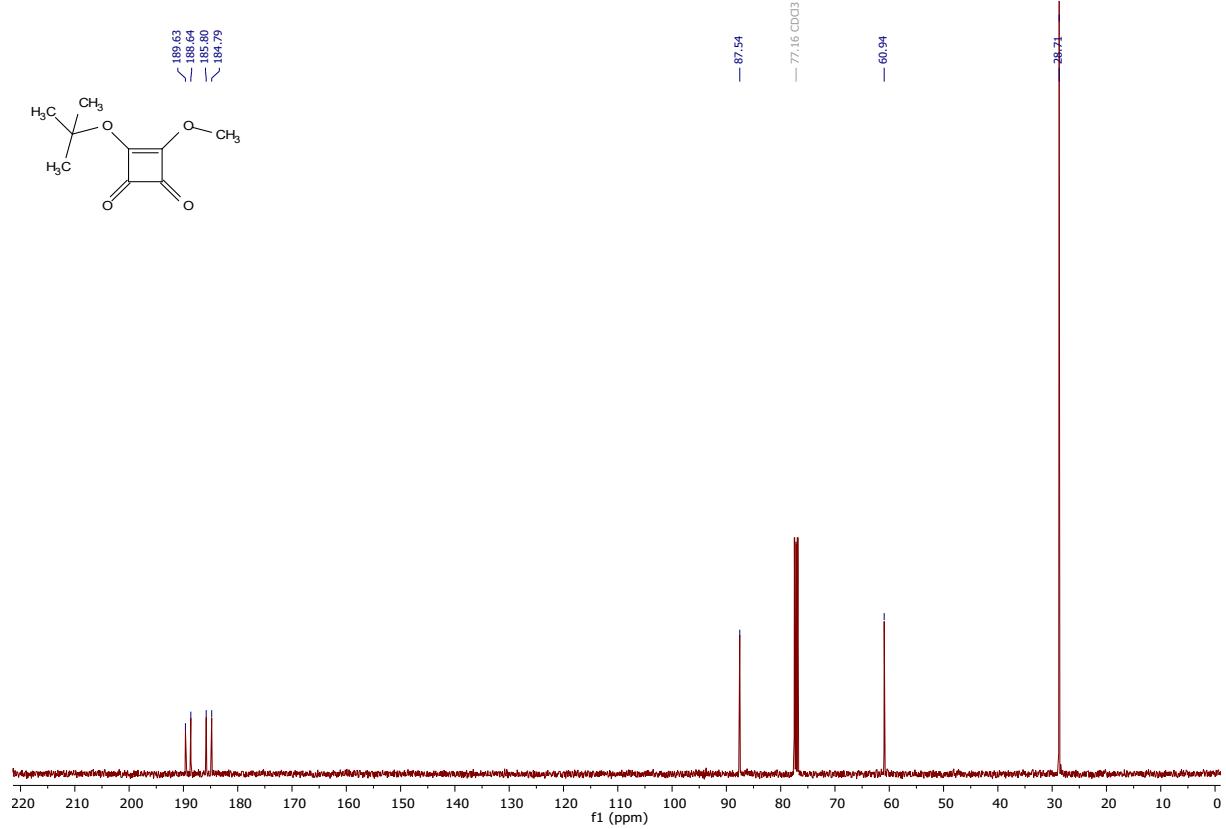


Fig S3. ^1H NMR spectra of 3-ethoxy-4-mercaptopcyclobut-3-ene-1,2-dione

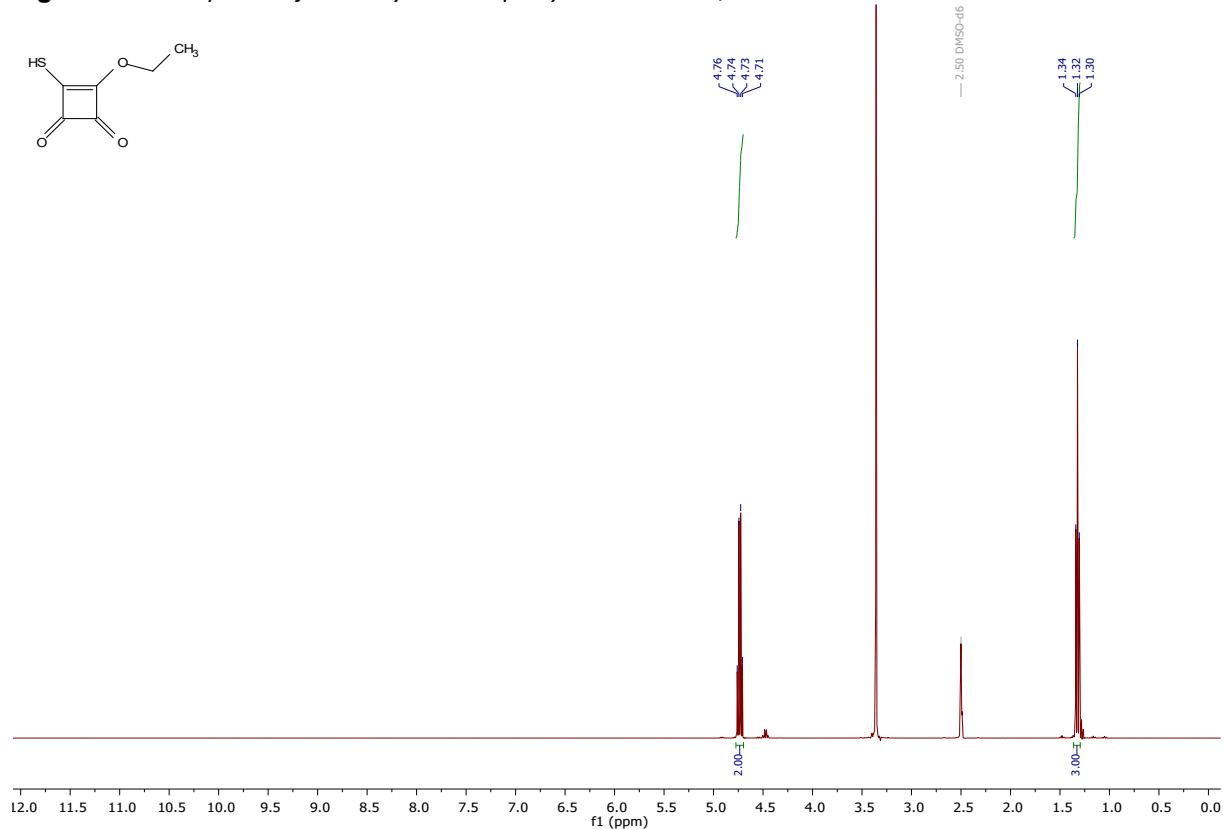


Fig S4. ^{13}C NMR spectra of 3-ethoxy-4-mercaptopcyclobut-3-ene-1,2-dione

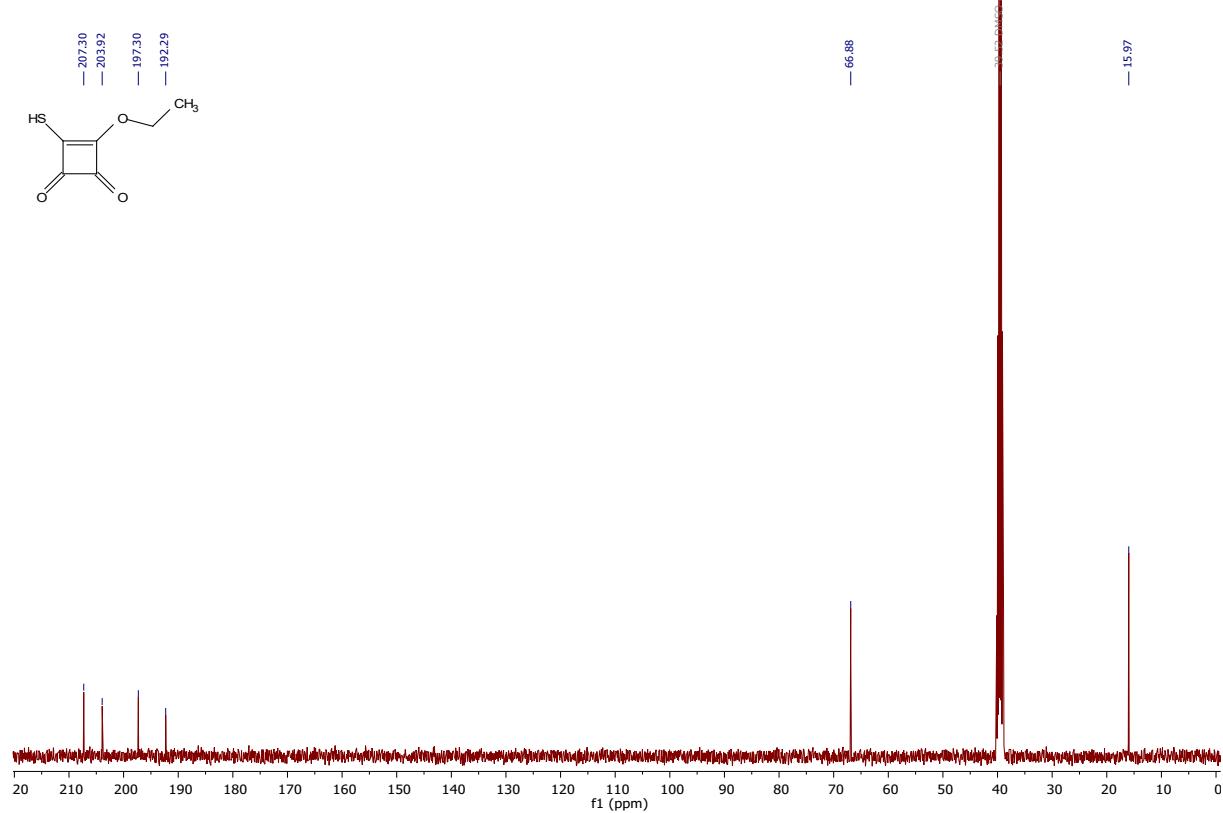


Fig S5. ^1H NMR spectra of 3-(benzylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6a**

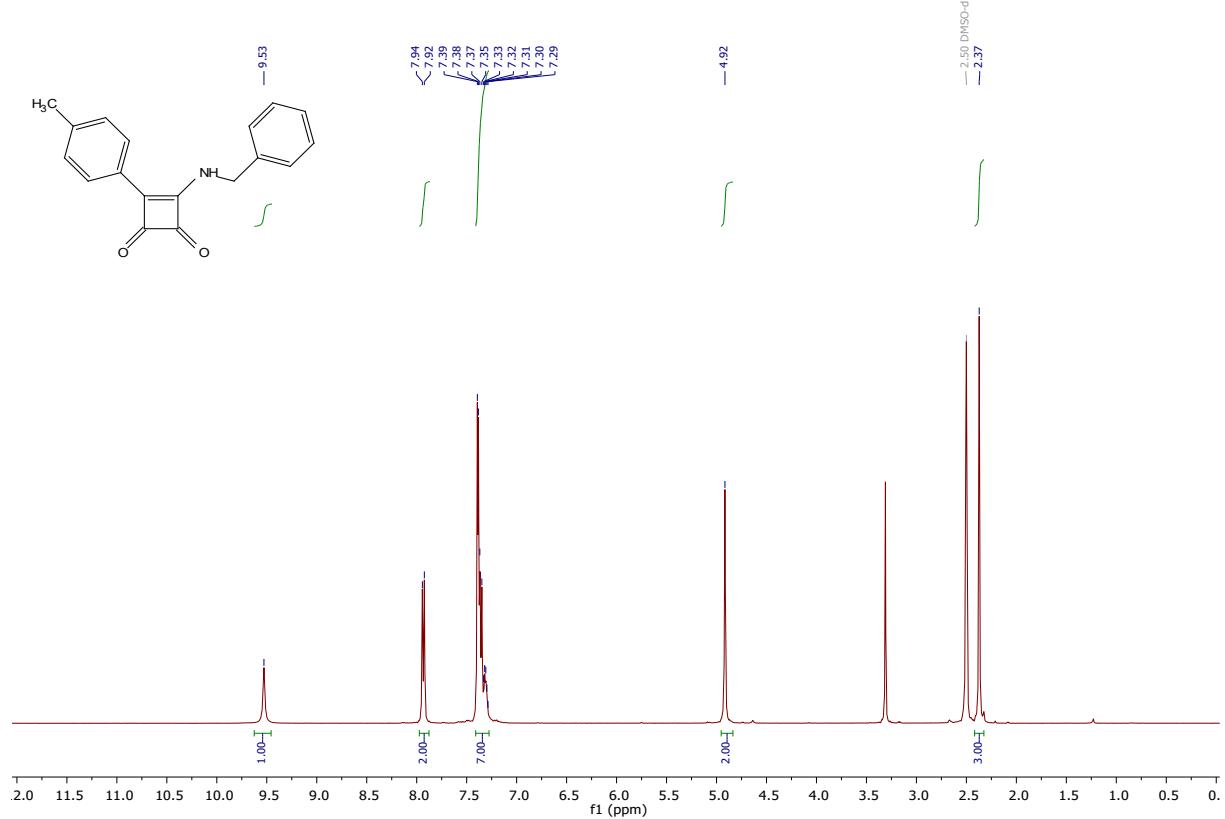


Fig S6. ^{13}C NMR spectra of 3-(benzylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6a**

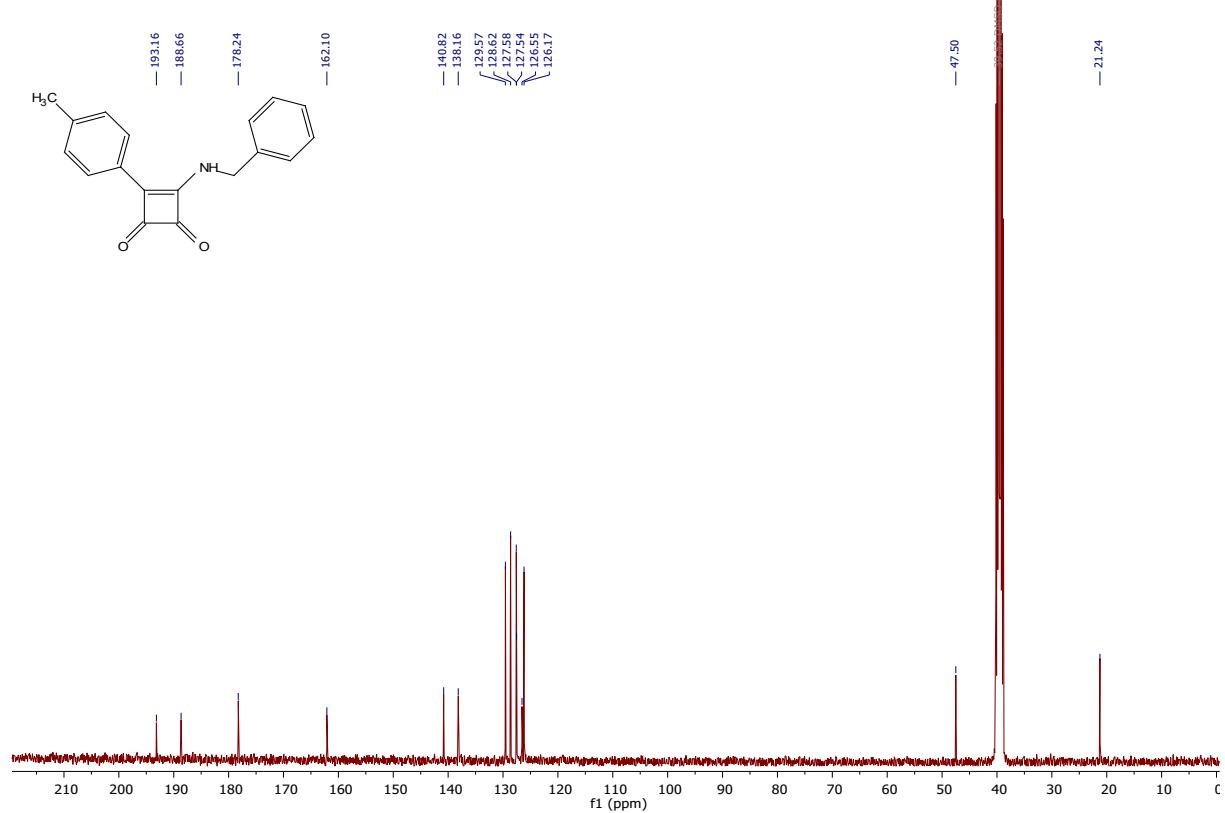


Fig S7. ^1H NMR spectra of 3-(benzylamino)-4-(4-methoxyphenyl)cyclobut-3-ene-1,2-dione **6b**

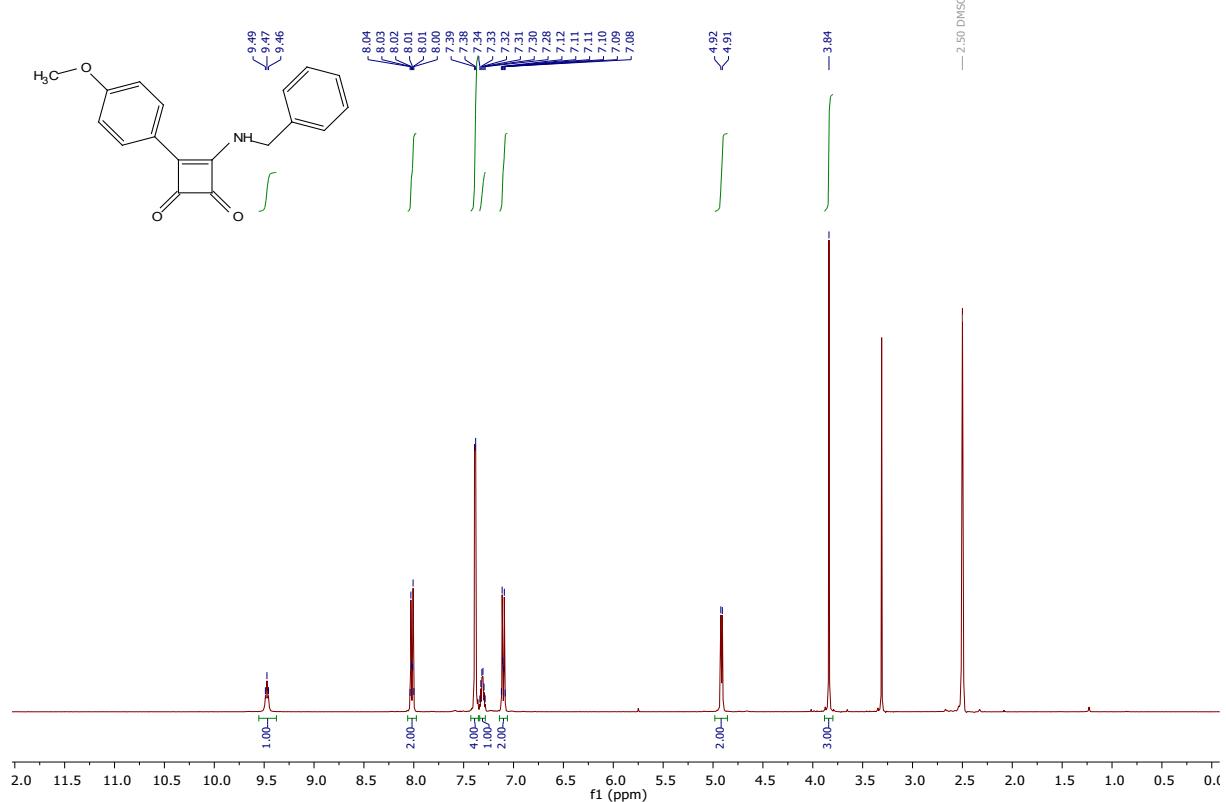


Fig S8. ^{13}C NMR spectra of 3-(benzylamino)-4-(4-methoxyphenyl)cyclobut-3-ene-1,2-dione **6b**

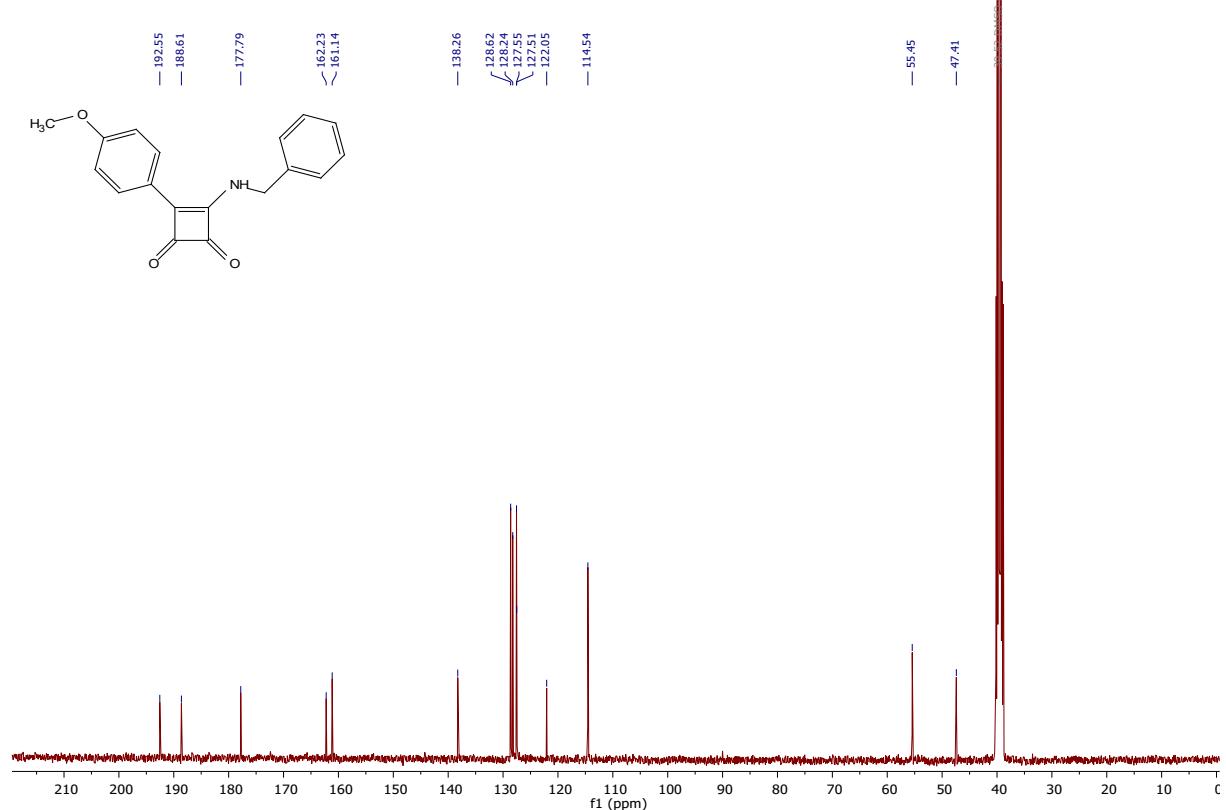


Fig S9. ^1H NMR spectra of 3-(benzylamino)-4-(4-(methylthio)phenyl)cyclobut-3-ene-1,2-dione **6c**

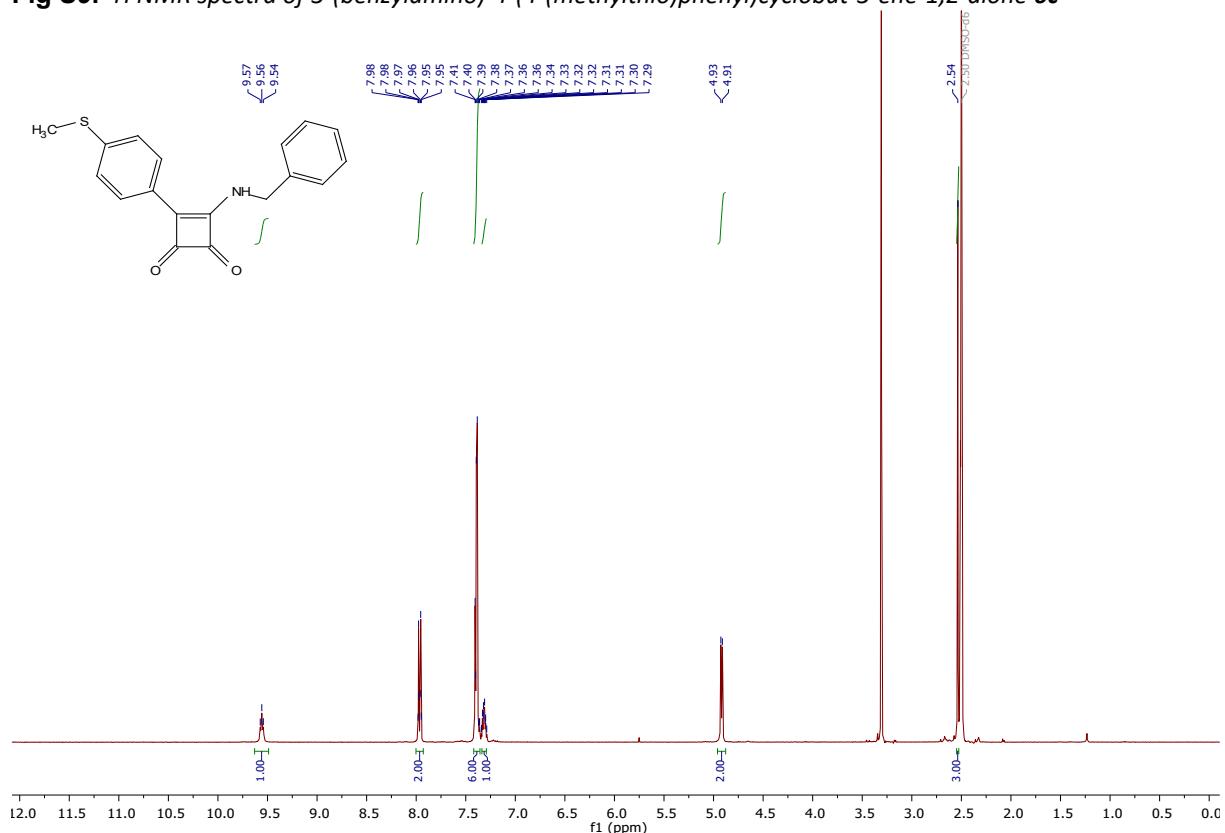


Fig S10. ^{13}C NMR spectra of 3-(benzylamino)-4-(4-(methylthio)phenyl)cyclobut-3-ene-1,2-dione **6c**

