Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.
This journal is © The Royal Society of Chemistry 2023

On the Brønsted Acid-Catalyzed *aza*-Michael Reaction of Isoxazol-5-ones to Enones: Reaction Optimization, Scope, Mechanistic Investigations and Scale-up

Marcelo M. de Siqueira,[a] Pedro P. de Castro, *[b] Juliana A. dos Santos, [a] Leonã S. Flores, [a] Walysson F. de Paiva, [c] Sergio A. Fernandes [c] and Giovanni W. Amarante *[a]

[a] Chemistry Department, Federal University of Juiz de Fora, Campus Martelos, Juiz de Fora, Minas Gerais, 36036-900, Brazil.

[b] Chemistry Department, Federal University of São Carlos, São Carlos, São Paulo, 13565-905, Brazil.

[c] Chemistry Department, Federal University of Viçosa, Viçosa, Minas Gerais, 36570-900, Brazil.

[*] Correspondence: pedro_possa@hotmail.com; giovanni.amarante@ufjf.br

Supplementary Information

Table of contents

1. NMR and IR spectra of isoxazol-5-ones (2a-2f) and its precursors

Figure S1. FT-IR (NaCl) of 3-phenylisoxazol-5(4*H*)-one

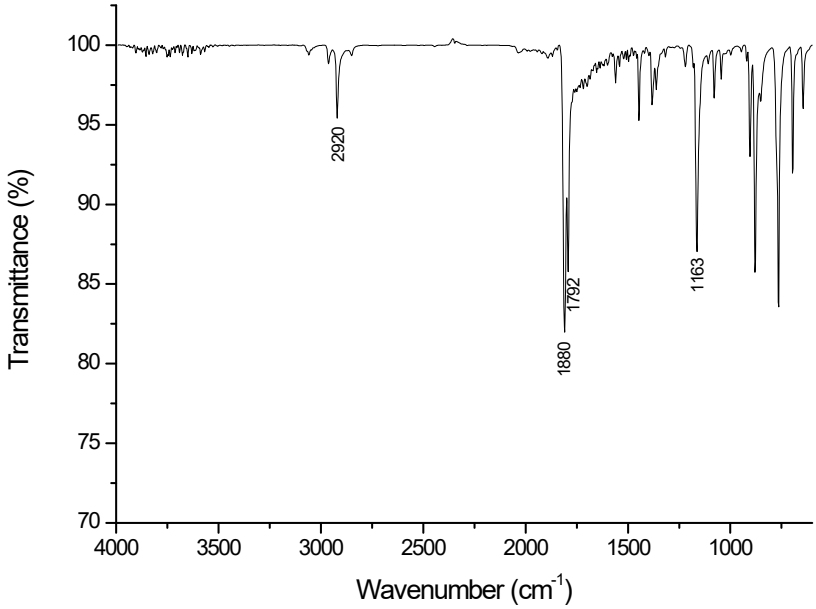


Figure S2. ^{1}H NMR (500 MHz, $CDCl_3$) of 3-phenylisoxazol-5(4*H*)-one

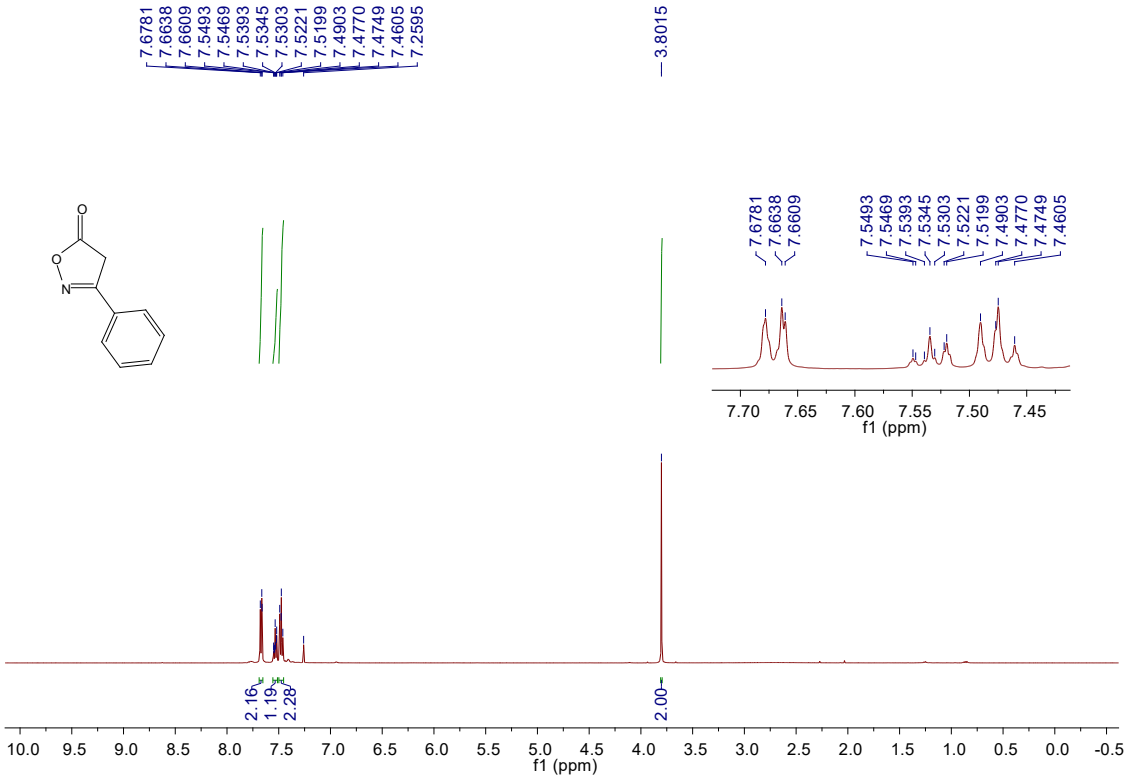


Figure S3. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of 3-phenylisoxazol-5(4*H*)-one