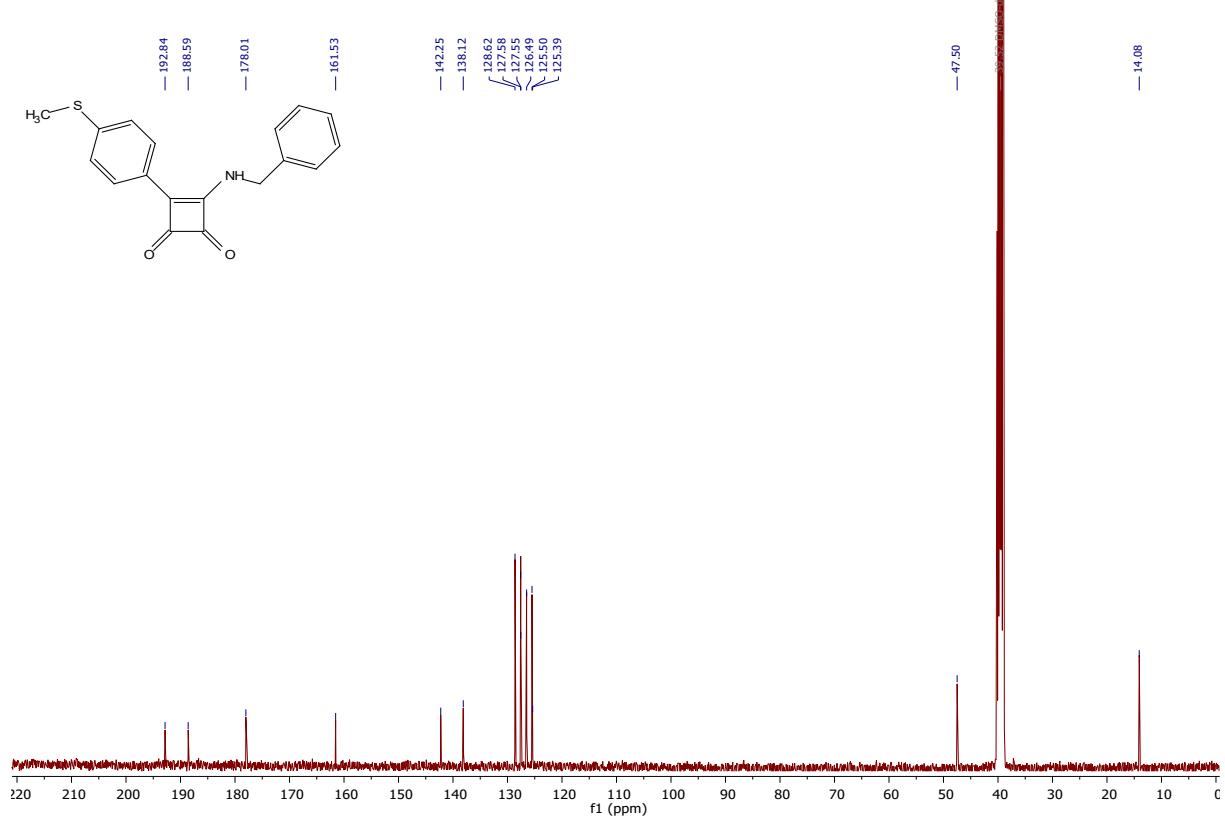


Fig S11. ^1H NMR spectra of 3-(benzylamino)-4-phenylcyclobut-3-ene-1,2-dione **6d**

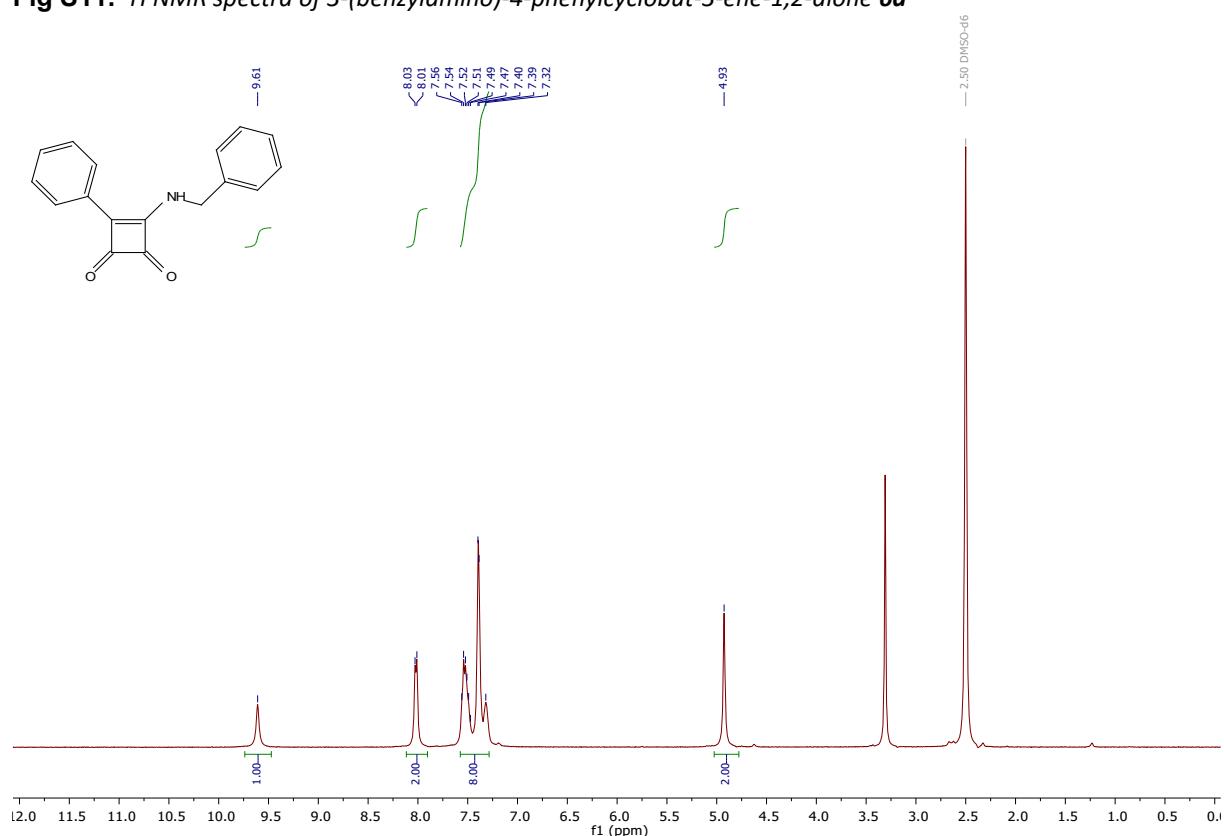


Fig S12. ^{13}C NMR spectra of 3-(benzylamino)-4-phenylcyclobut-3-ene-1,2-dione **6d**

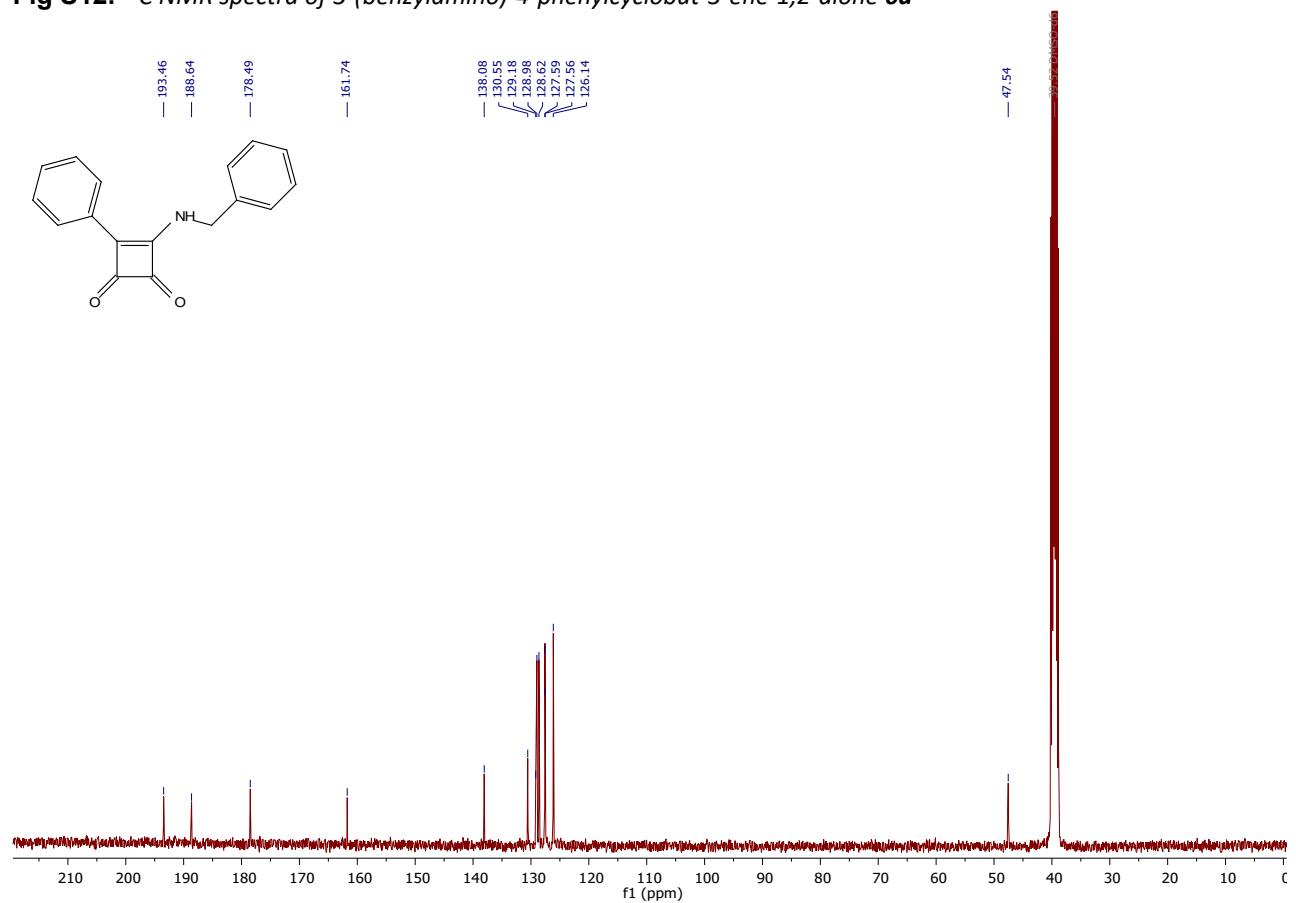


Fig S13. ^1H NMR spectra of 3-(benzylamino)-4-(4-nitrophenyl)cyclobut-3-ene-1,2-dione **6e**

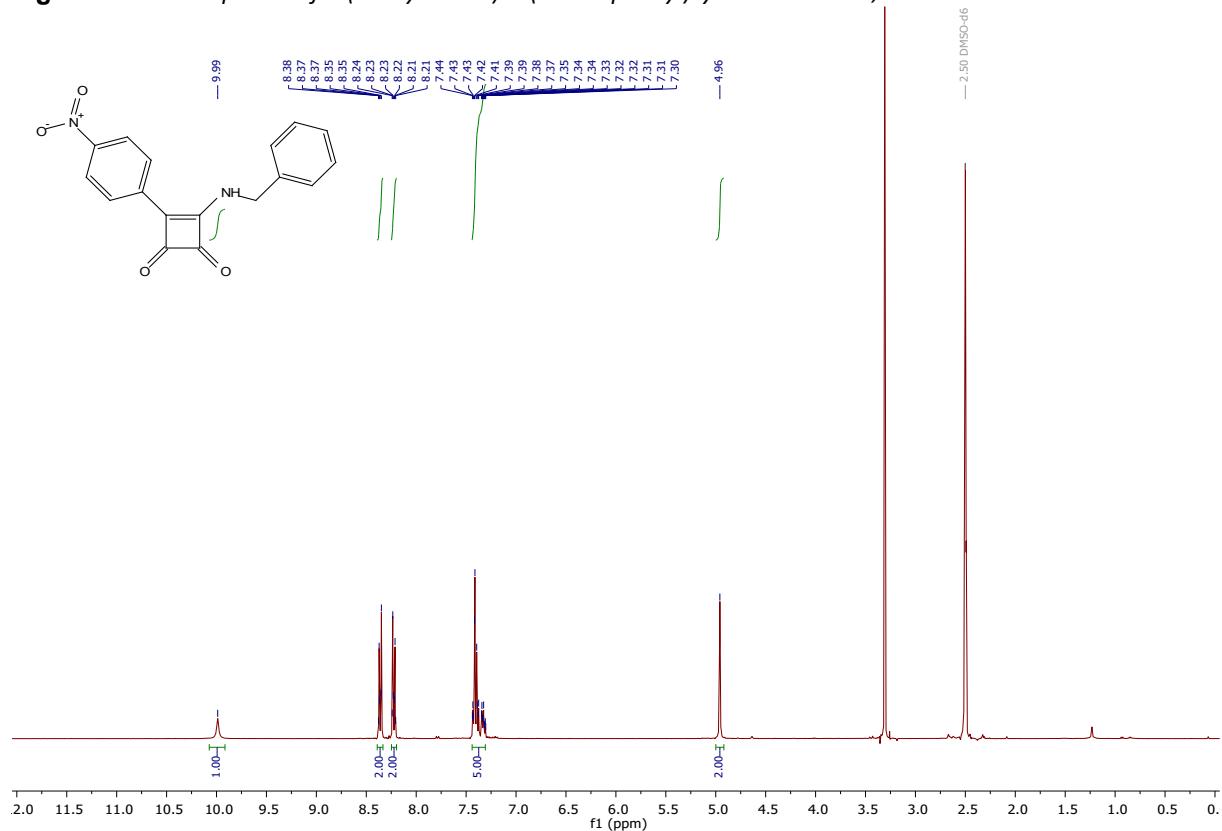


Fig S14. ^{13}C NMR spectra of 3-(benzylamino)-4-(4-nitrophenyl)cyclobut-3-ene-1,2-dione **6e**

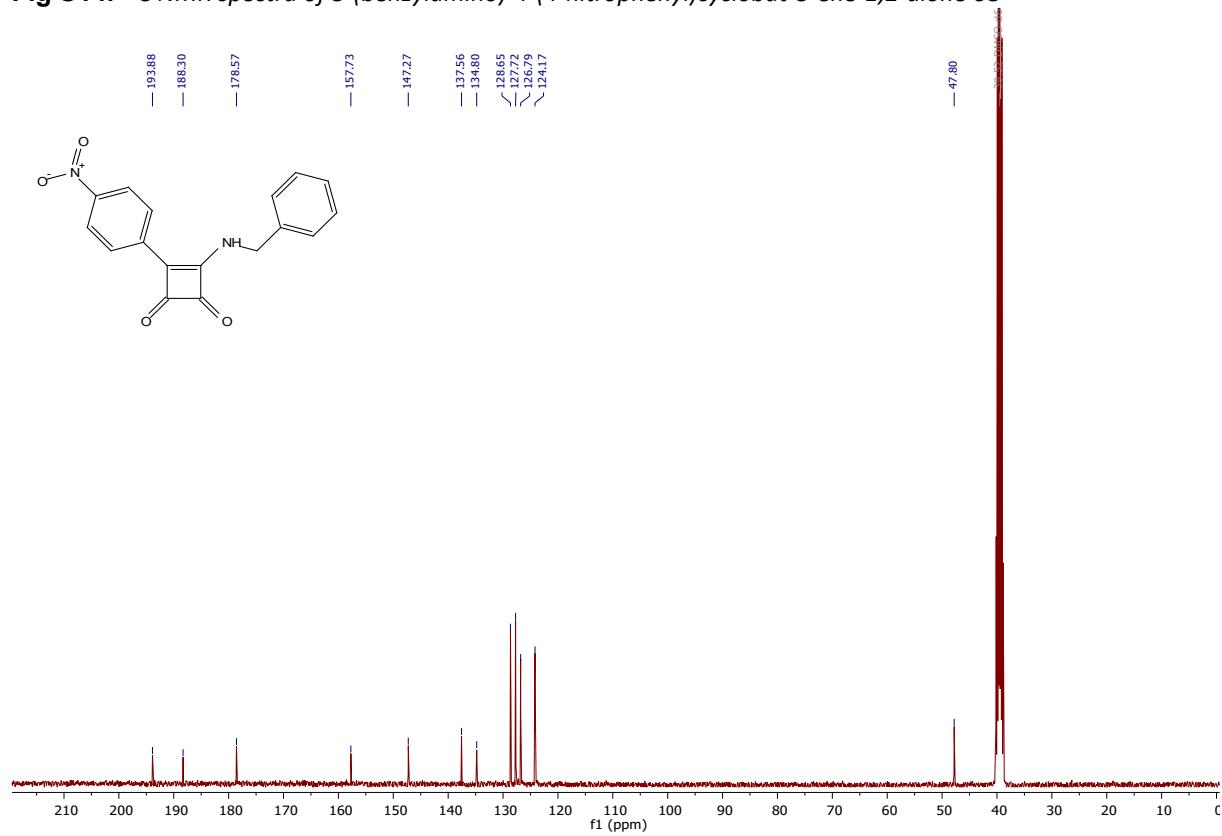


Fig S15. ^1H NMR spectra of 3-(benzylamino)-4-(4-(trifluoromethyl)phenyl)cyclobut-3-ene-1,2-dione **6f**

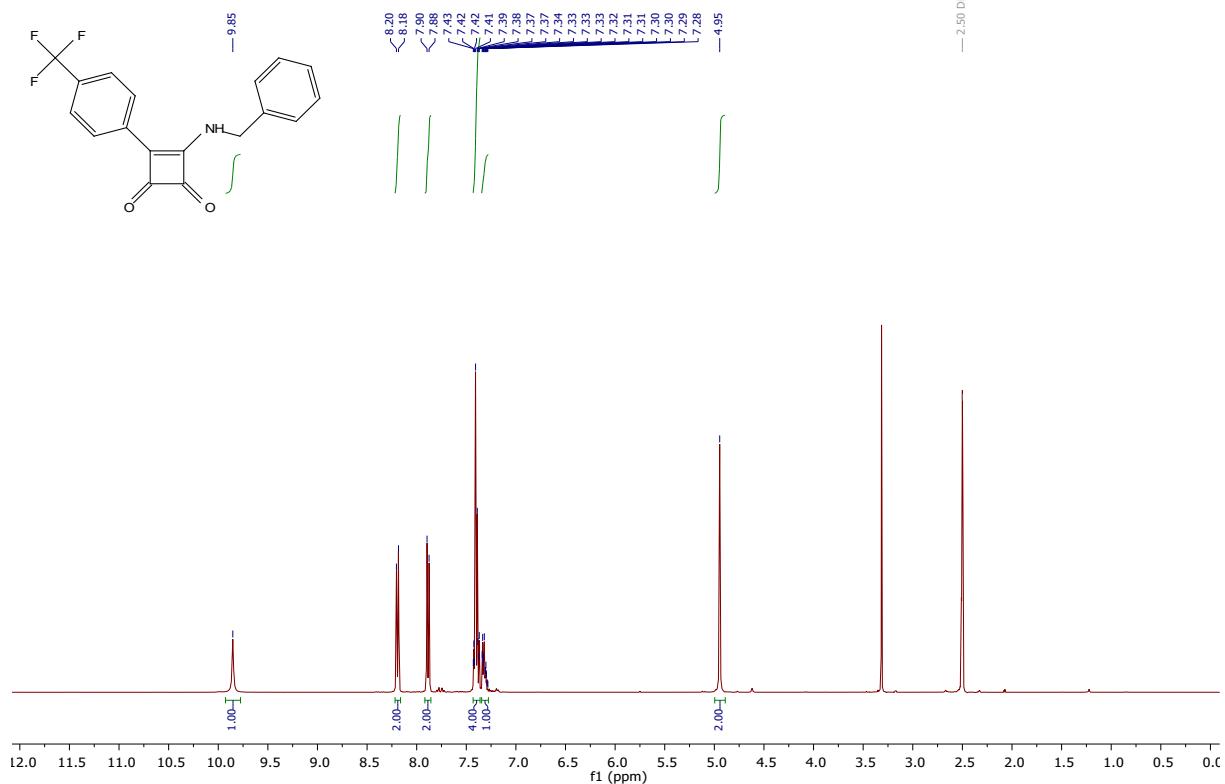


Fig S16. ^{13}C NMR spectra of 3-(benzylamino)-4-(4-(trifluoromethyl)phenyl)cyclobut-3-ene-1,2-dione **6f**

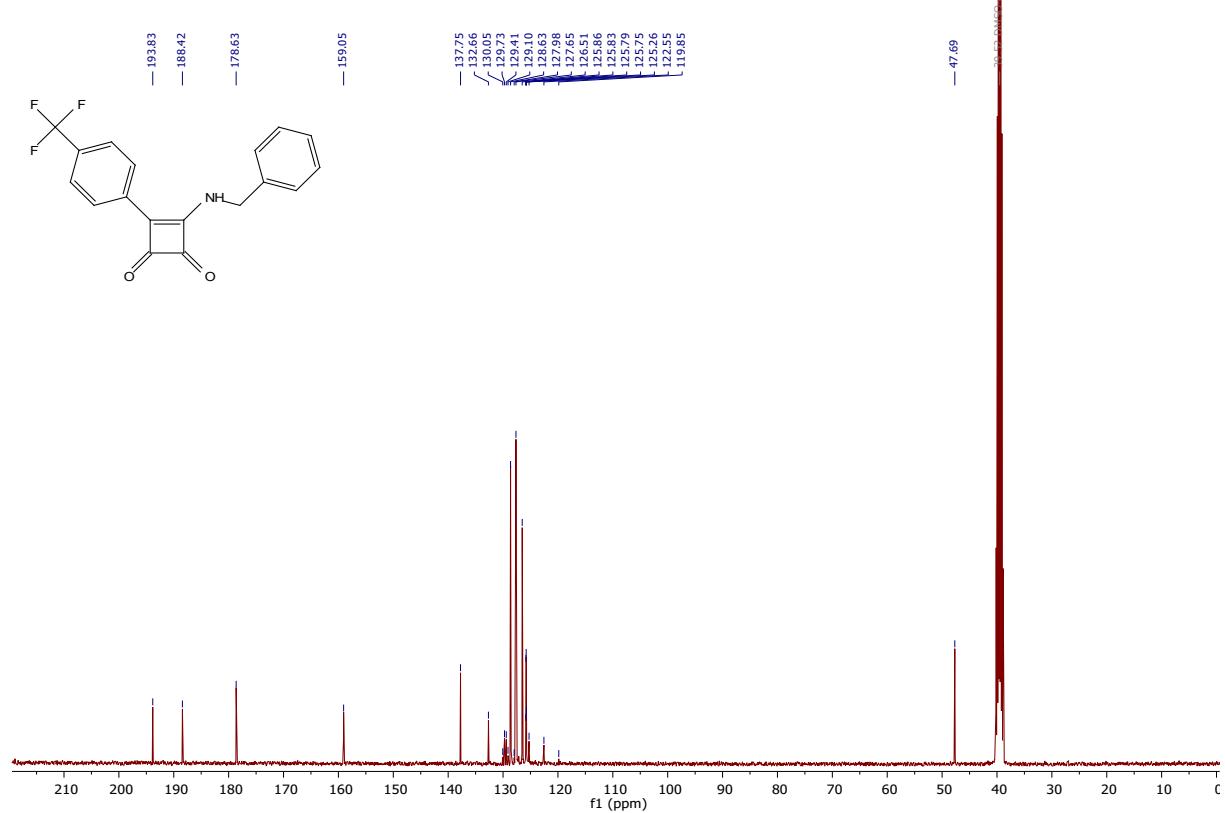


Fig S17. ^1H NMR spectra of 4-(2-(benzylamino)-3,4-dioxocyclobut-1-en-1-yl)benzaldehyde **6g**

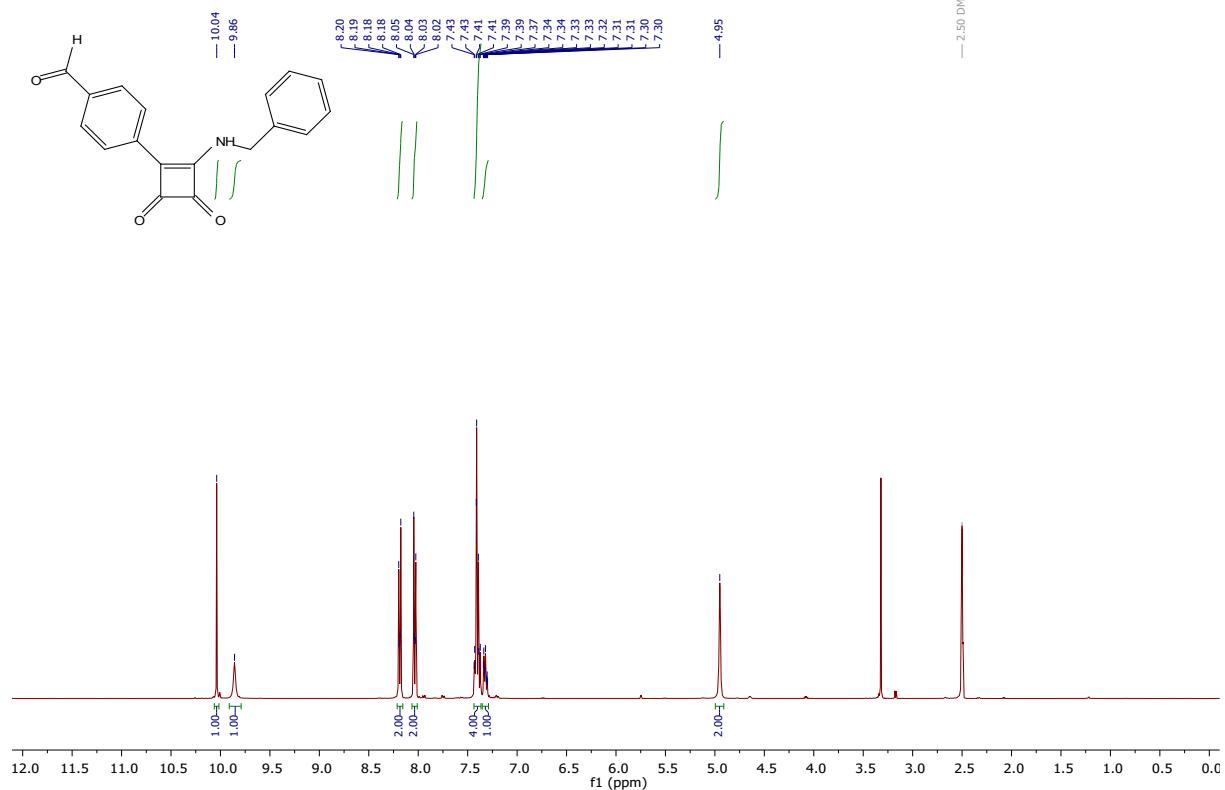


Fig S18. ^{13}C NMR spectra of 4-(2-(benzylamino)-3,4-dioxocyclobut-1-en-1-yl)benzaldehyde **6g**

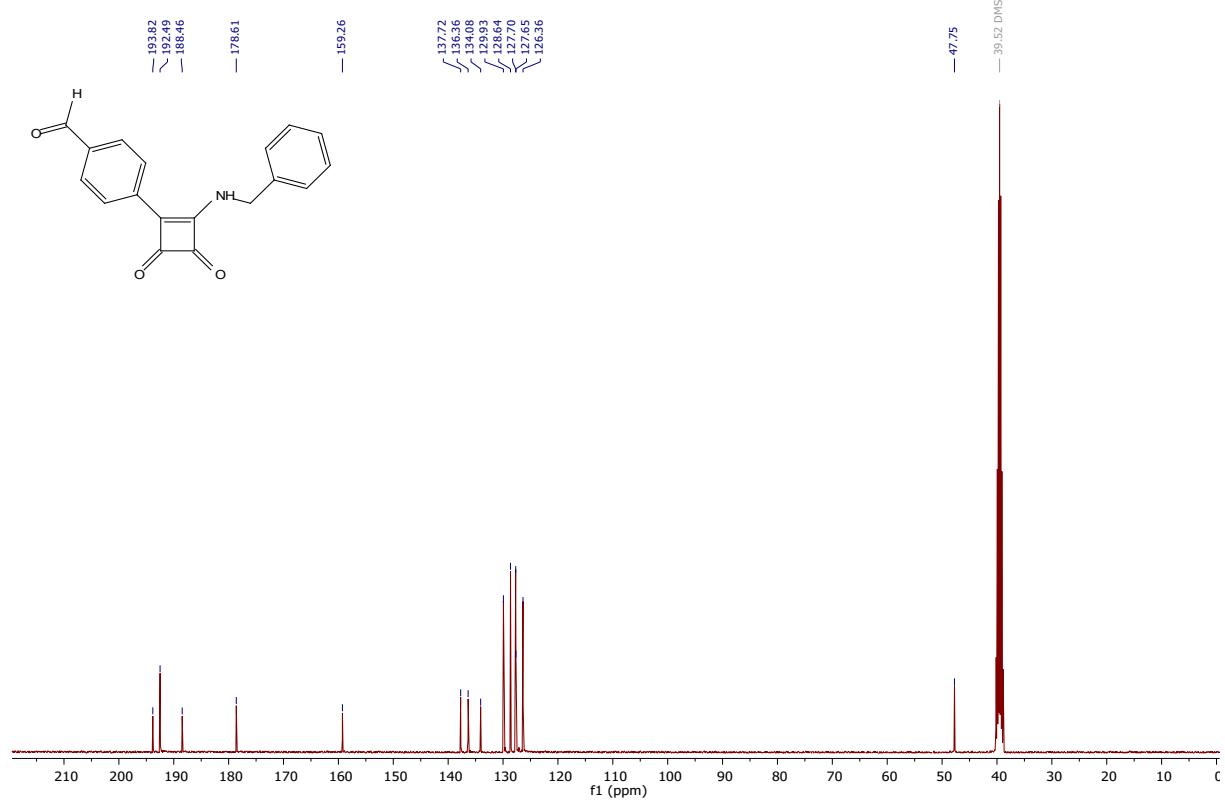


Fig S19. ^1H NMR spectra of 3-(benzylamino)-4-(4-bromophenyl)cyclobut-3-ene-1,2-dione **6h**

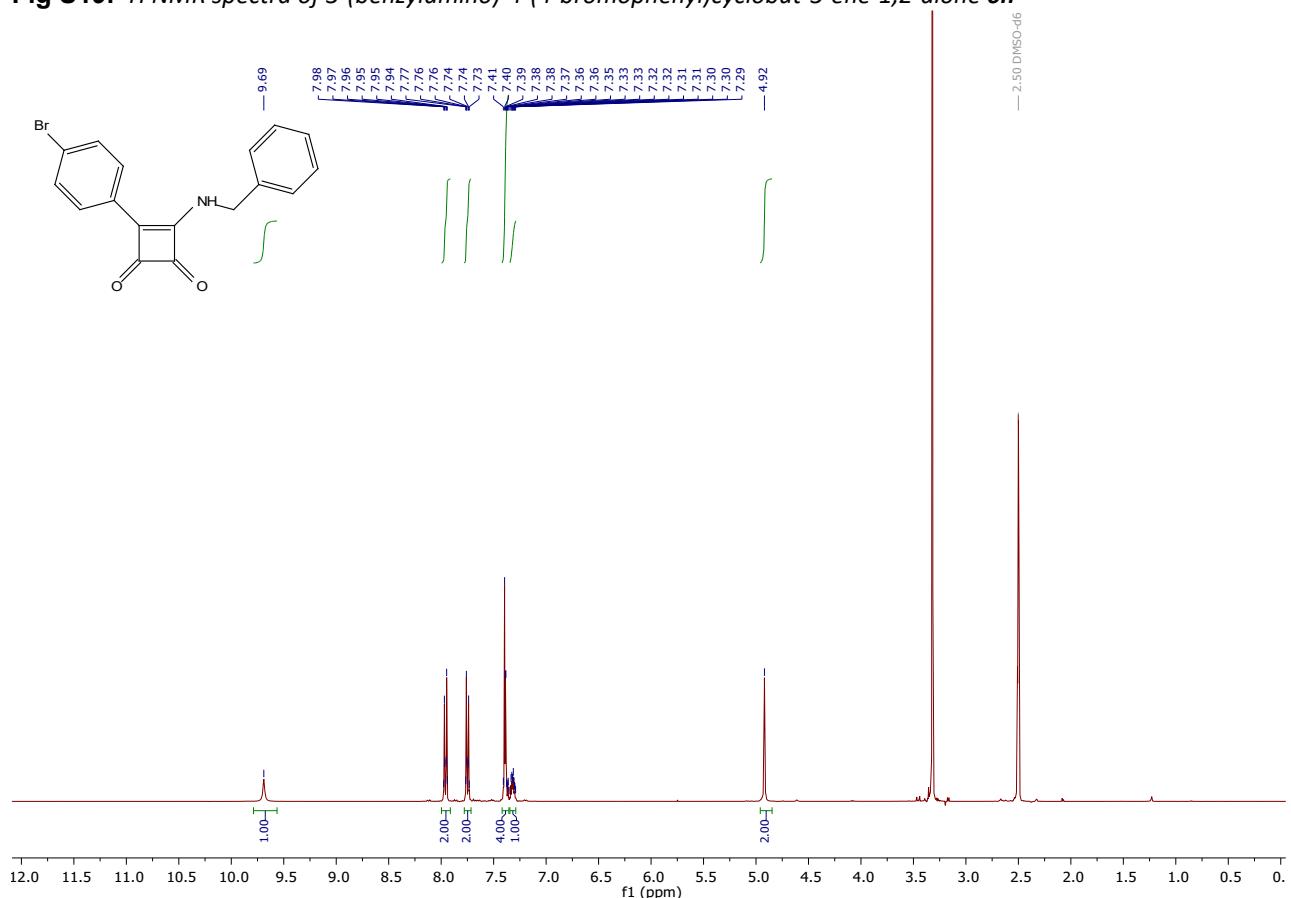


Fig S20. ^{13}C NMR spectra of 3-(benzylamino)-4-(4-bromophenyl)cyclobut-3-ene-1,2-dione **6h**

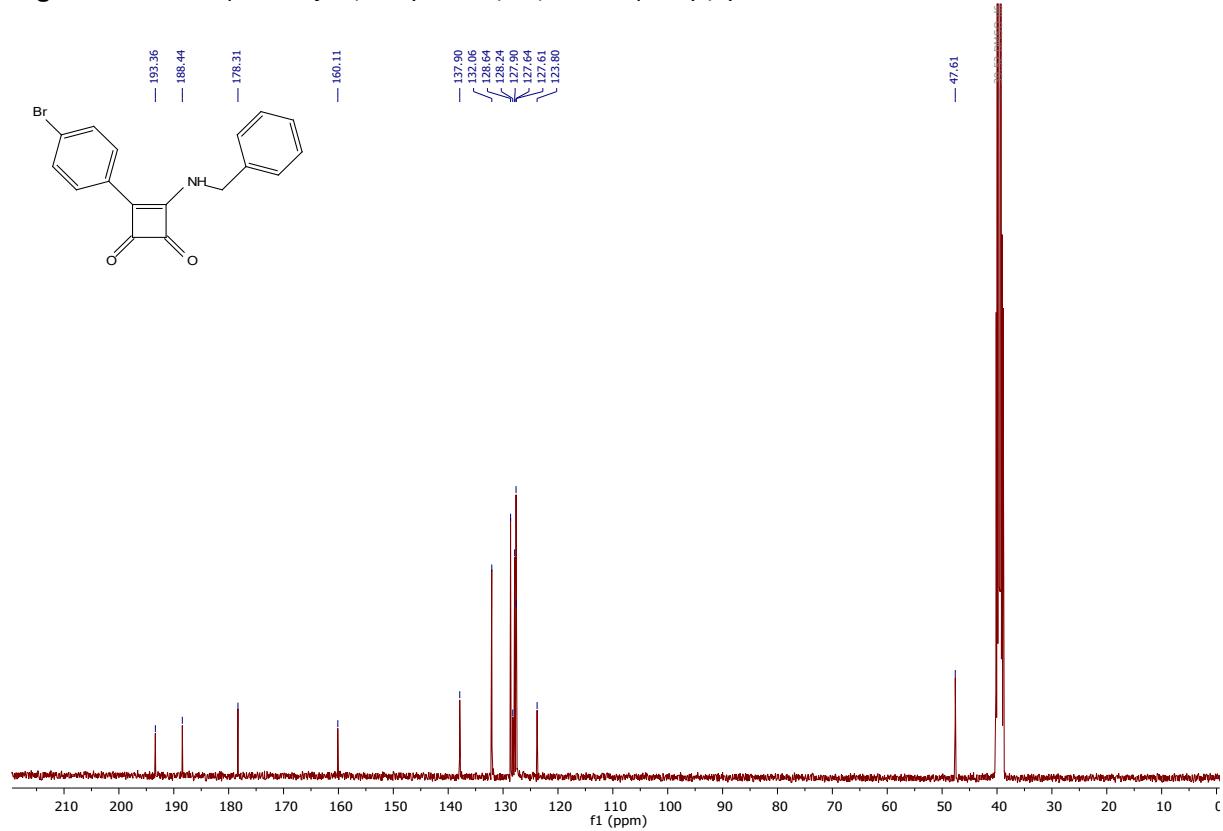


Fig S21. ^1H NMR spectra of 3-(benzylamino)-4-(furan-3-yl)cyclobut-3-ene-1,2-dione **6i**

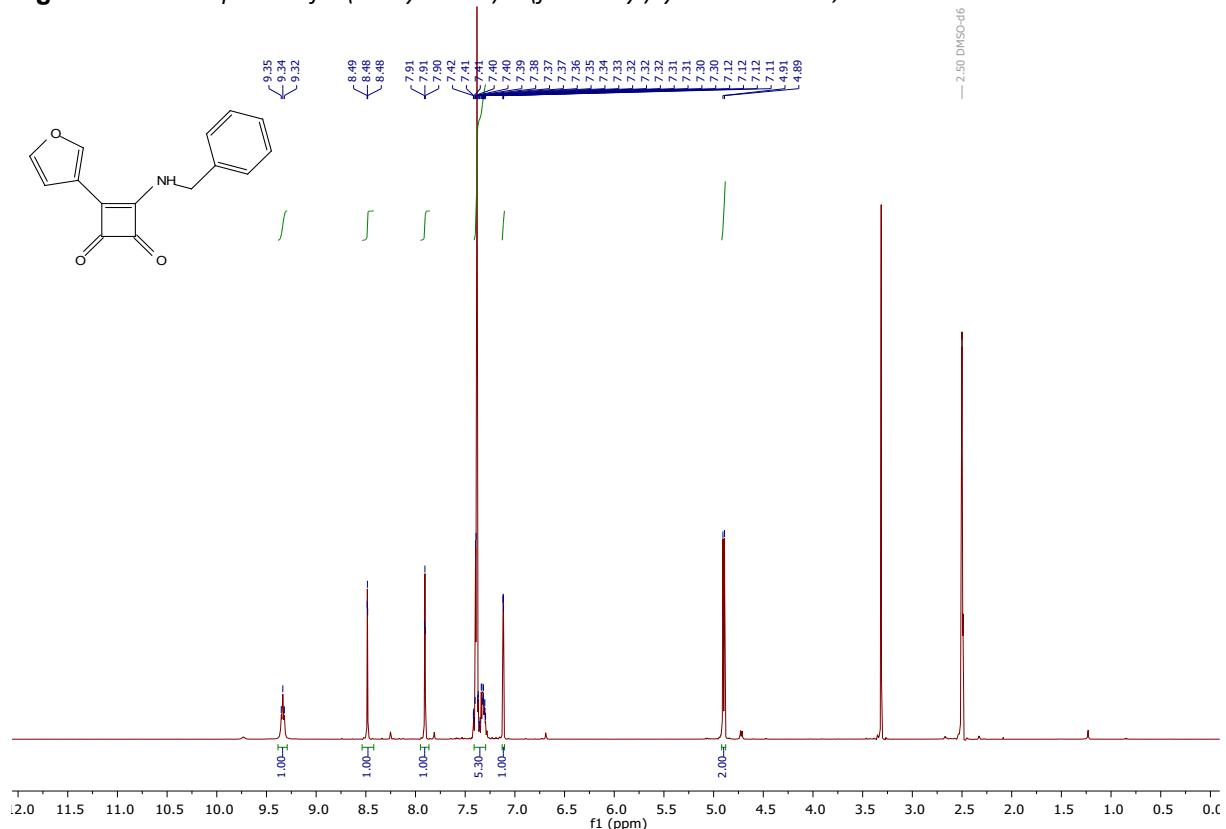


Fig S22. ^{13}C NMR spectra of 3-(benzylamino)-4-(furan-3-yl)cyclobut-3-ene-1,2-dione **6i**

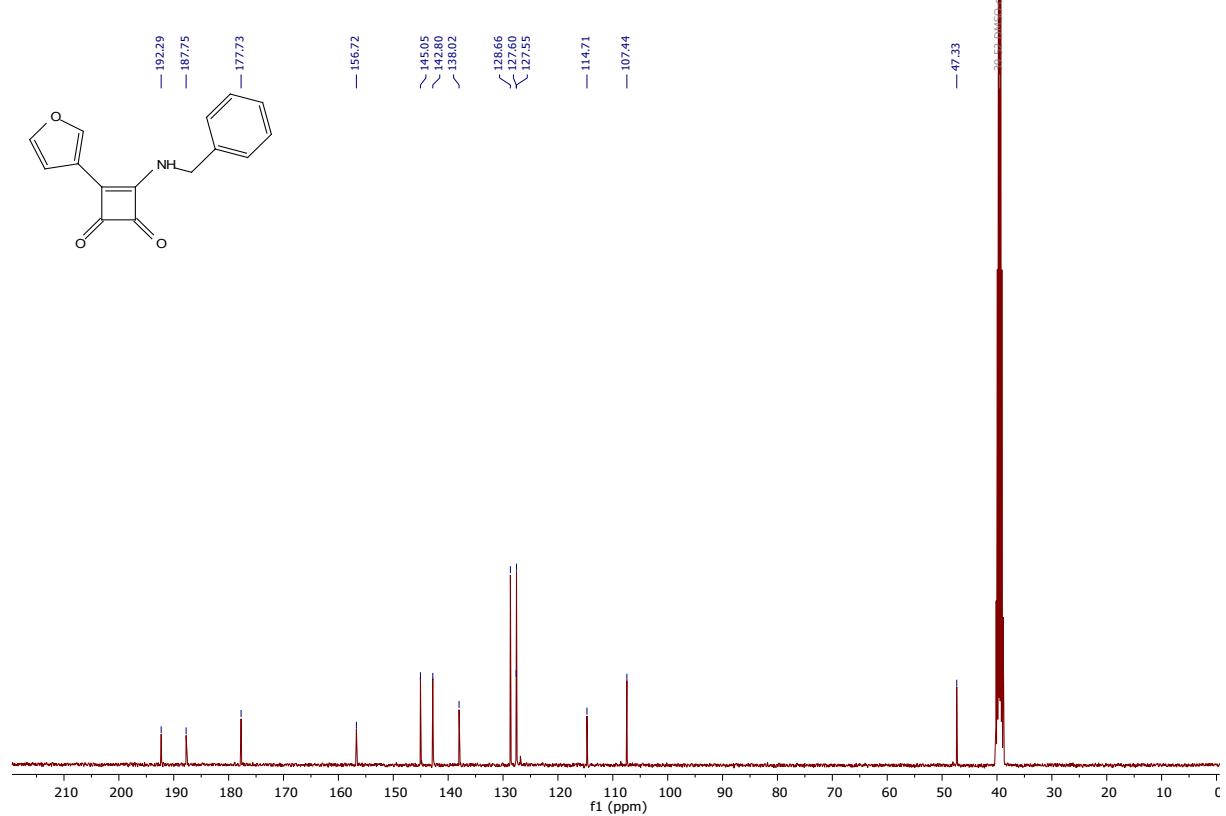


Fig S23. ^1H NMR spectra of 3-(benzylamino)-4-(thiophen-3-yl)cyclobut-3-ene-1,2-dione **6k**

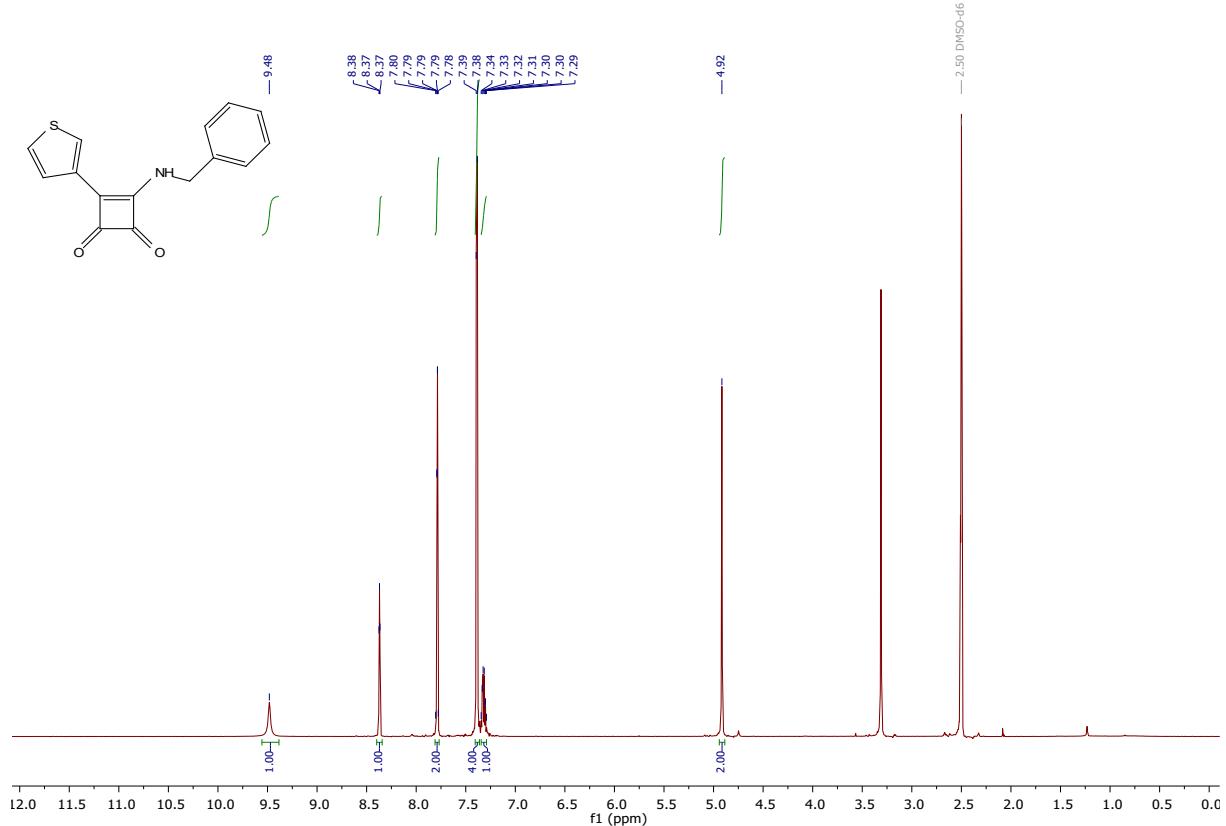


Fig S24. ^{13}C NMR spectra of 3-(benzylamino)-4-(thiophen-3-yl)cyclobut-3-ene-1,2-dione **6k**

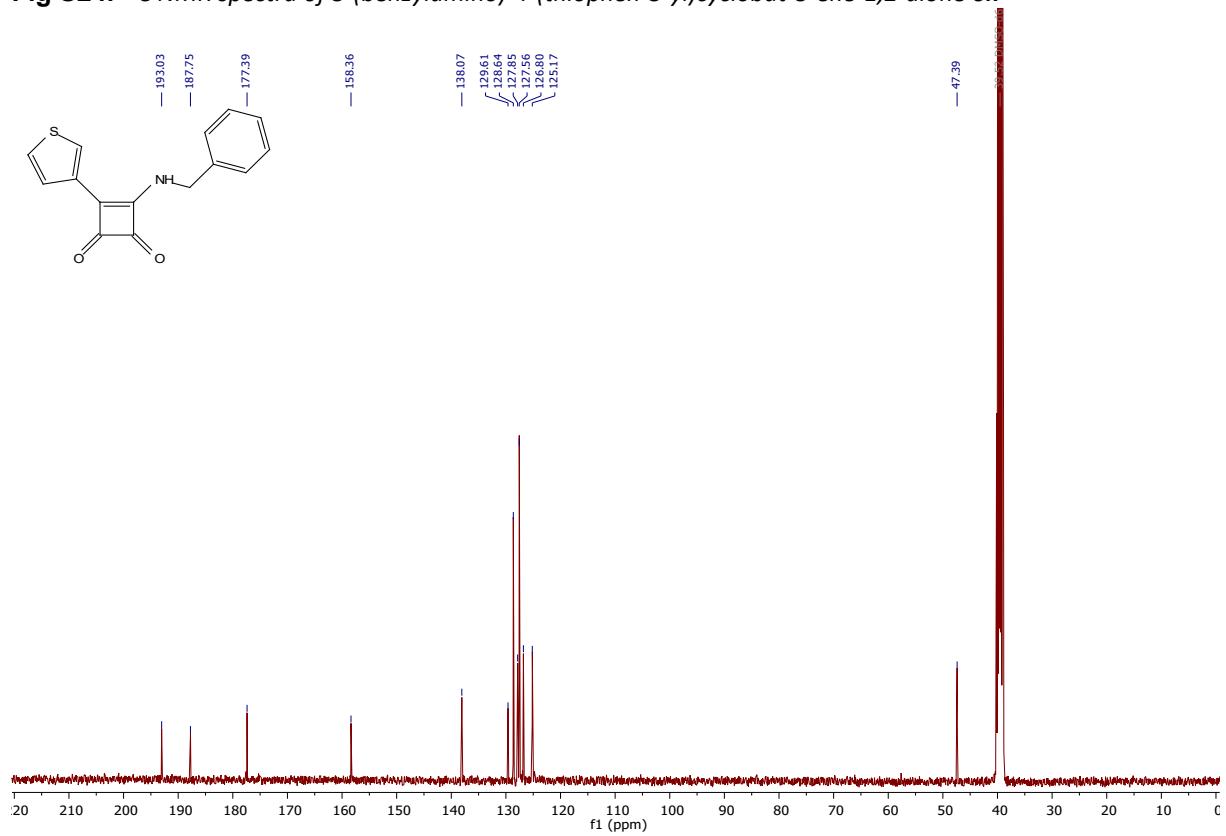


Fig S25. ^1H NMR spectra of 3-(benzylamino)-4-(thiophen-2-yl)cyclobut-3-ene-1,2-dione **6I**

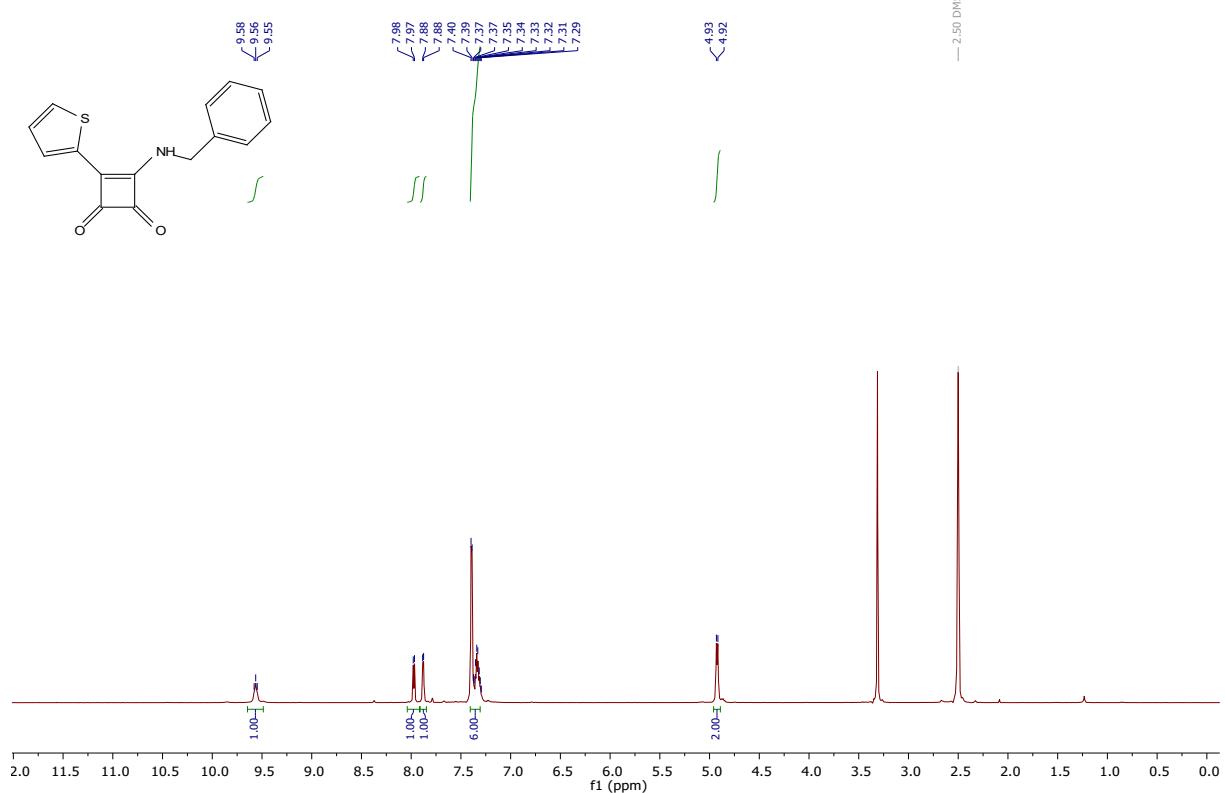


Fig S26. ^{13}C NMR spectra of 3-(benzylamino)-4-(thiophen-2-yl)cyclobut-3-ene-1,2-dione **6I**