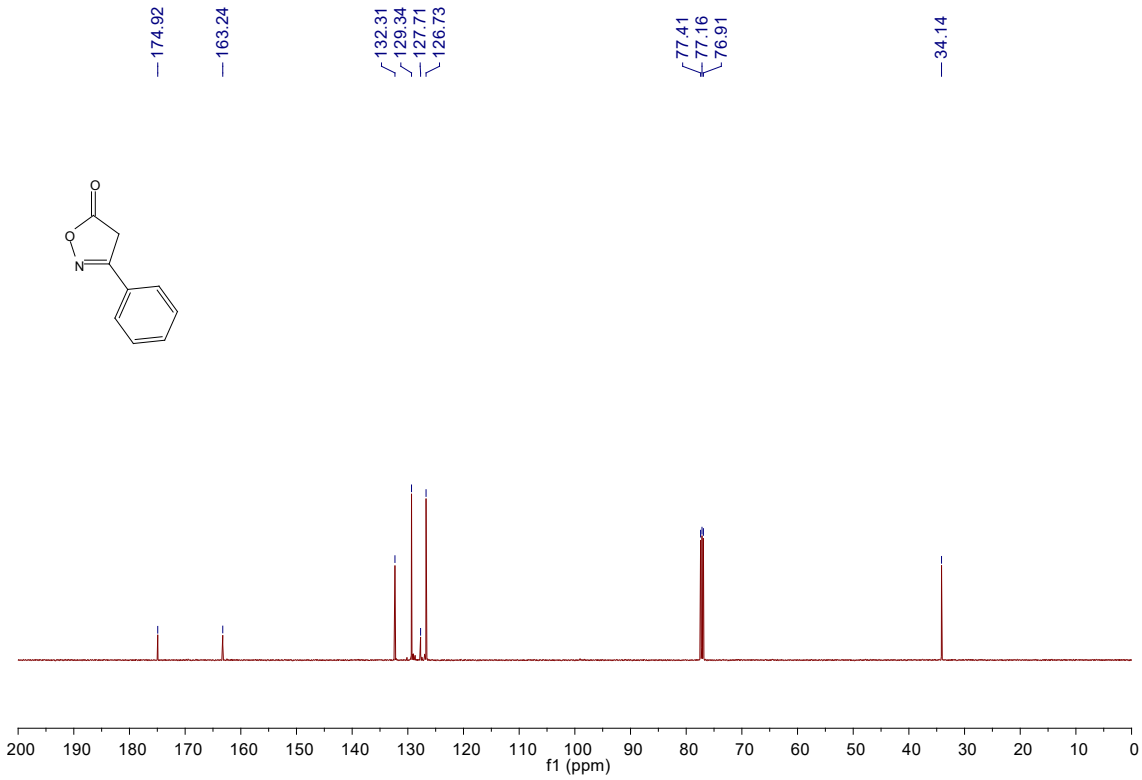


Figure S4. FT-IR (NaCl) of *(Z)-4-(benzylidene)-3-phenylisoxazol-5(4H)-one*

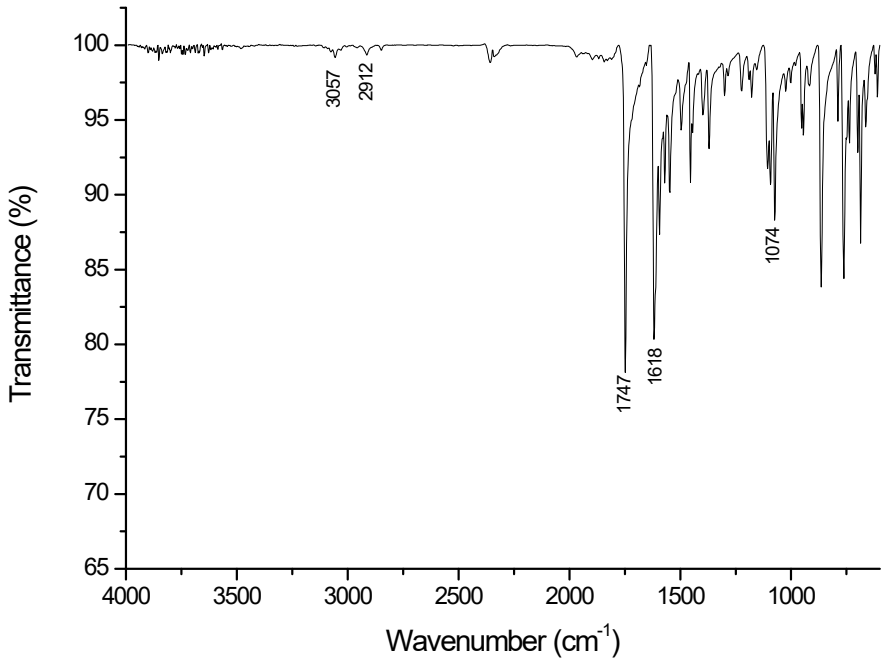


Figure S5. ^{1}H NMR (500 MHz, $CDCl_3$) of *(Z)-4-(benzylidene)-3-phenylisoxazol-5(4H)-one*