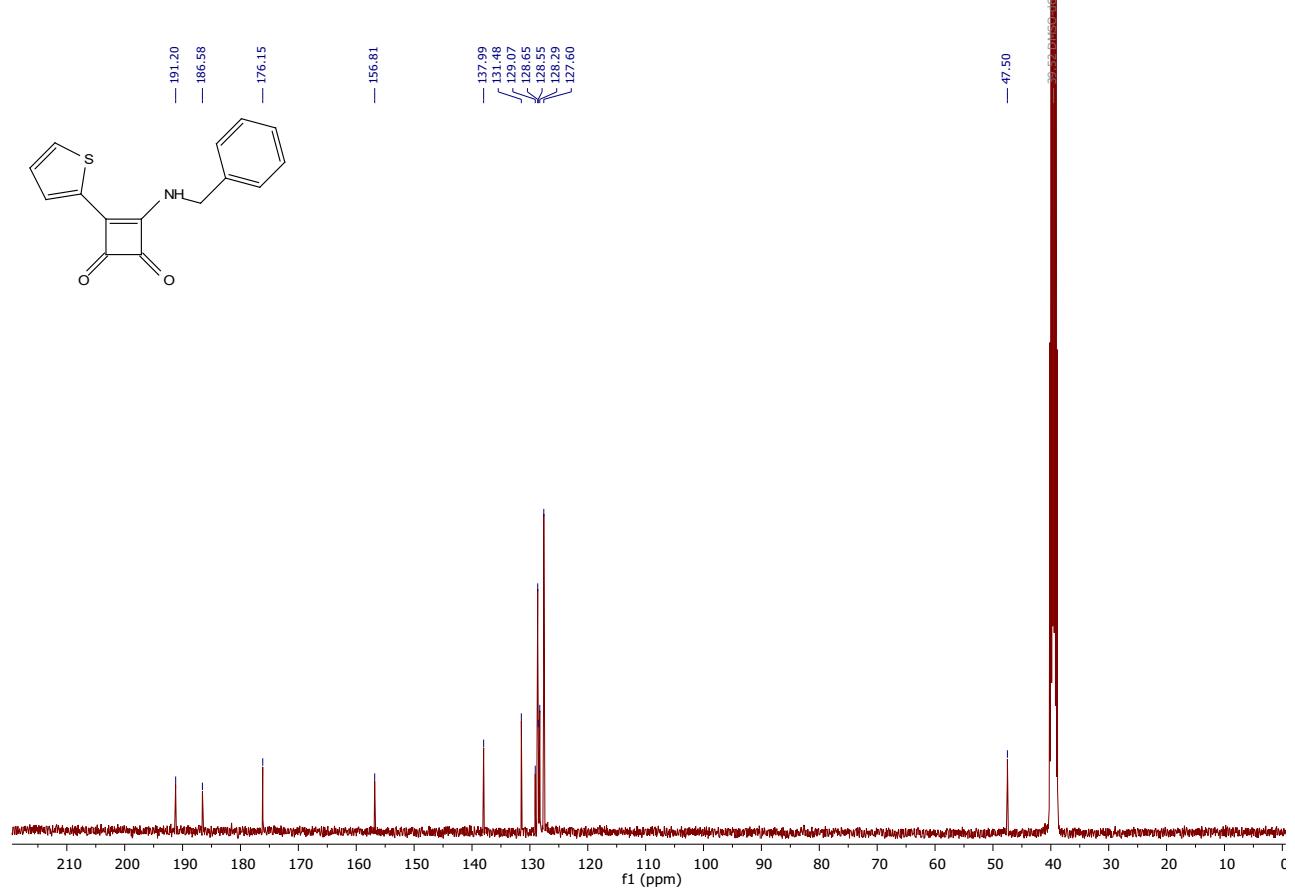


Fig S27. ^1H NMR spectra of (*E*)-3-(benzylamino)-4-styrylcyclobut-3-ene-1,2-dione **6m**

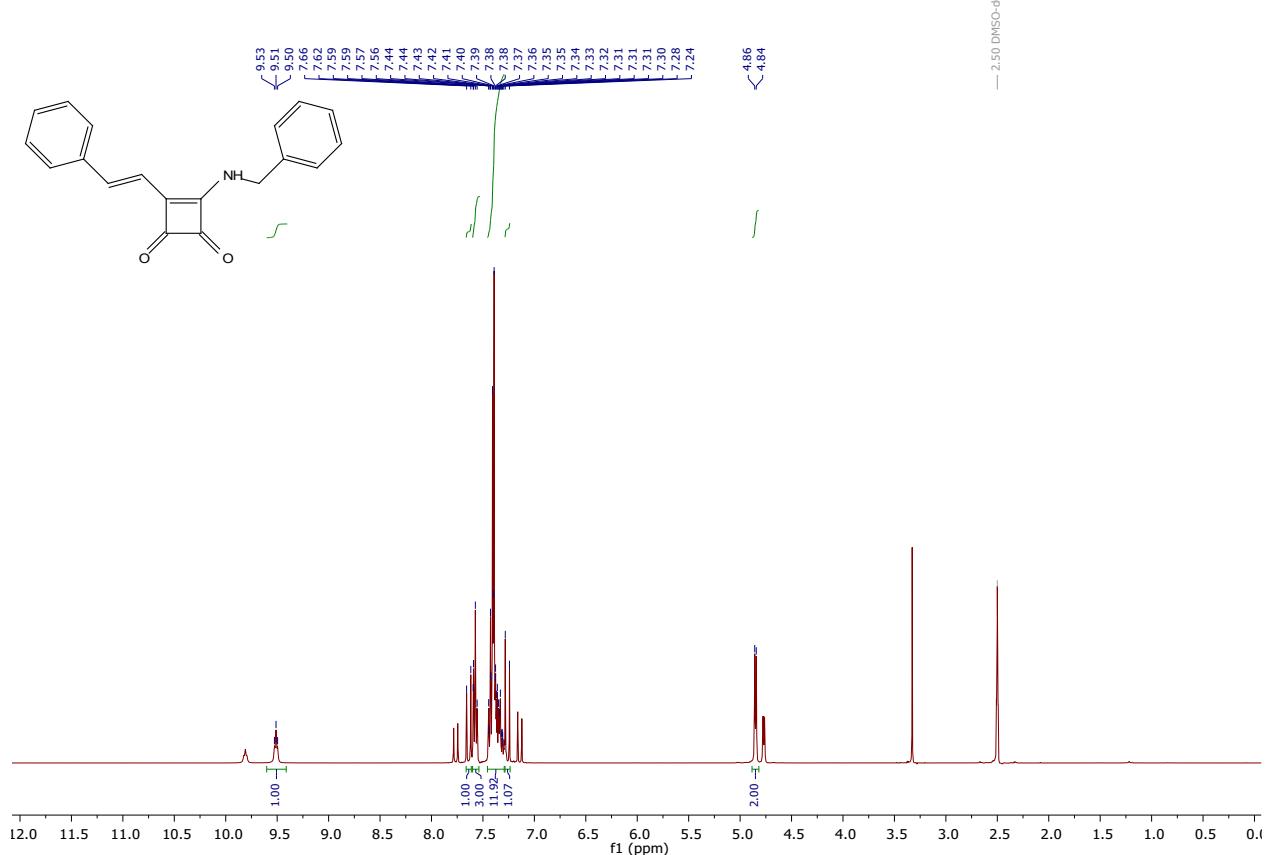


Fig S28. ^{13}C NMR spectra of (*E*)-3-(benzylamino)-4-styrylcyclobut-3-ene-1,2-dione **6m**

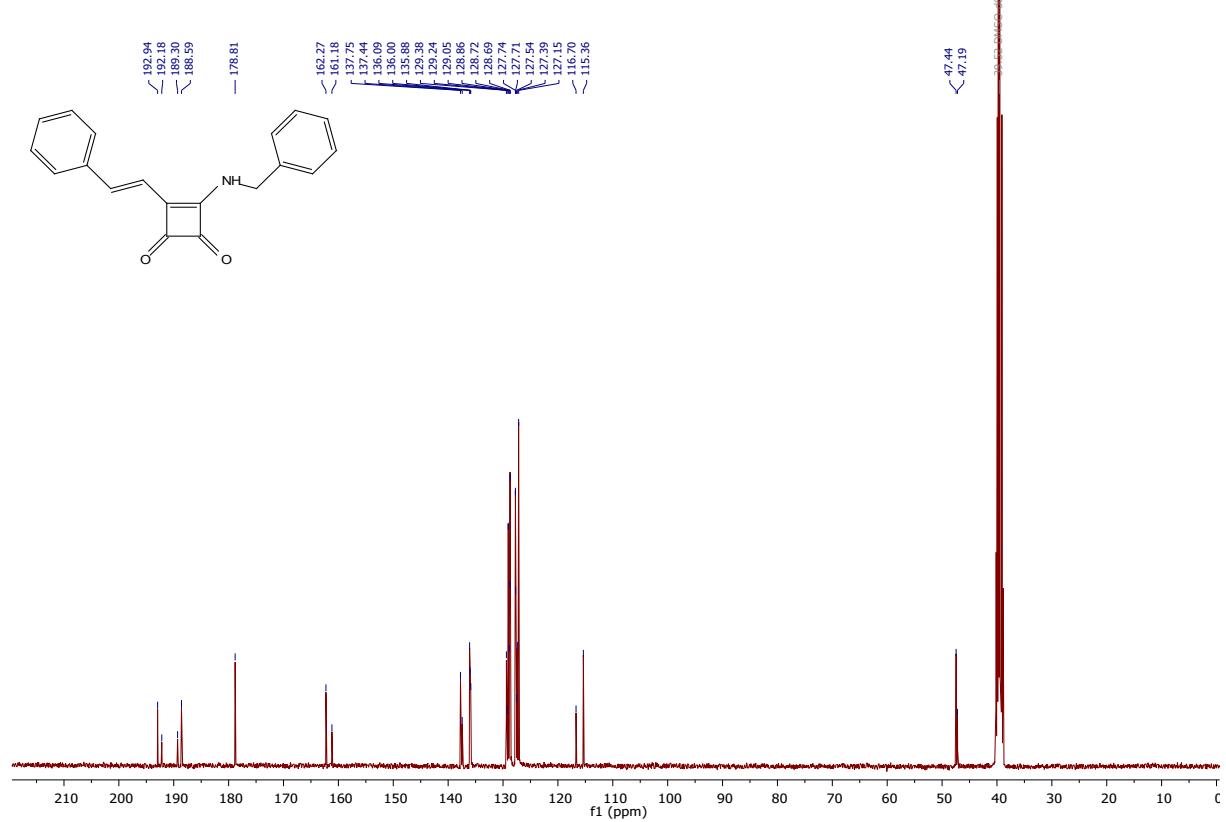


Fig S29. ^1H NMR spectra of 3-(benzylamino)-4-(2,6-dimethylphenyl)cyclobut-3-ene-1,2-dione **6n**

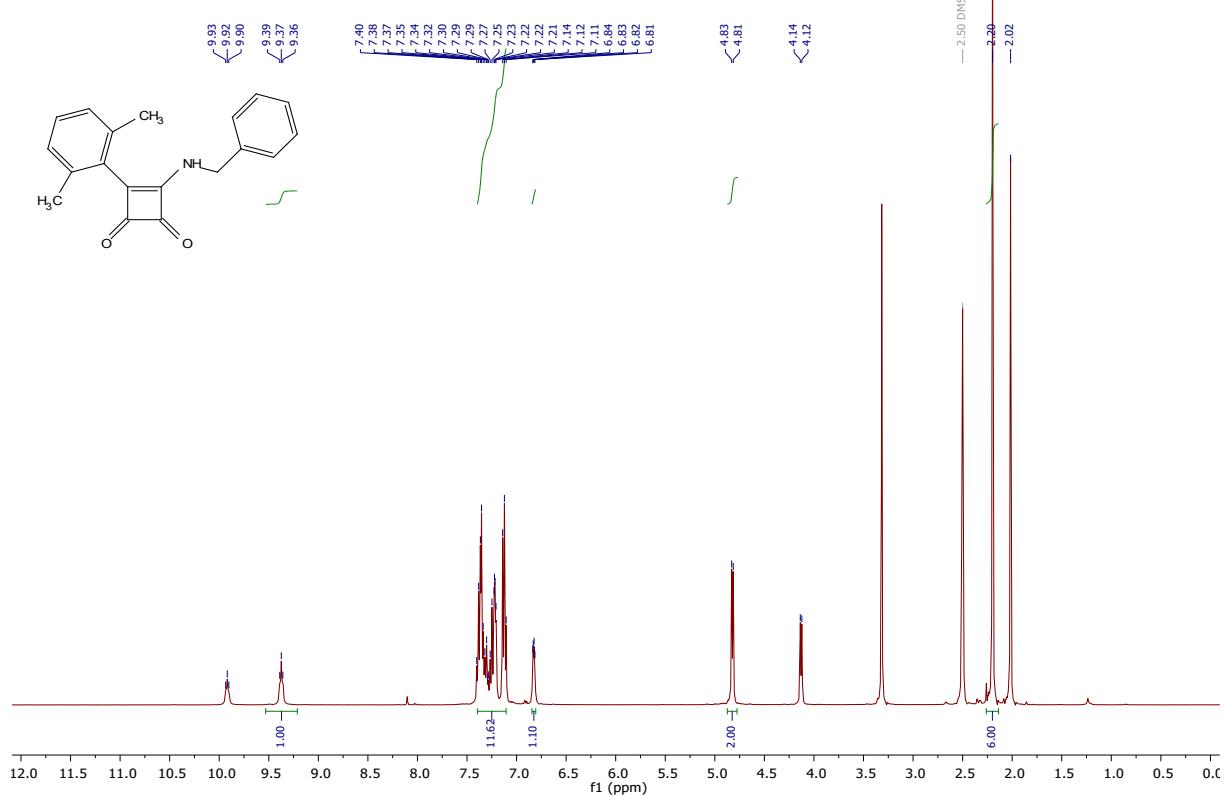


Fig S30. ^{13}C NMR spectra of 3-(benzylamino)-4-(2,6-dimethylphenyl)cyclobut-3-ene-1,2-dione **6n**

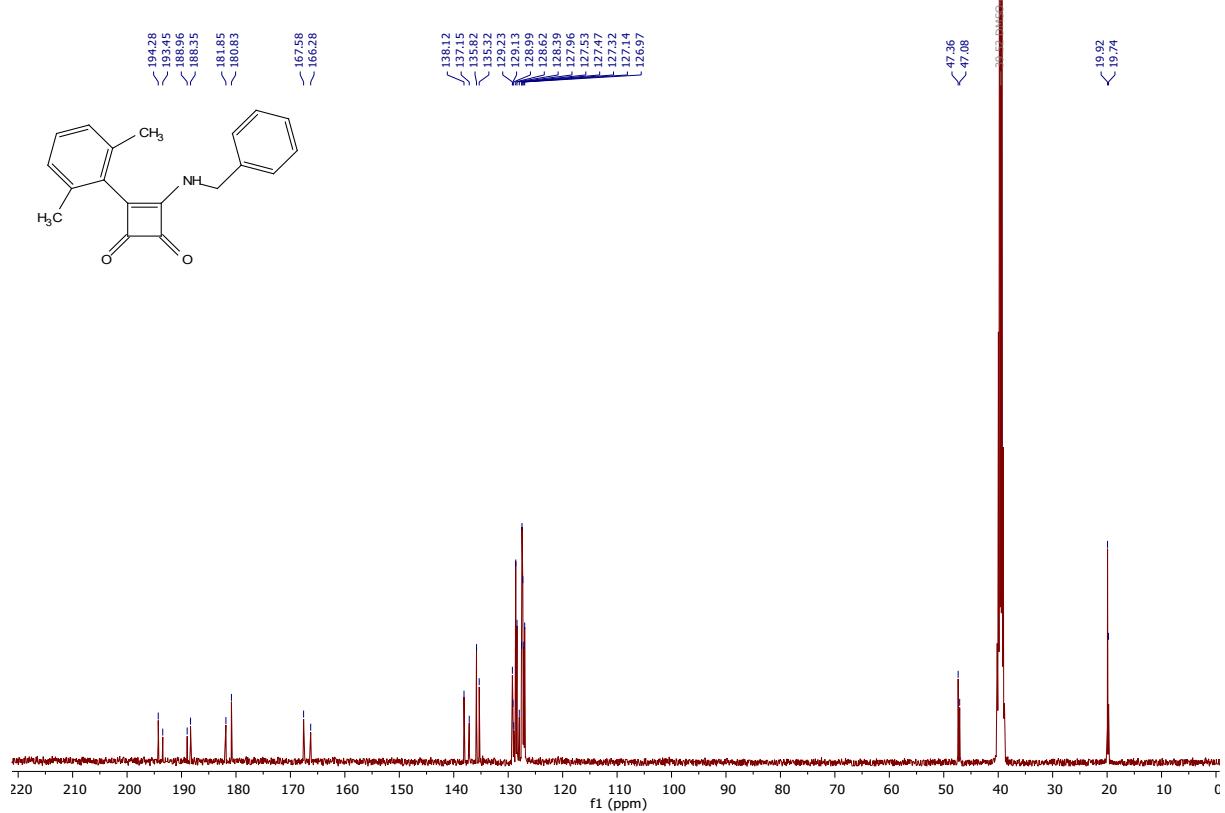


Fig S31. ^1H NMR spectra of 3-(benzylamino)-4-(6-ethoxynaphthalen-2-yl)cyclobut-3-ene-1,2-dione **6o**

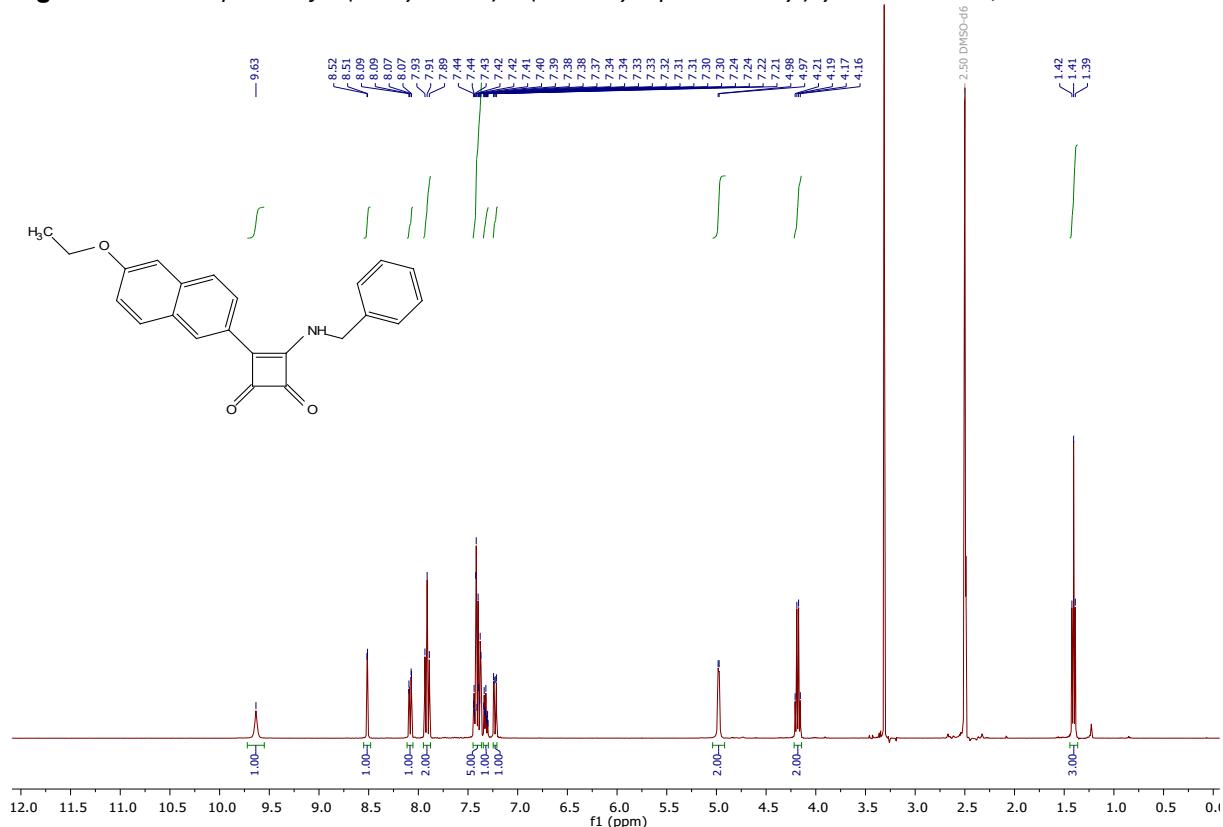


Fig S32. ^{13}C NMR spectra of 3-(benzylamino)-4-(6-ethoxynaphthalen-2-yl)cyclobut-3-ene-1,2-dione **6o**

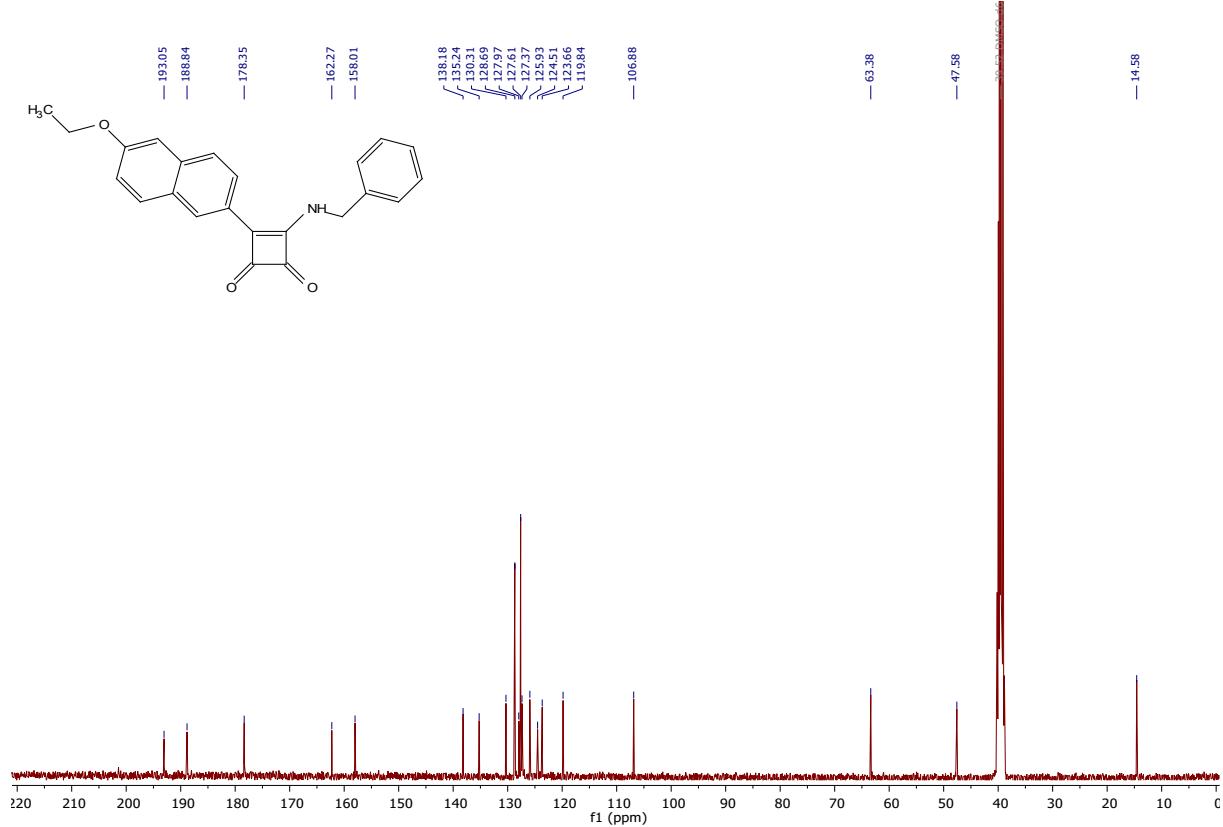


Fig S33. ^1H NMR spectra of 3-((pyridin-2-ylmethyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6p**

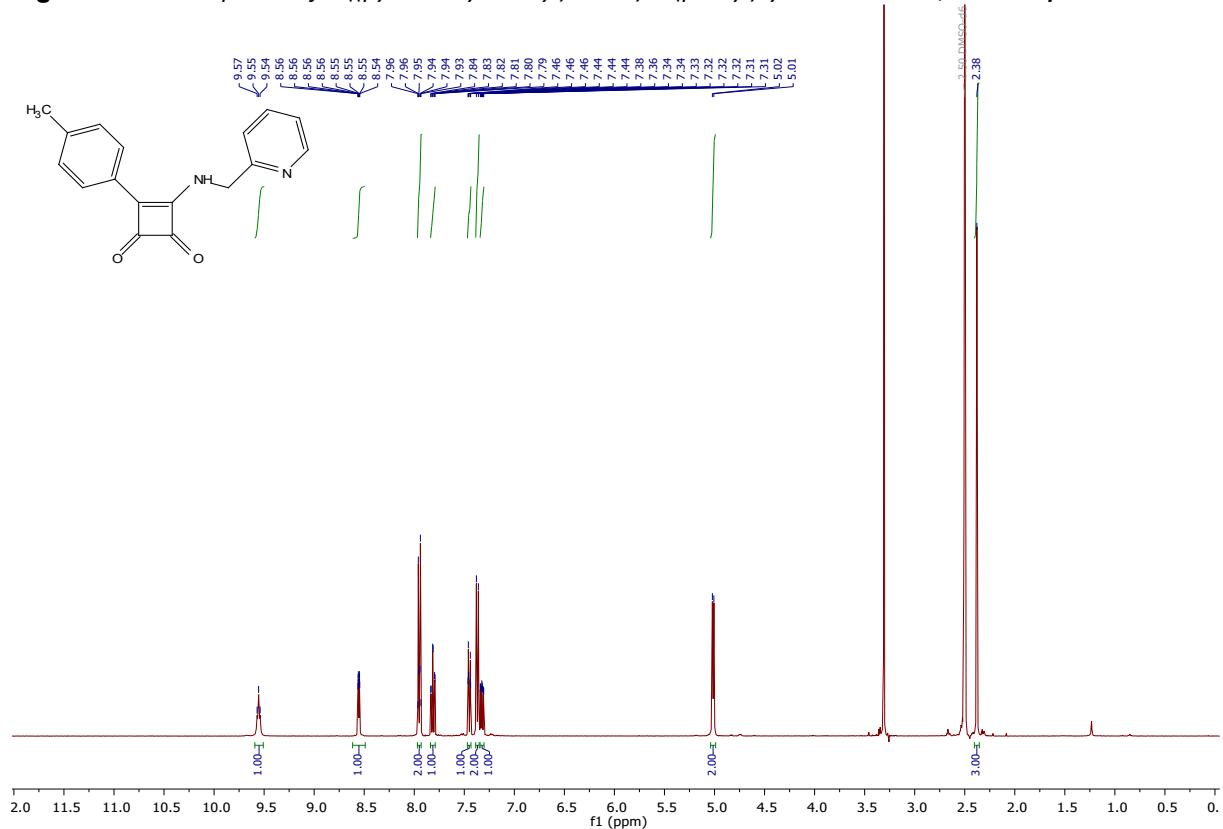


Fig S34. ^{13}C NMR spectra of 3-((pyridin-2-ylmethyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6p**

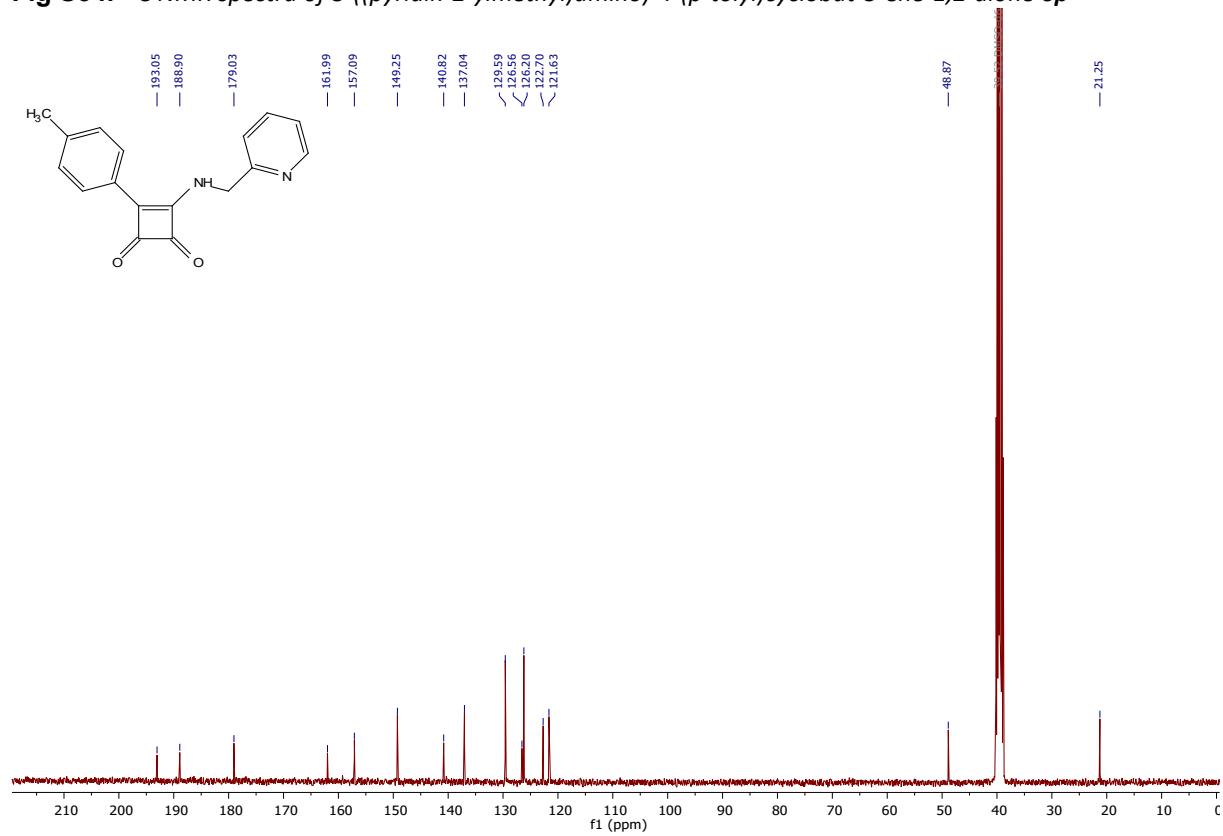


Fig S35. ^1H NMR spectra of 3-((4-bromobenzyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6q**

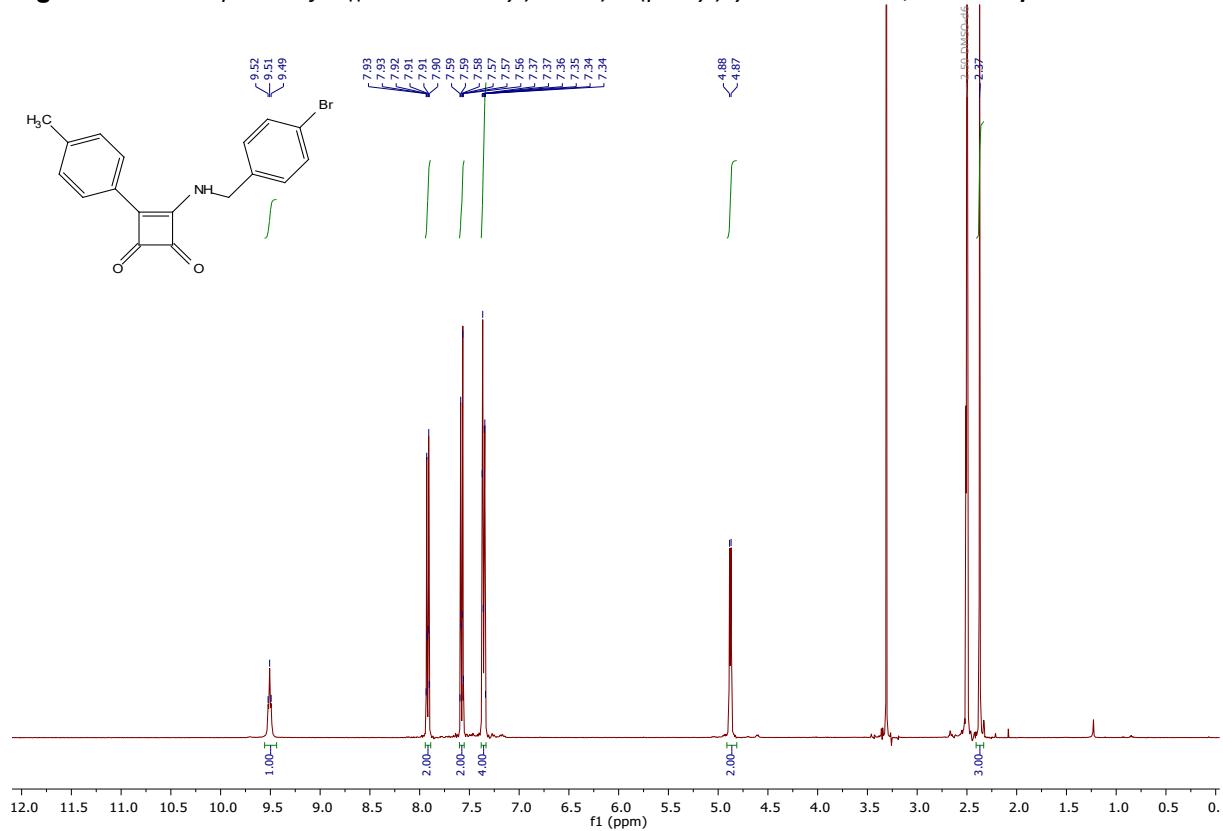


Fig S36. ^{13}C NMR spectra of 3-((4-bromobenzyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6q**

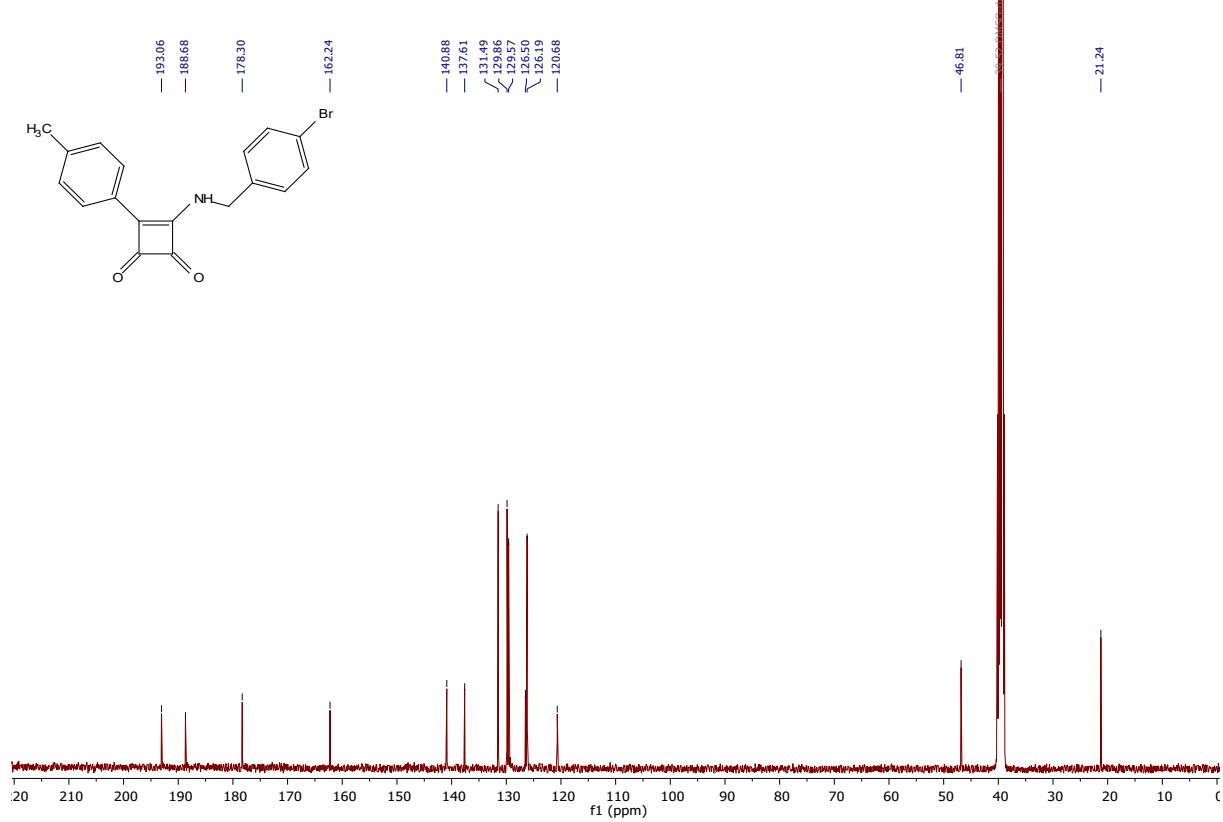


Fig S37. ^1H NMR spectra of 3-(propylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6r**

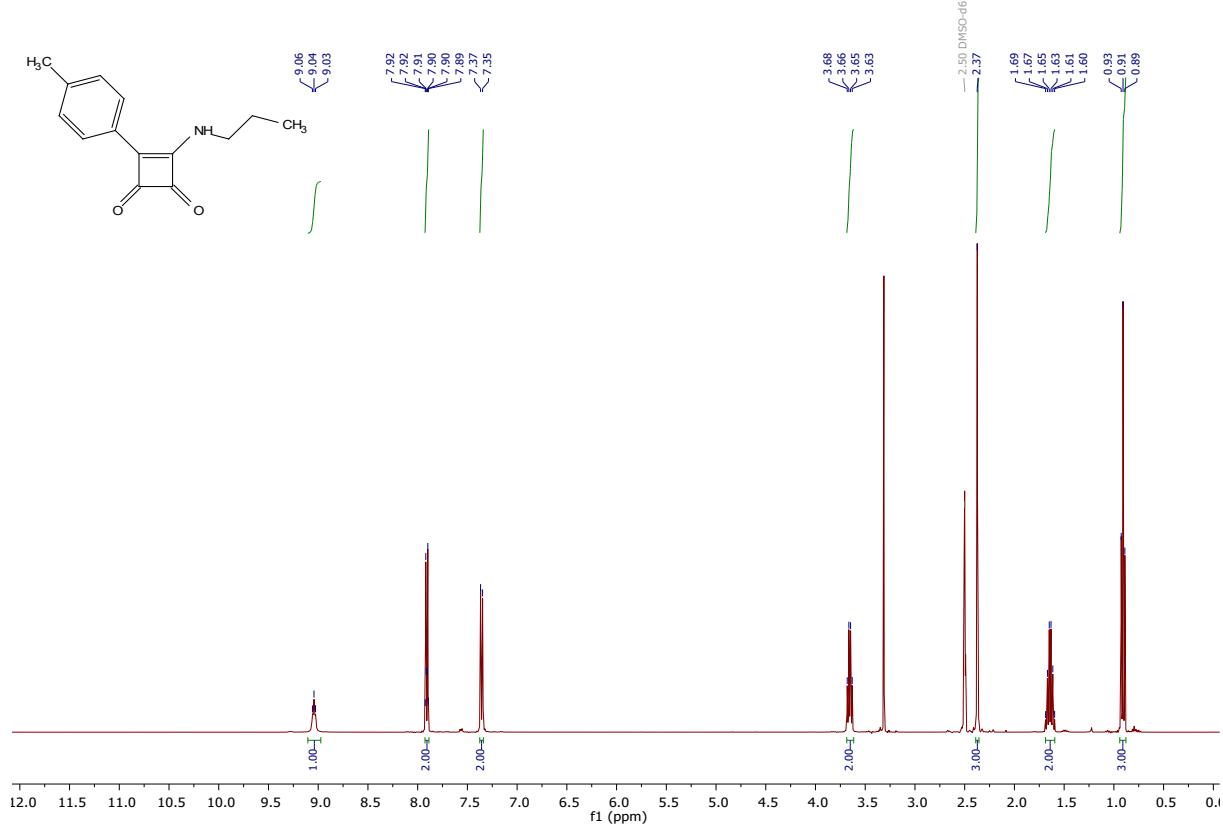


Fig S38. ^{13}C NMR spectra of 3-(propylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6r**

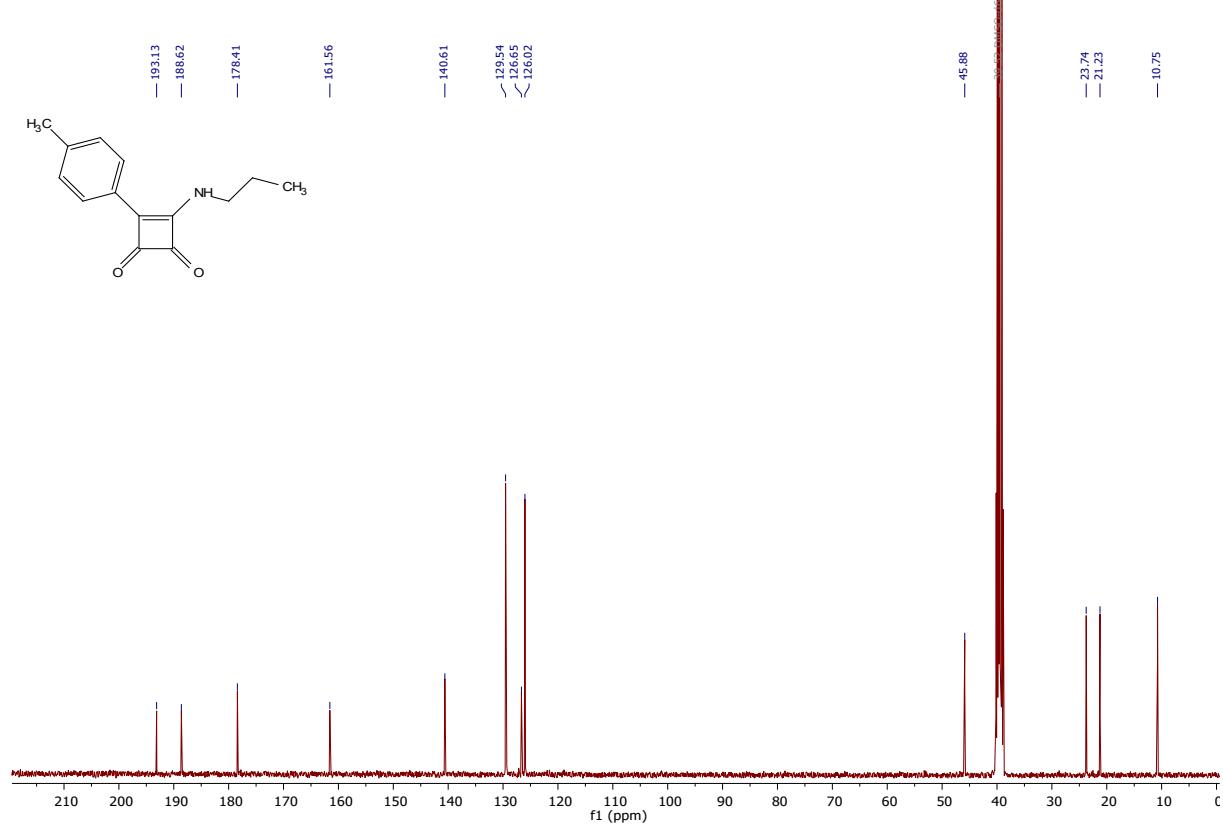


Fig S39. ^1H NMR spectra of 3-(cyclohexylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6s**

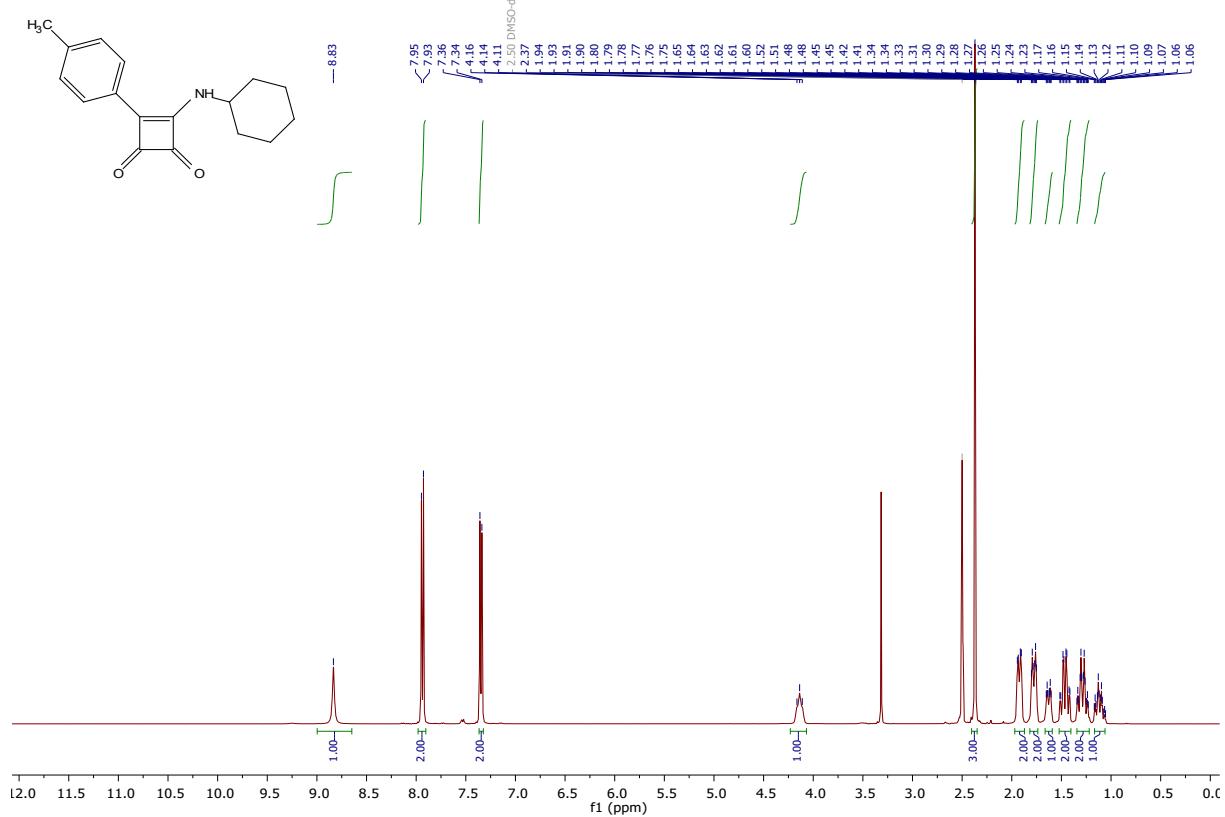


Fig S40. ^{13}C NMR spectra of 3-(cyclohexylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6s**

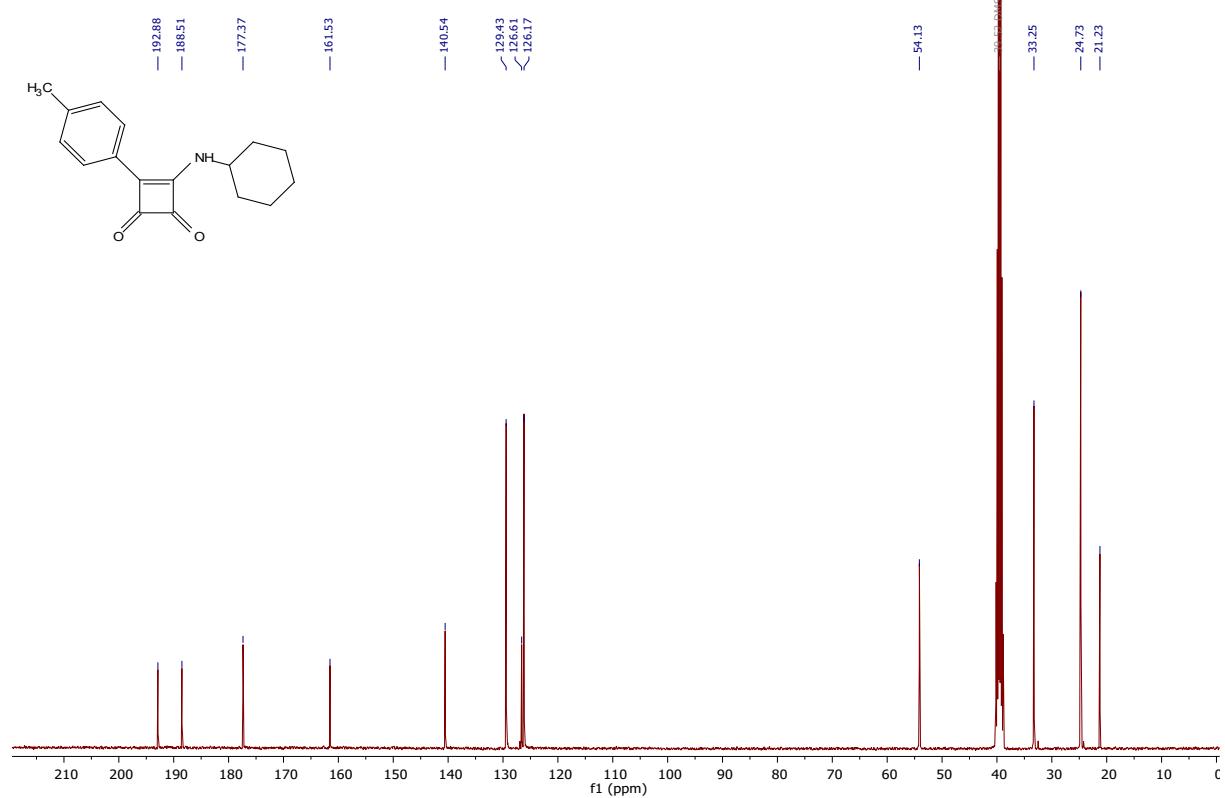


Fig S41. ^1H NMR spectra of 3-(phenylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6t**

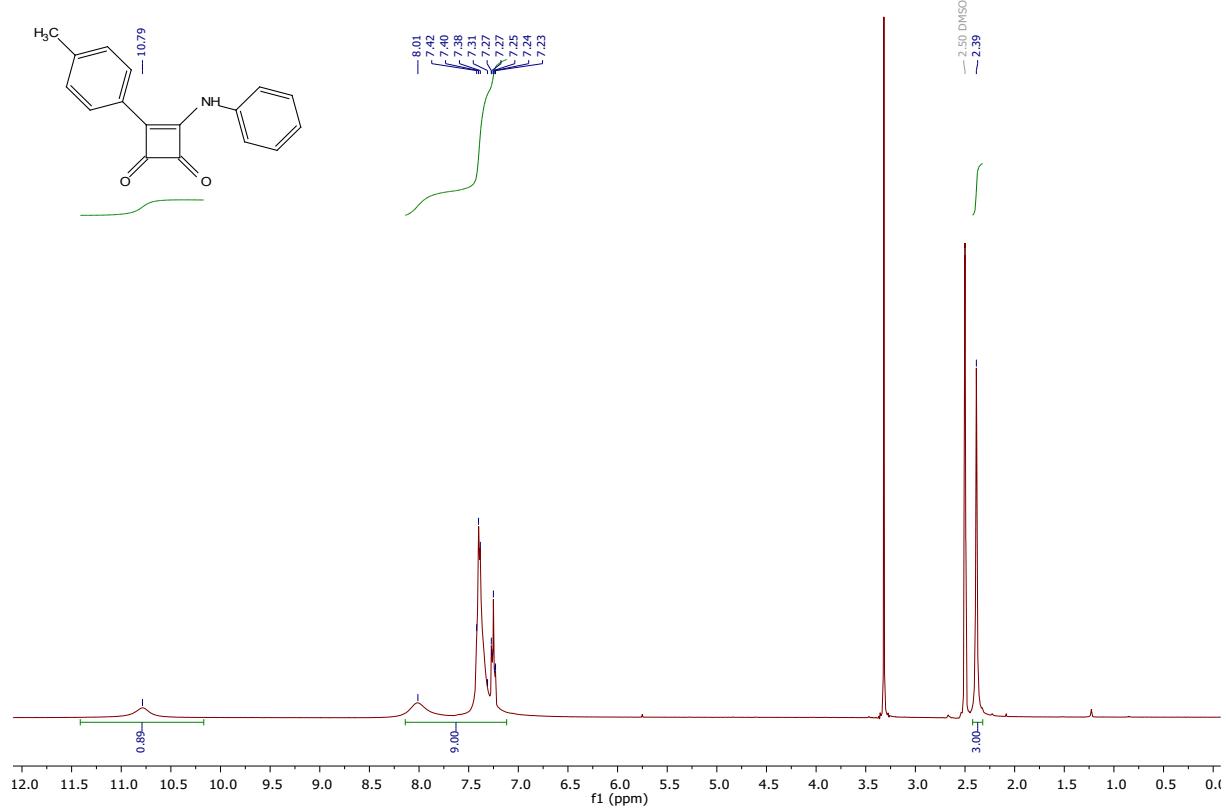


Fig S42. ^{13}C NMR spectra of 3-(phenylamino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6t**