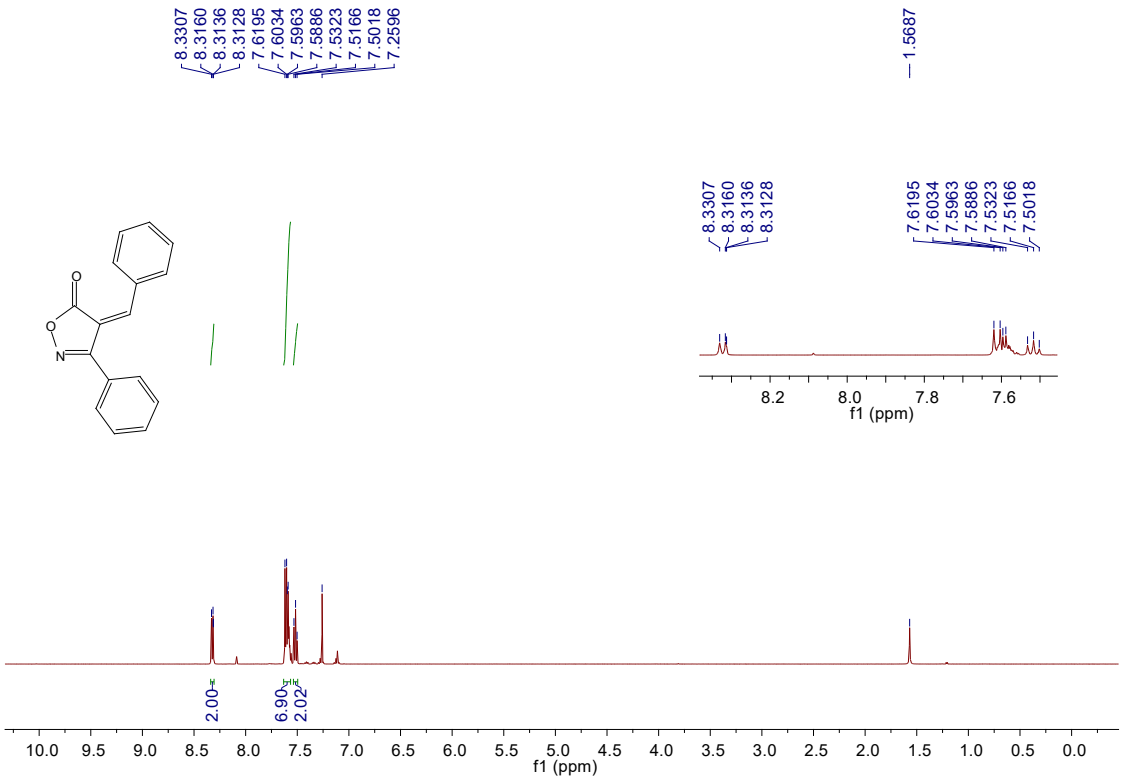


Figure S6. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of (Z)-4-(benzylidene)-3-phenylisoxazol-5(4H)-one

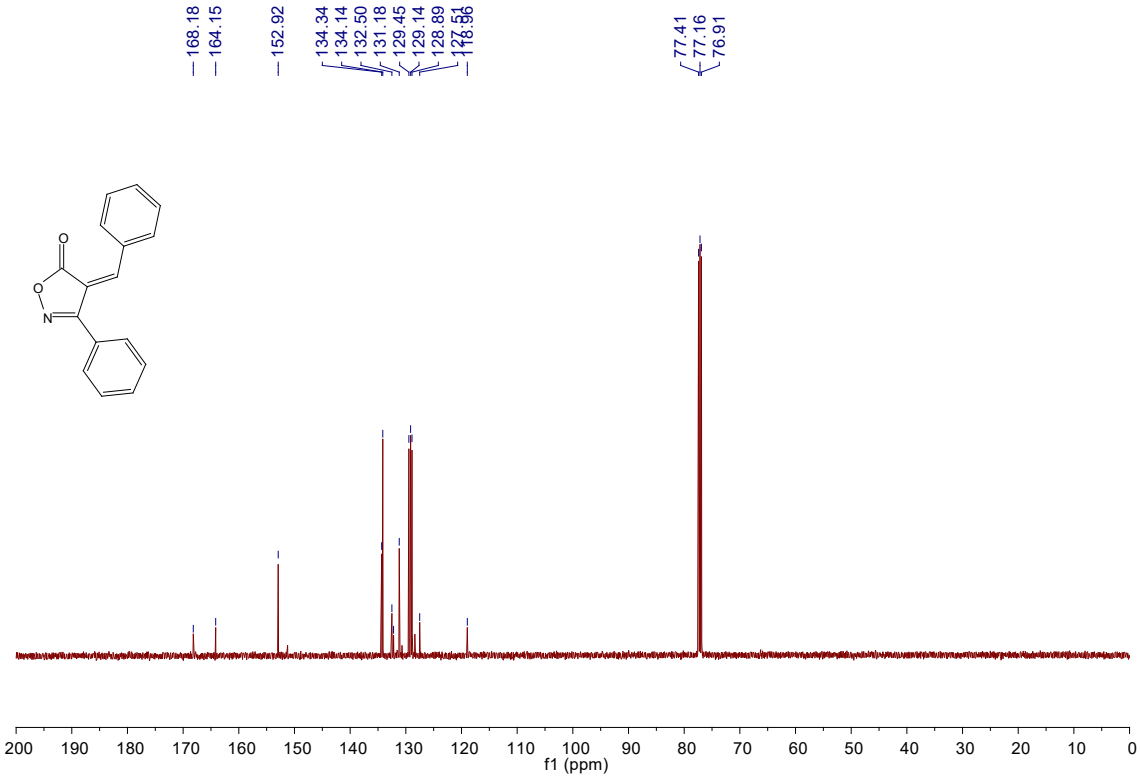


Figure S7. FT-IR (NaCl) of (Z)-4-(2-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one