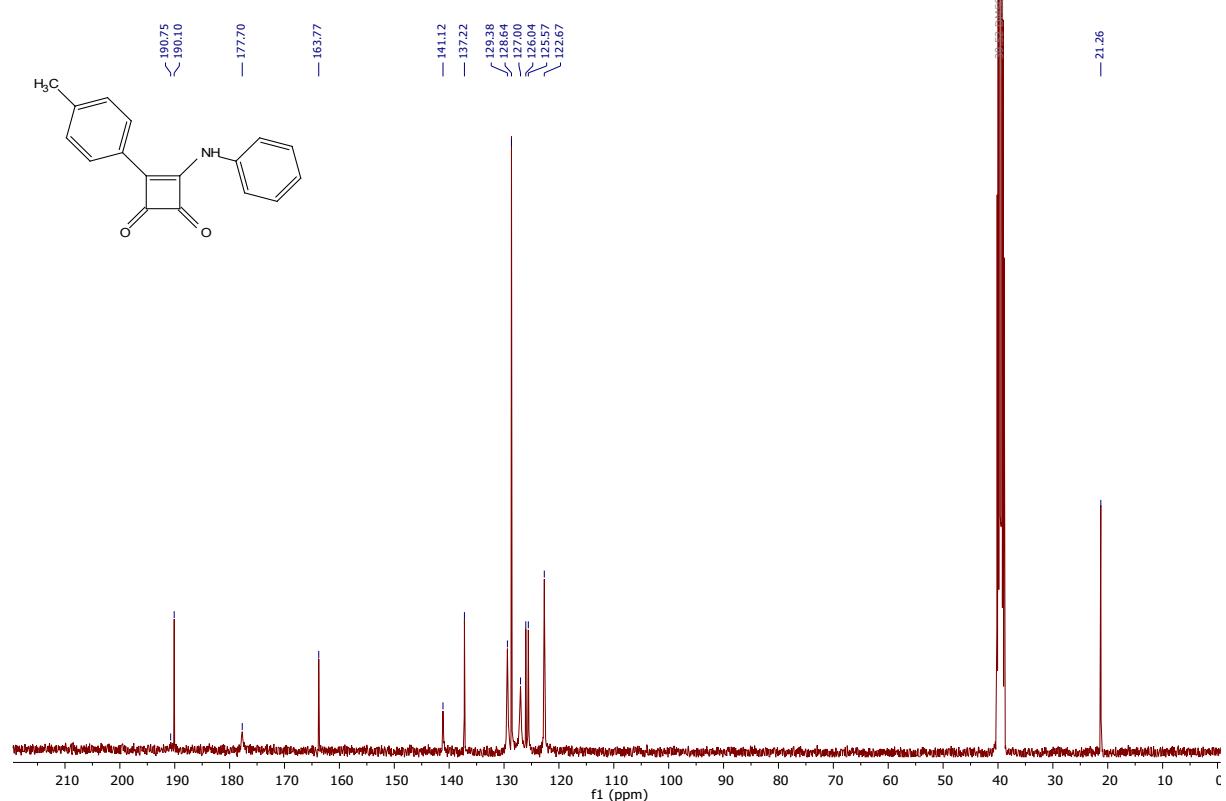


Fig S43. ^1H NMR spectra of 3-((4-methoxyphenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6u**

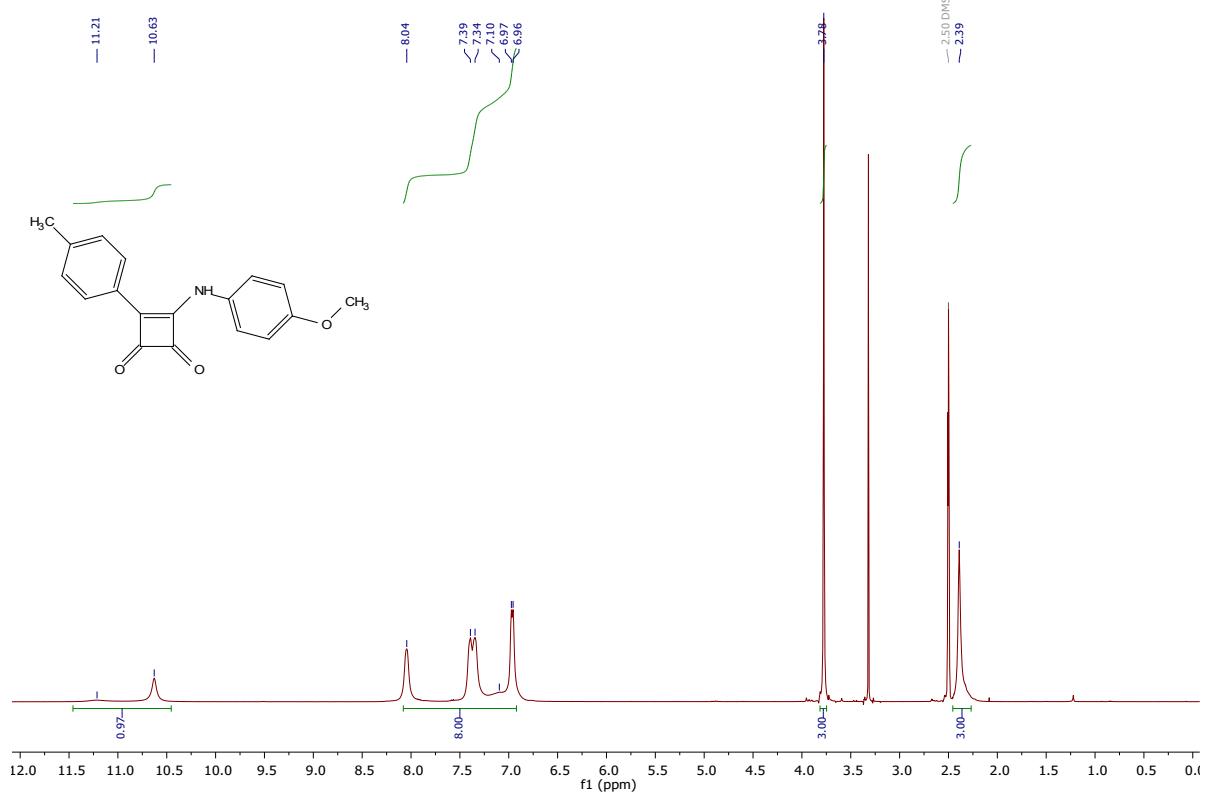


Fig S44. ^{13}C NMR spectra of 3-((4-methoxyphenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6u**

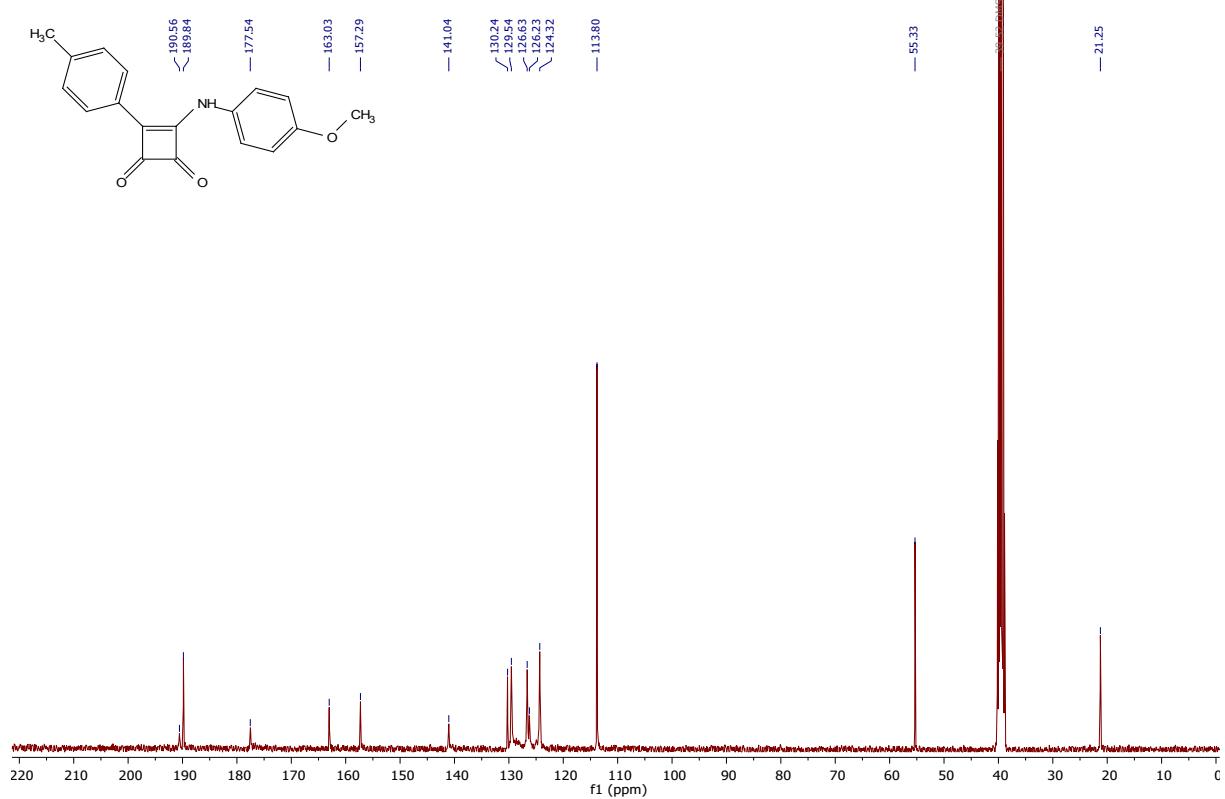


Fig S45. ^1H NMR spectra of methyl (3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)-*L*-tyrosinate **6y**

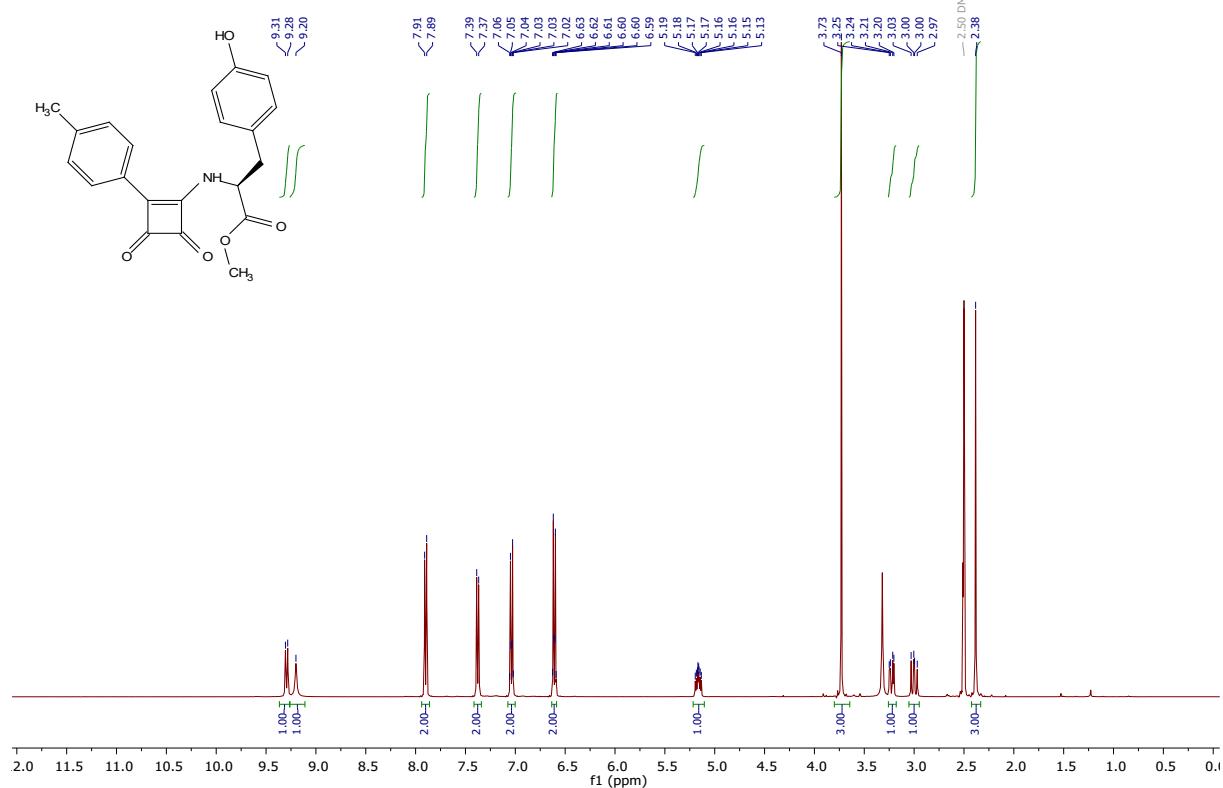


Fig S46. ^{13}C NMR spectra of methyl (3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)-*L*-tyrosinate **6y**

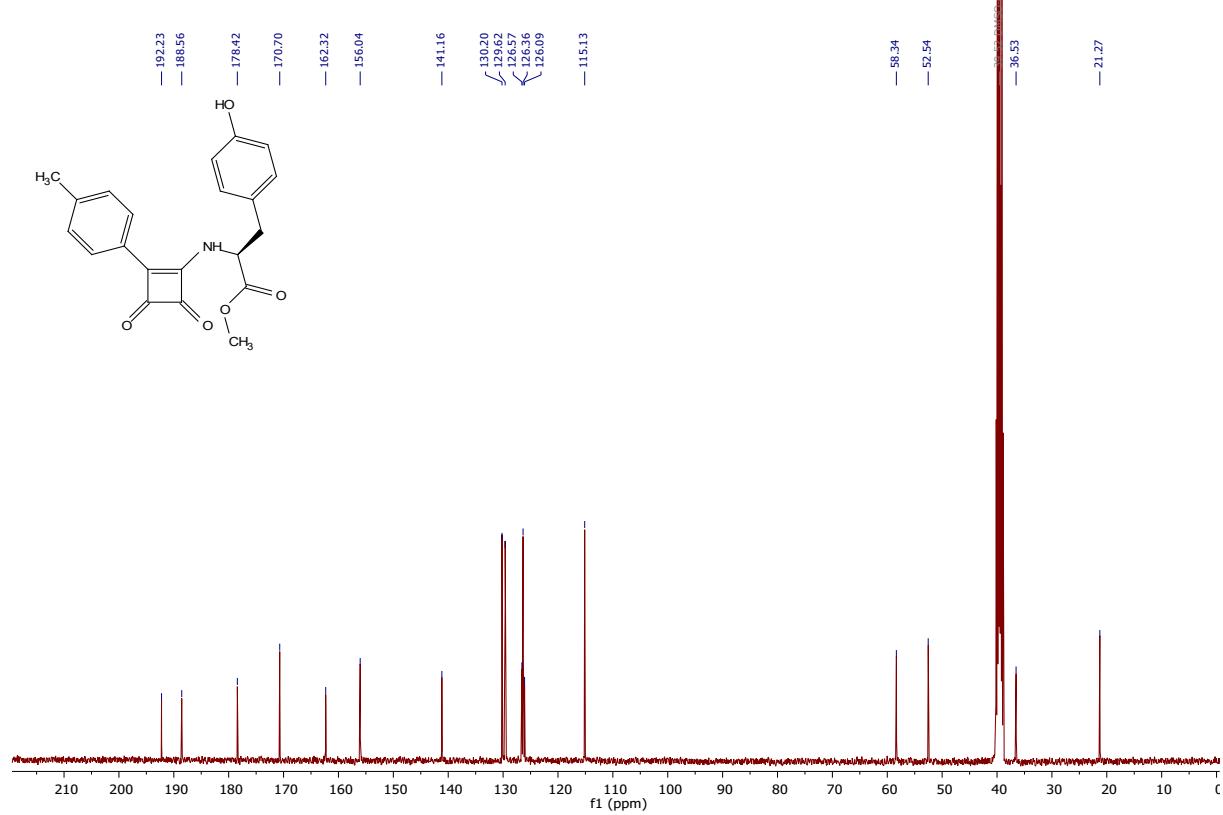


Fig S47. ^1H NMR spectra of 3-ethoxy-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6aa**

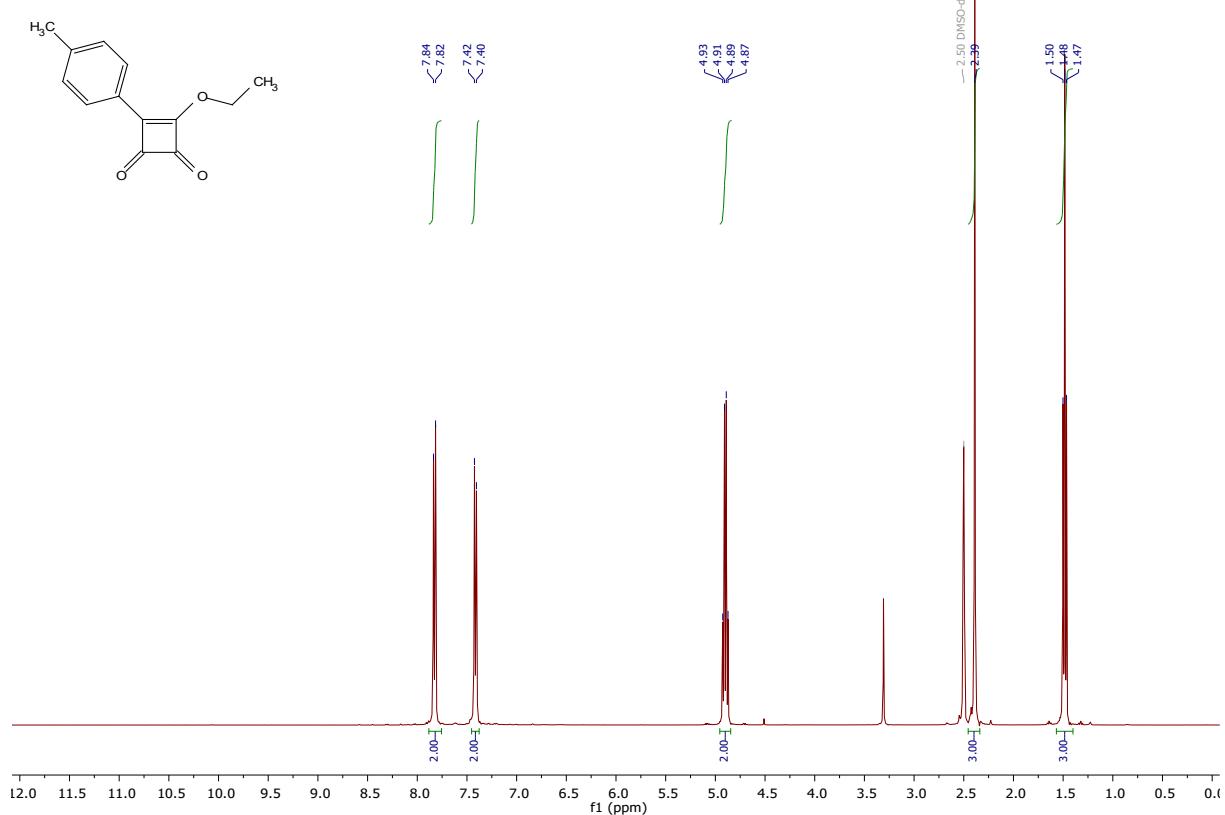


Fig S48. ^{13}C NMR spectra of 3-ethoxy-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6aa**

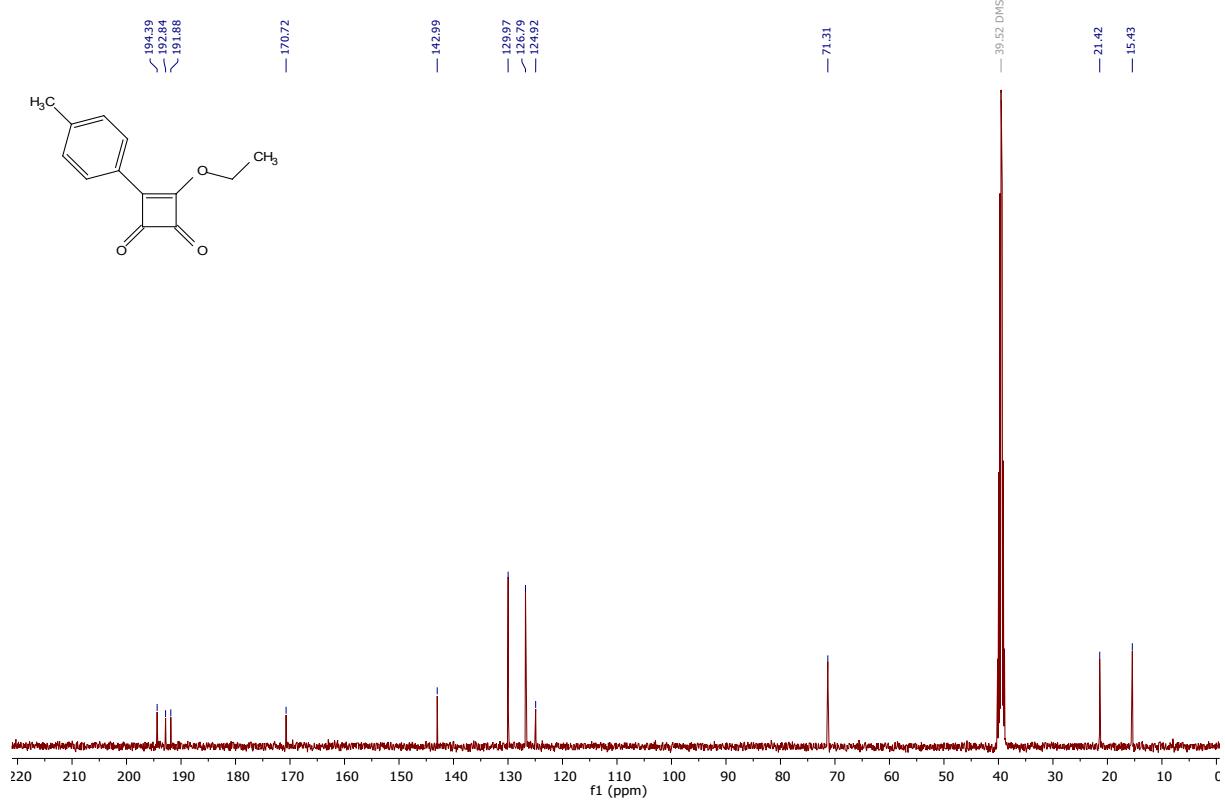


Fig S49. ^1H NMR spectra of 3-((4-bromophenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ab**

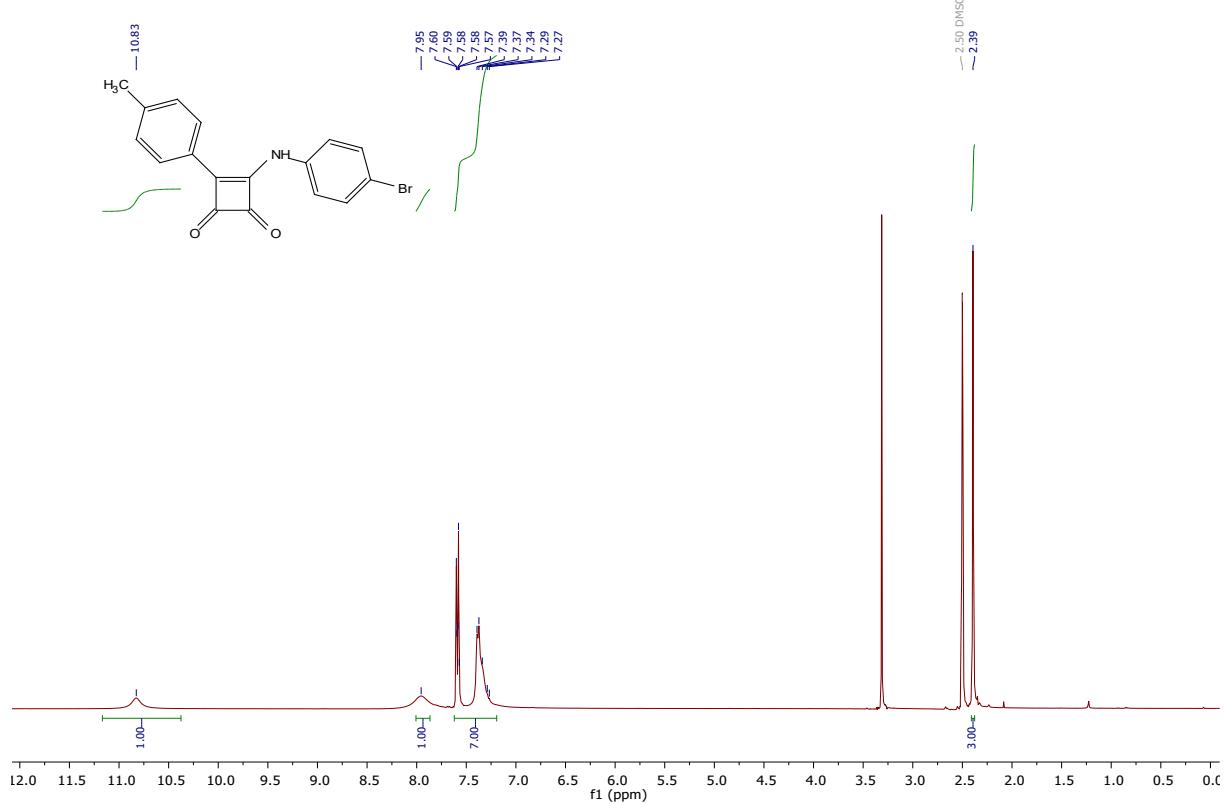


Fig S50. ^{13}C NMR spectra of 3-((4-bromophenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ab**

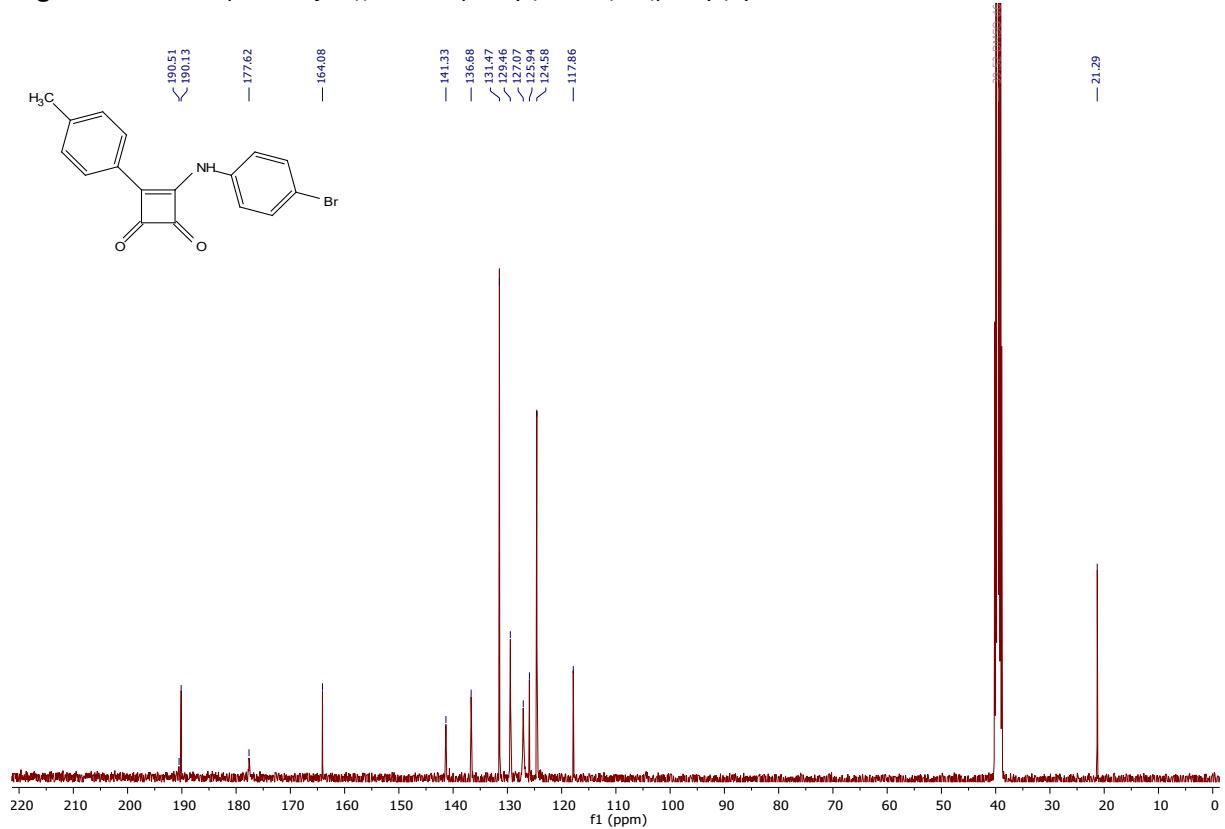


Fig S51. ^1H NMR spectra of 3-((4-morpholinophenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ac**

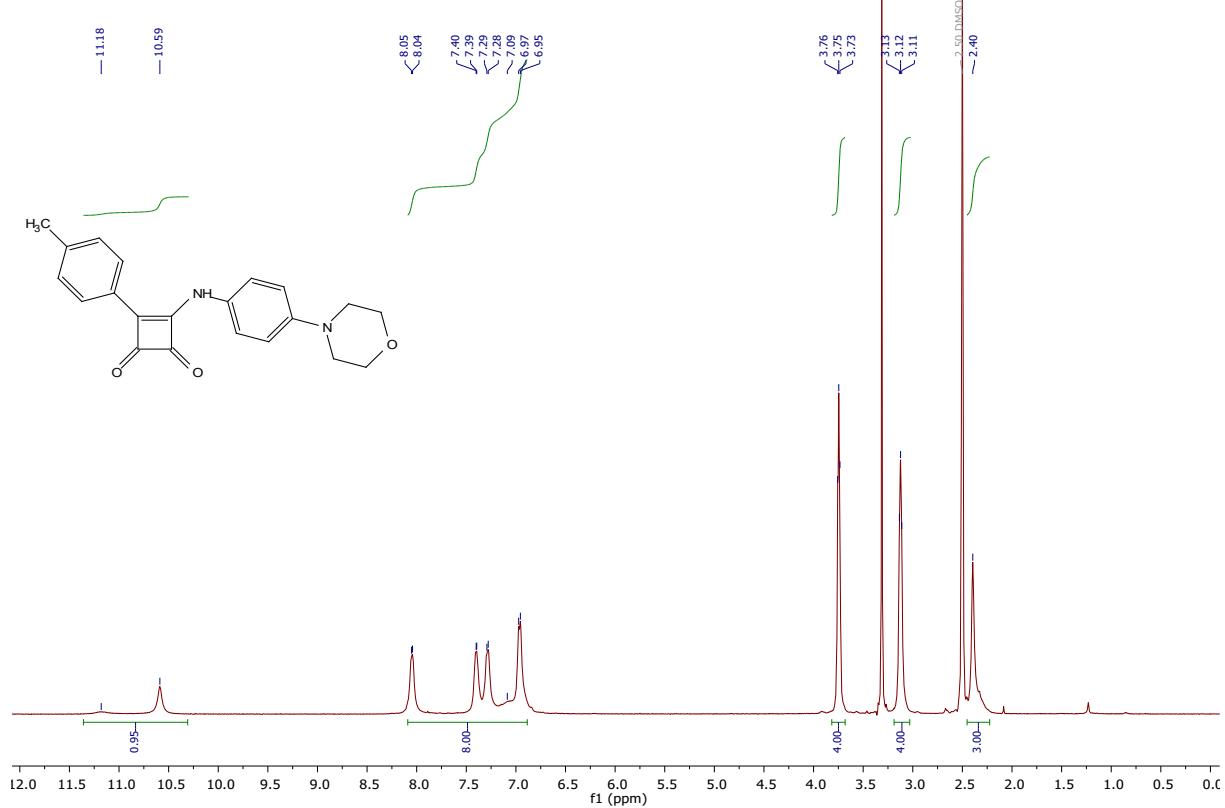


Fig S52. ^{13}C NMR spectra of 3-((4-morpholinophenyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ac**

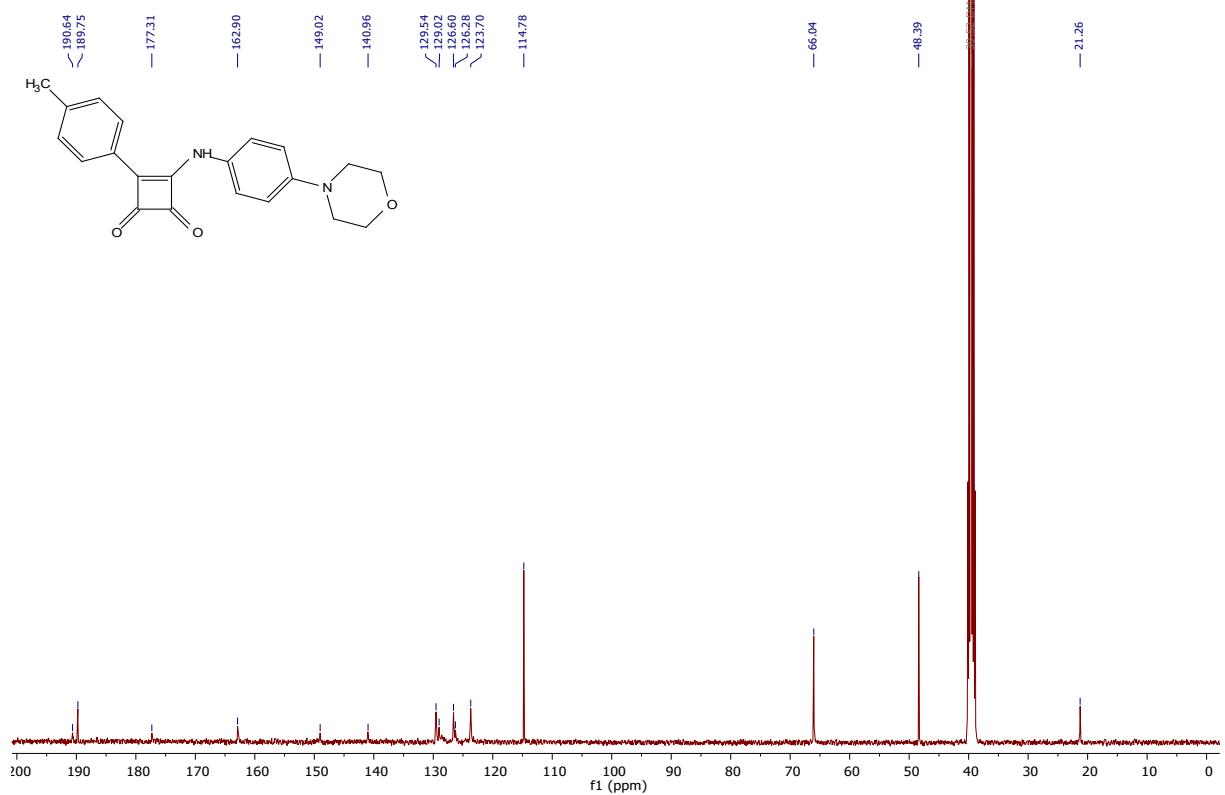


Fig S53. ^1H NMR spectra of ethyl 3-((3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)amino)propanoate **6ad**

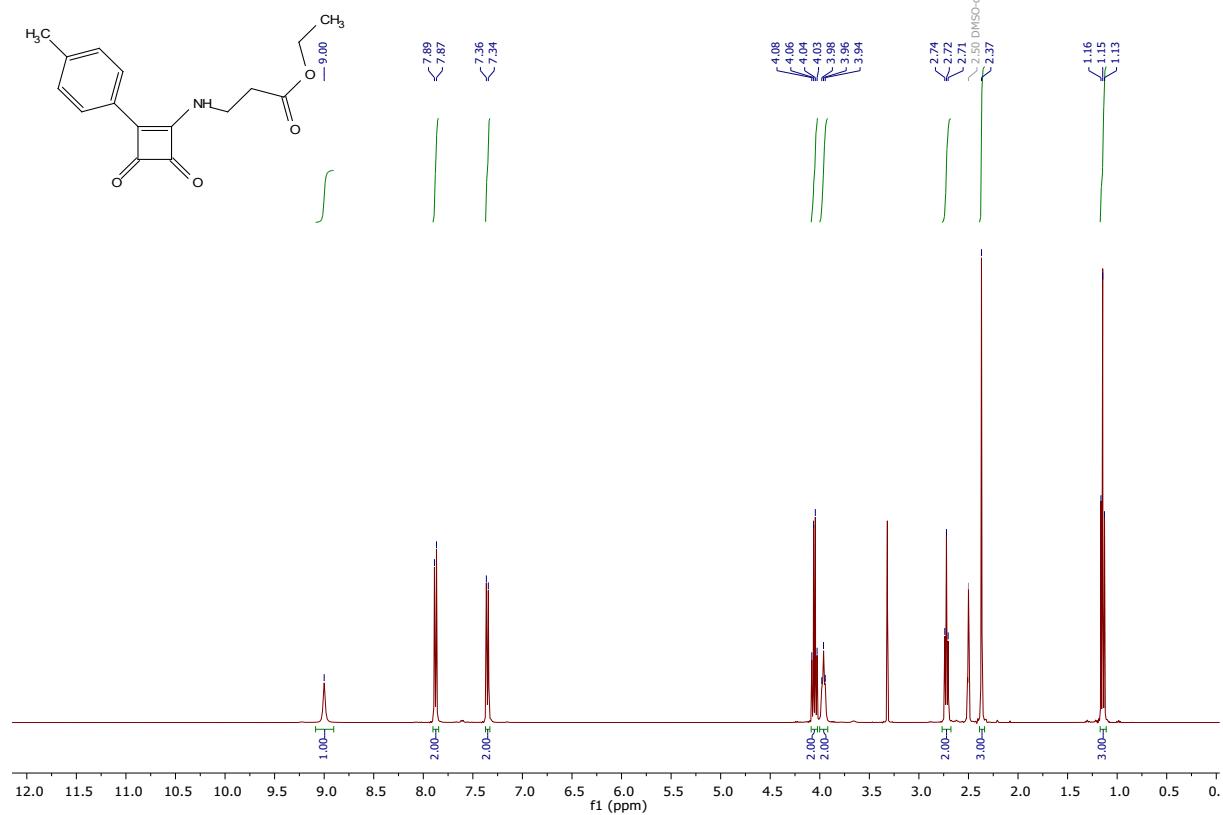


Fig S54. ^{13}C NMR spectra of ethyl 3-((3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)amino)propanoate **6ad**

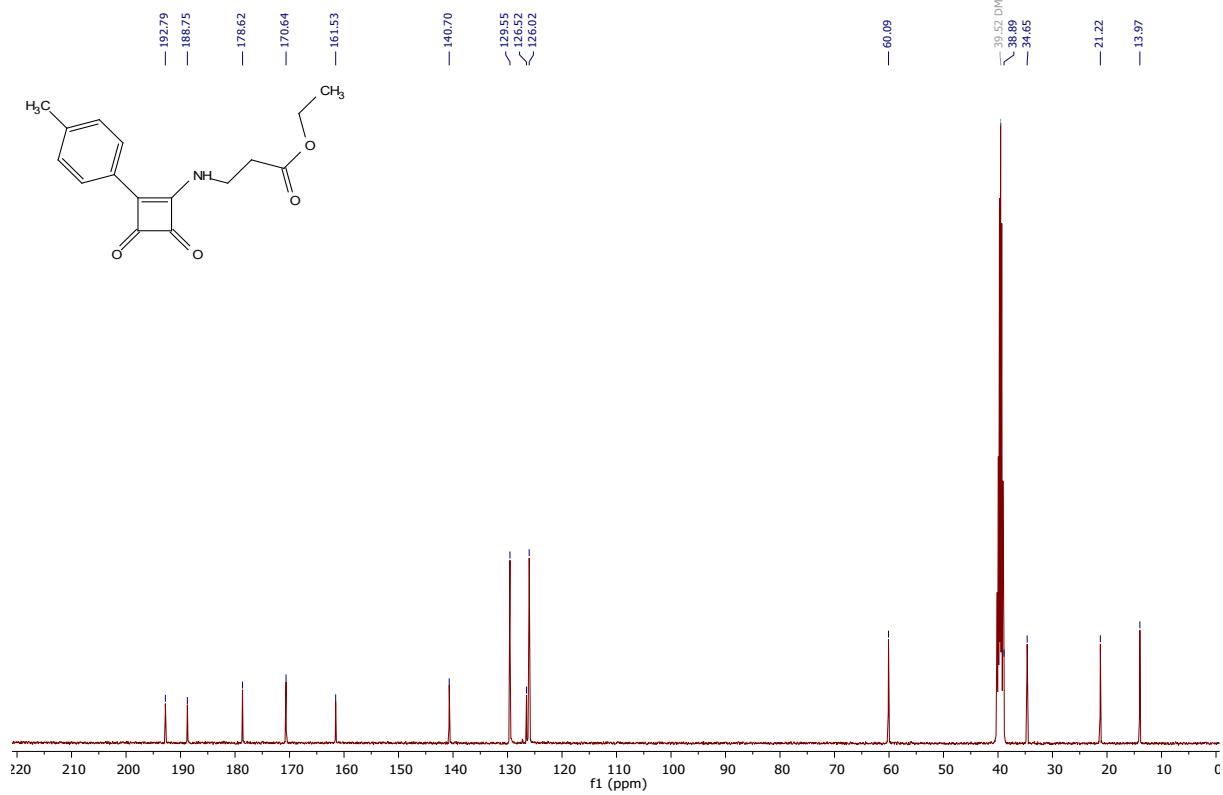


Fig S55. ^1H NMR spectra of 3-(benzyl(hydroxy)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ae**

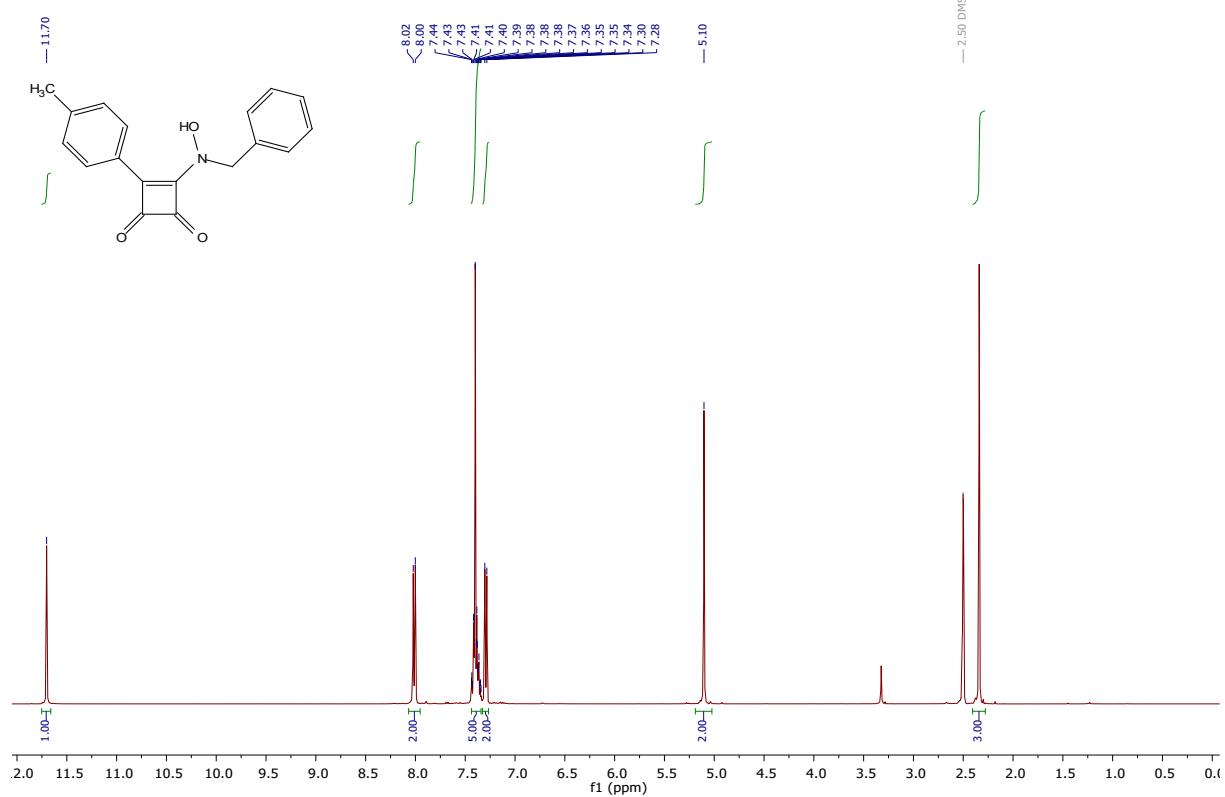


Fig S56. ^{13}C NMR spectra of 3-(benzyl(hydroxy)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ae**

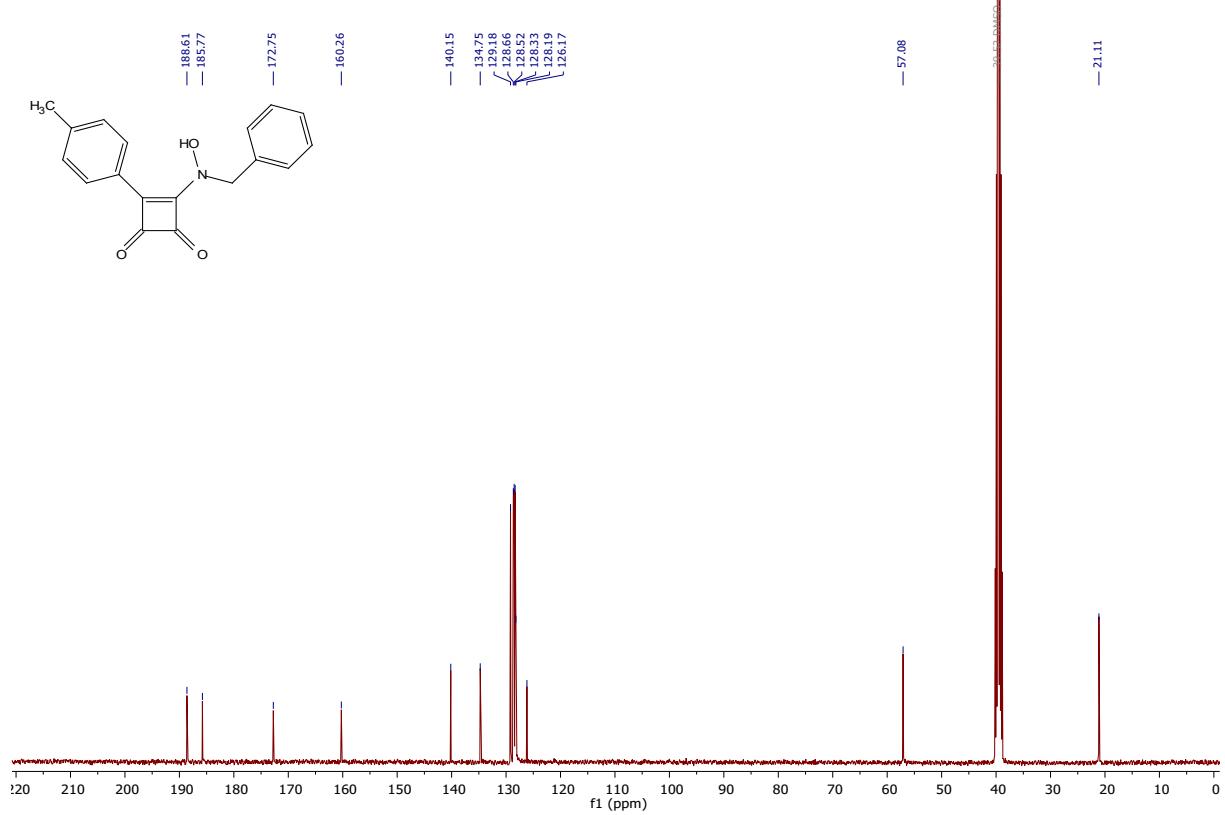


Fig S57. ^1H NMR spectra of 3-(methoxy(methyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6af**

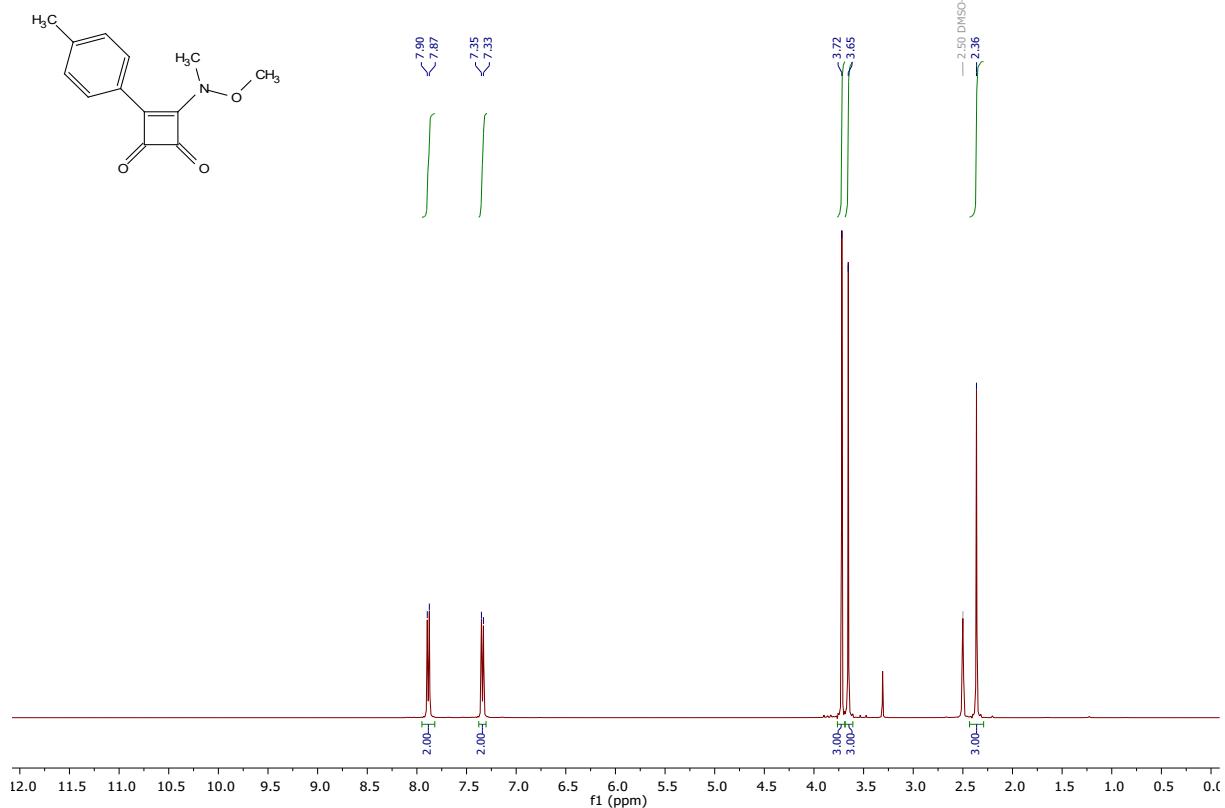


Fig S58. ^{13}C NMR spectra of 3-(methoxy(methyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6af**