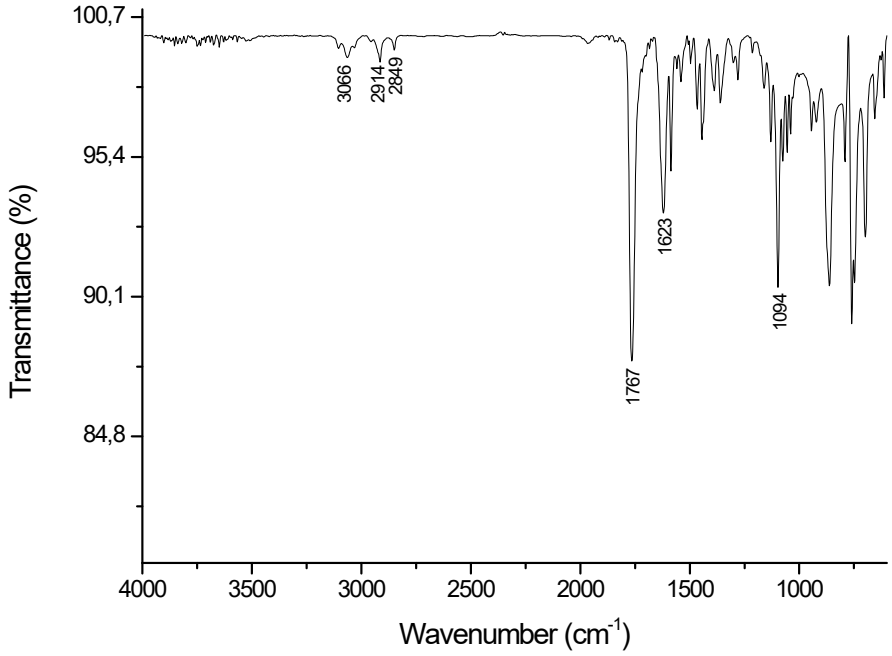


Figure S8. ^{1}H NMR (500 MHz, $CDCl_3$) of (Z)-4-(2-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one]