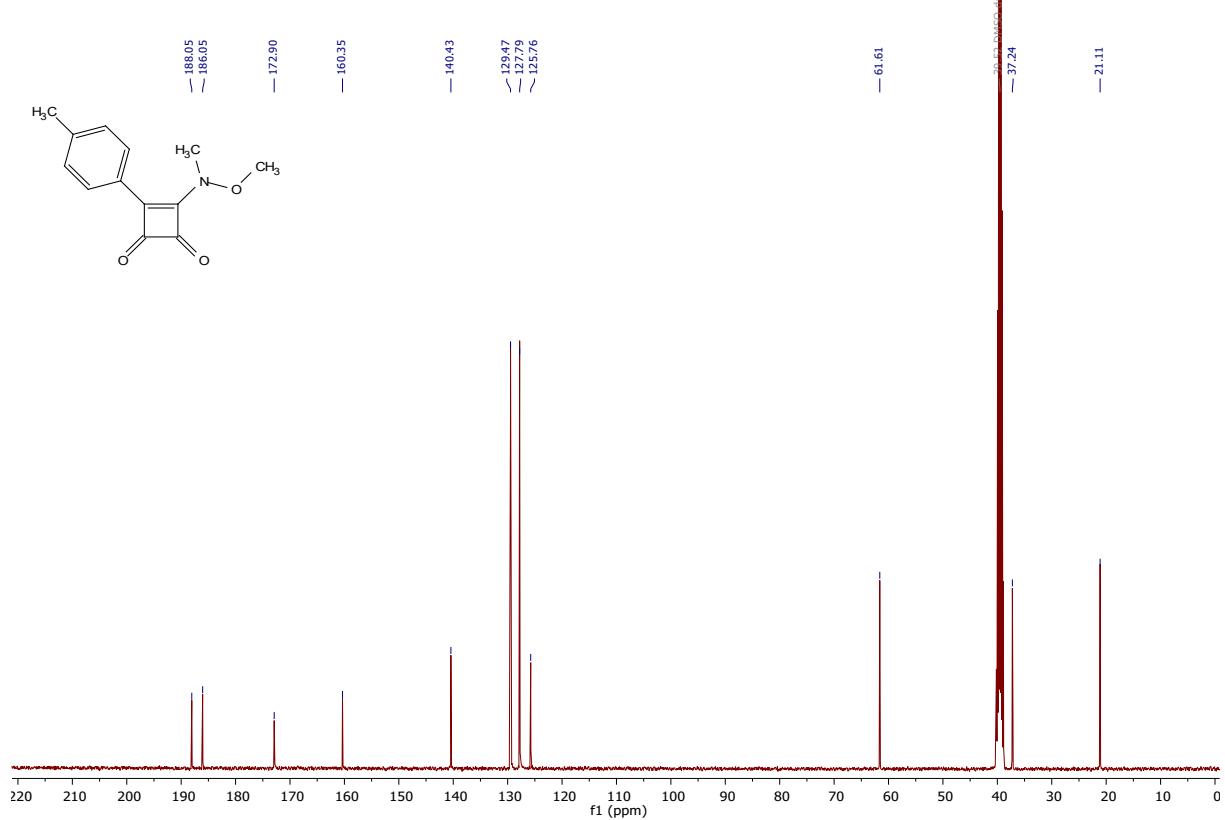


Fig S59. ^1H NMR spectra of 3-morpholino-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ag**

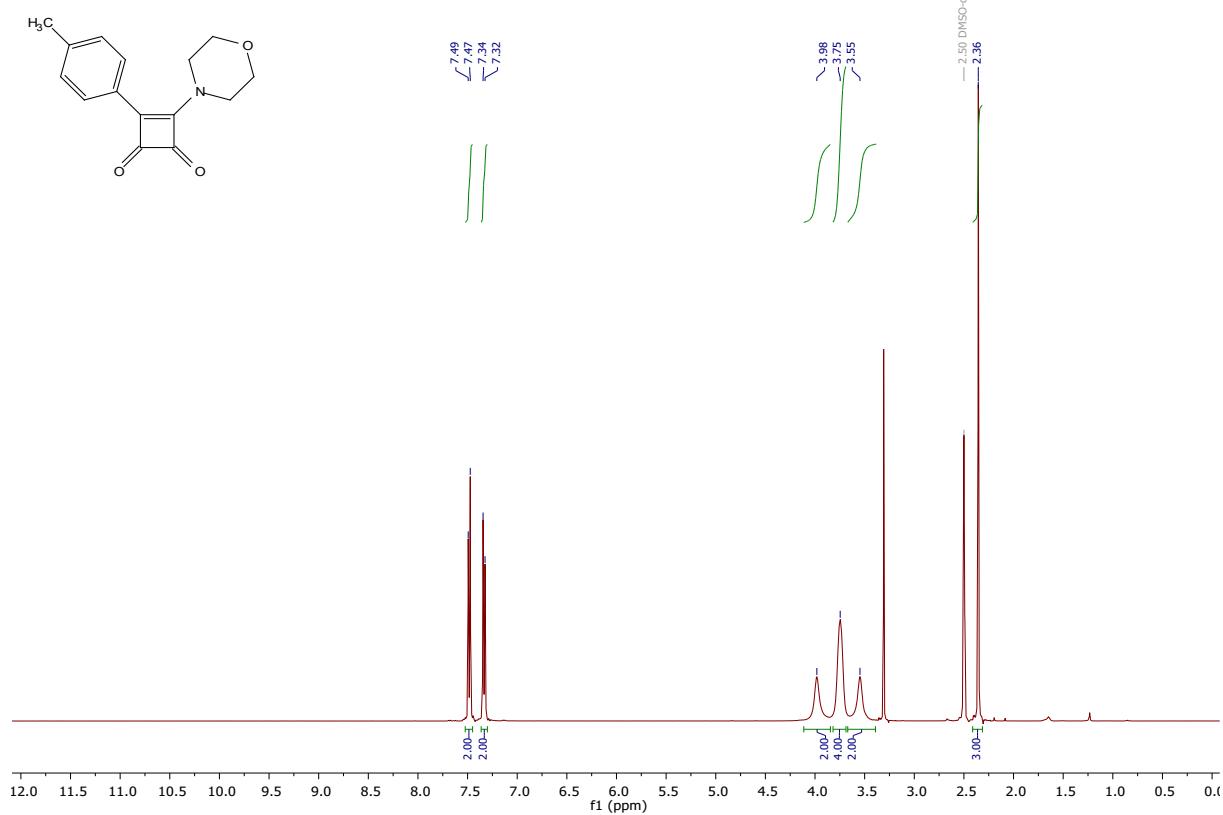


Fig S60. ^{13}C NMR spectra of 3-morpholino-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6ag**

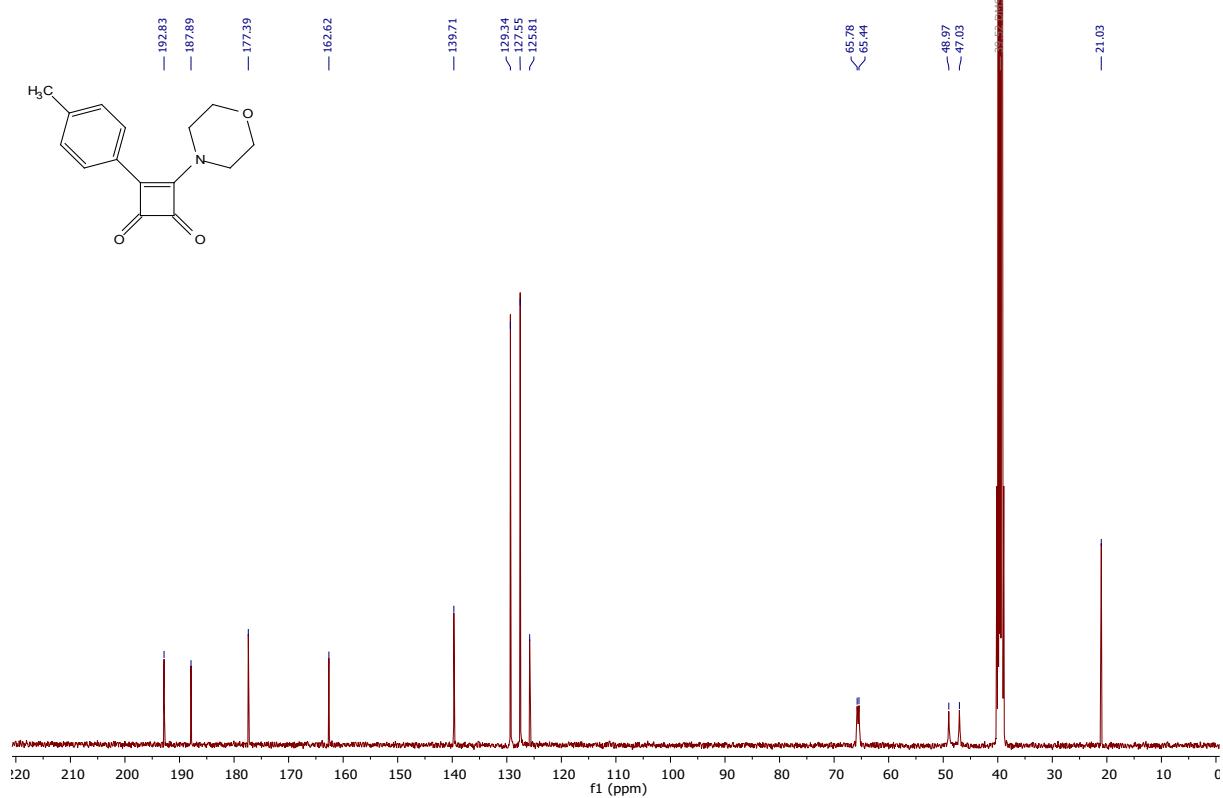


Fig S61. ^1H NMR spectra of tert-butyl 4-(3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)piperazine-1-carboxylate **6ai**

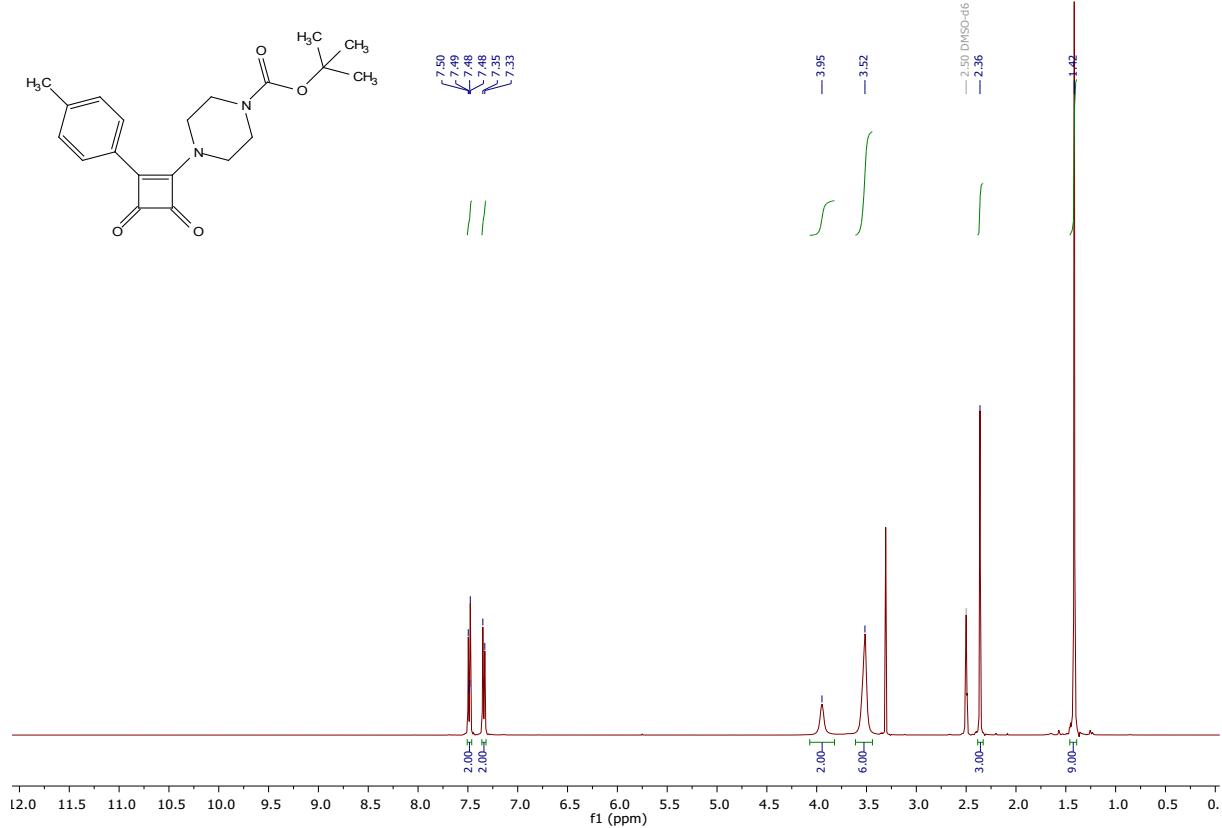


Fig S62. ^{13}C NMR spectra of tert-butyl 4-(3,4-dioxo-2-(*p*-tolyl)cyclobut-1-en-1-yl)piperazine-1-carboxylate **6ai**

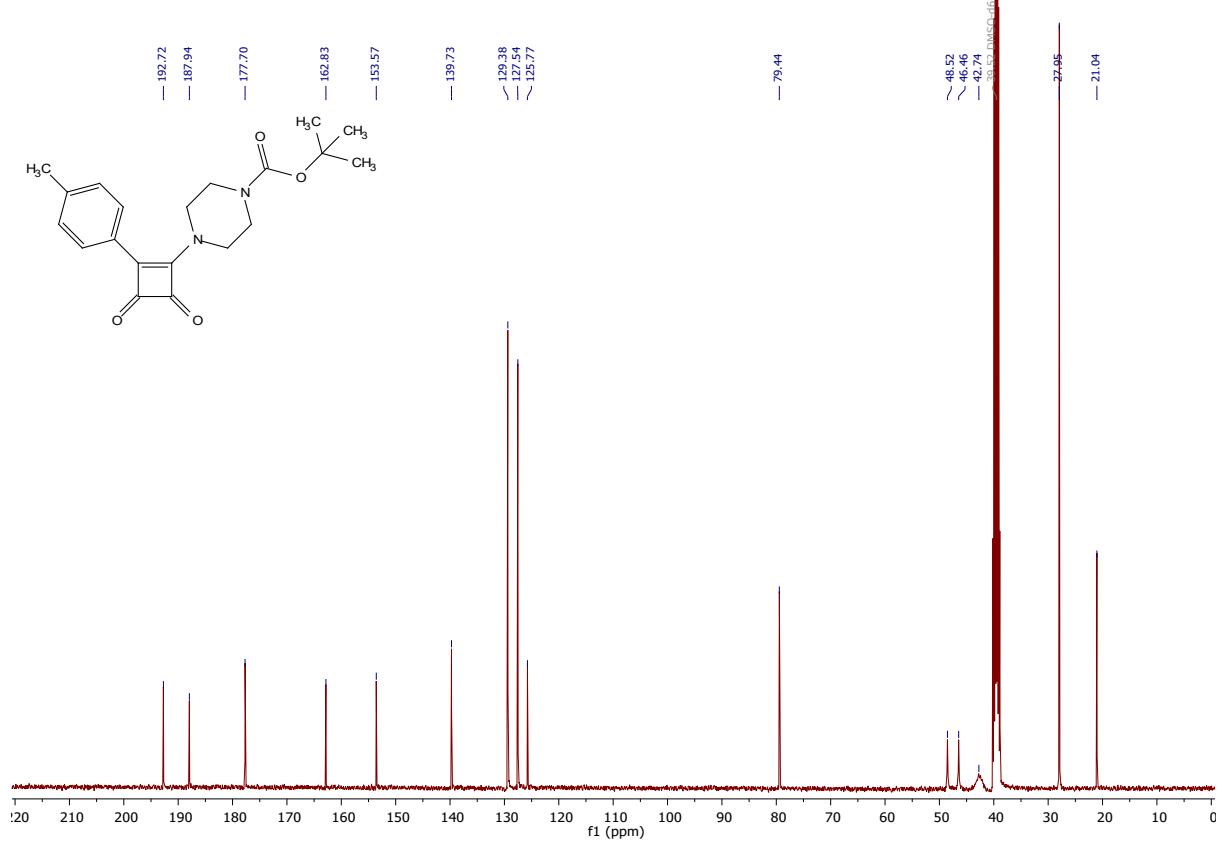


Fig S63. ^1H NMR spectra of 3-((furan-2-ylmethyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6aj**

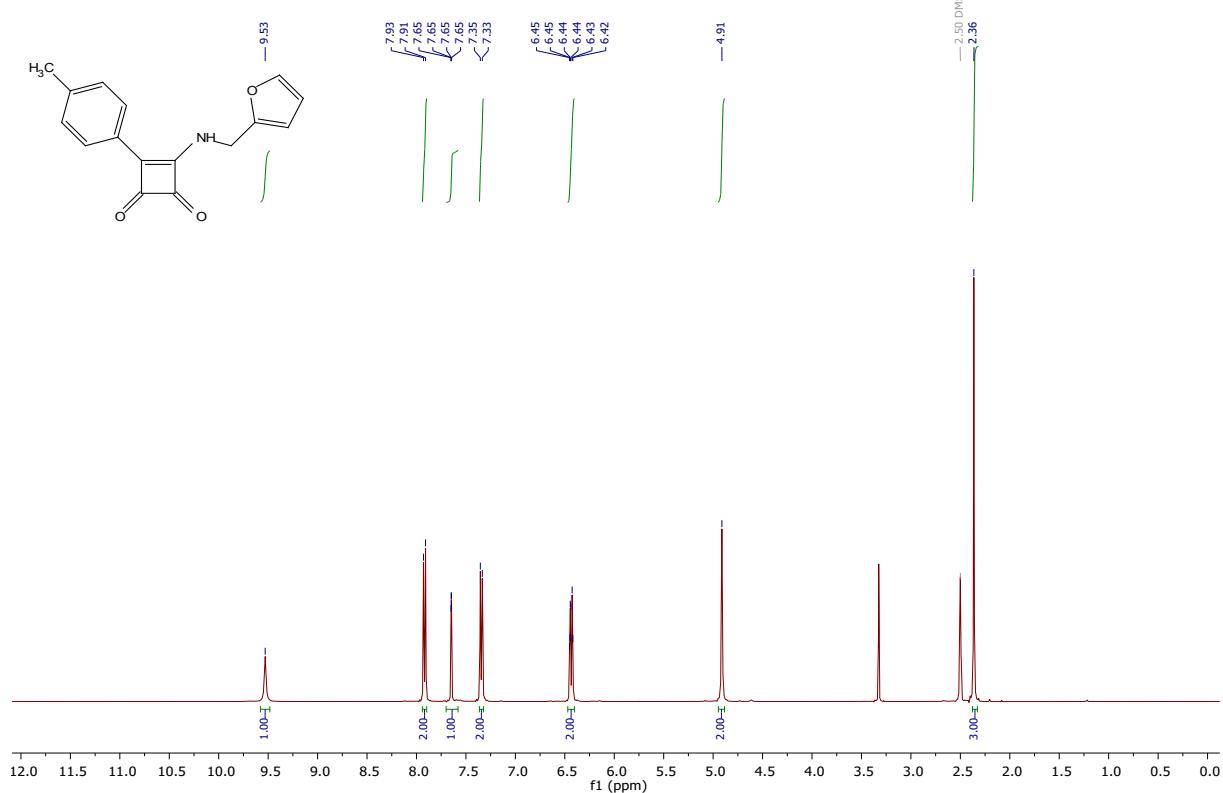


Fig S64. ^{13}C NMR spectra of 3-((furan-2-ylmethyl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6aj**

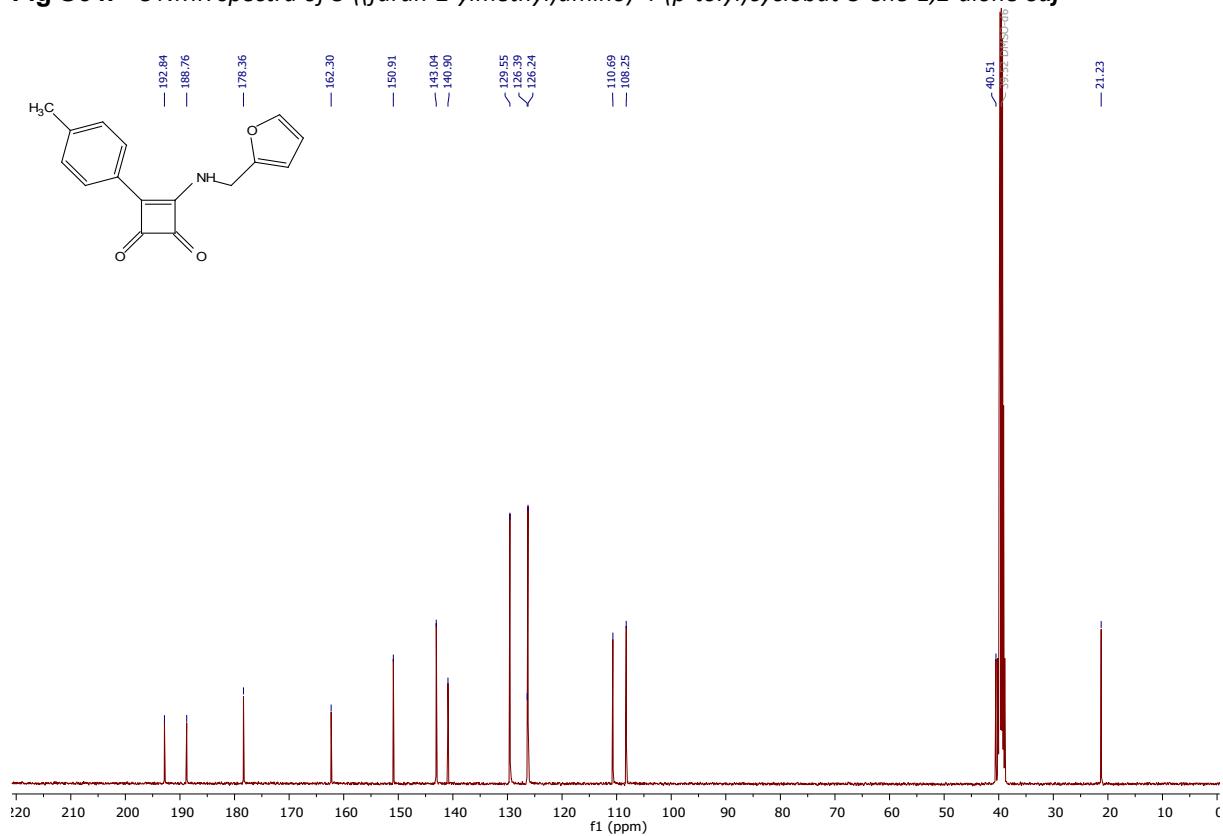


Fig S65. ^1H NMR spectra of 3-((4'-methoxy-[1,1'-biphenyl]-4-yl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6am**

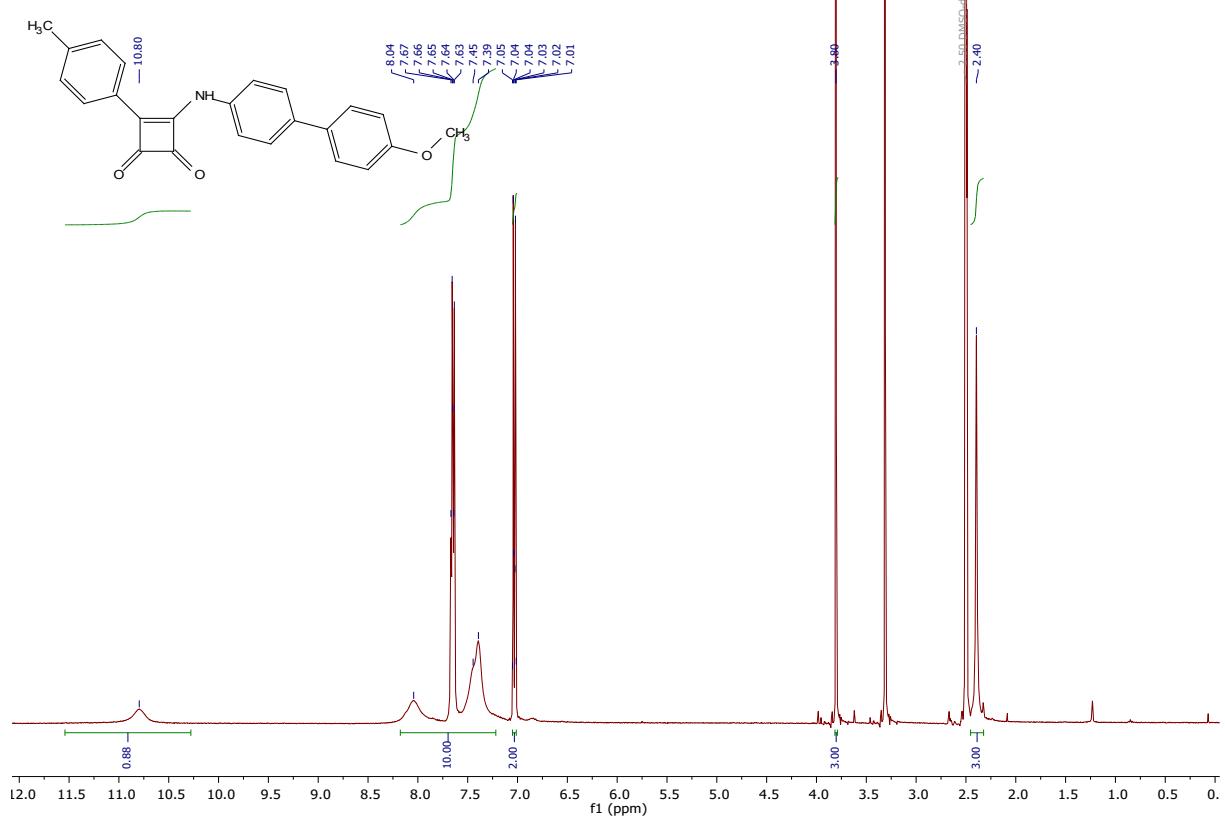


Fig S66. ^{13}C NMR spectra of 3-((4'-methoxy-[1,1'-biphenyl]-4-yl)amino)-4-(*p*-tolyl)cyclobut-3-ene-1,2-dione **6am**