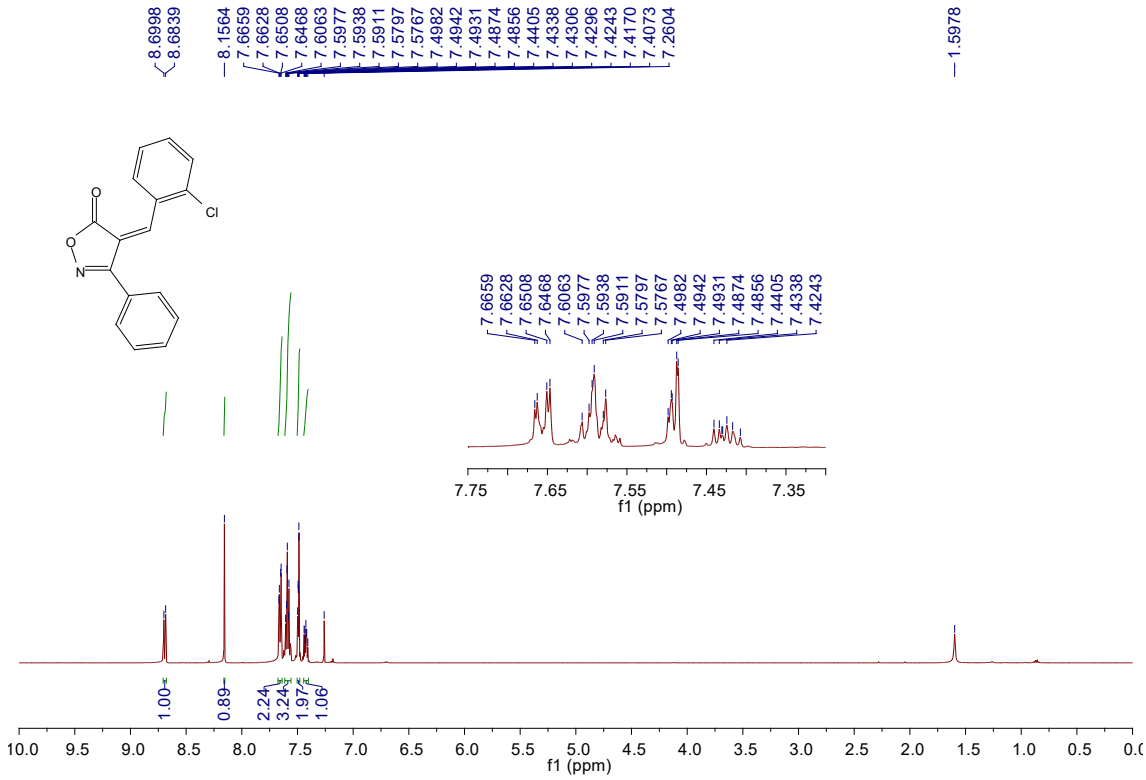


Figure S9. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(Z)-4-(2-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

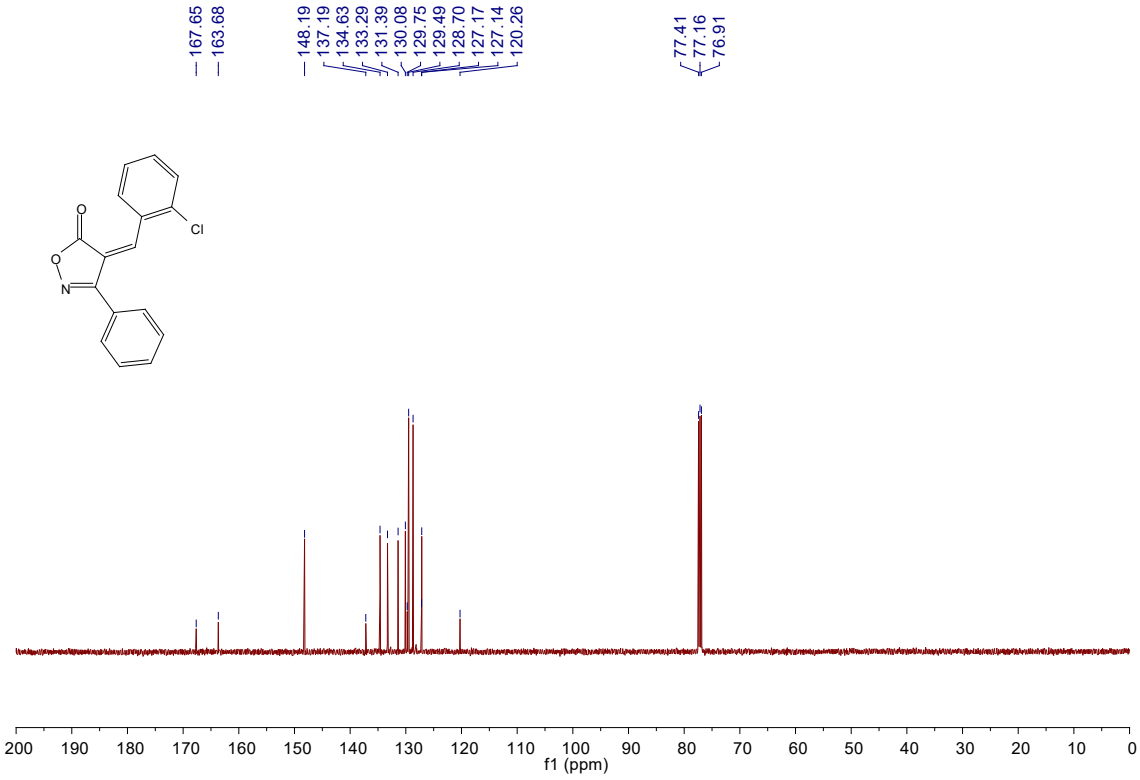


Figure S10. FT-IR (NaCl) of (Z)-4-(3-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one

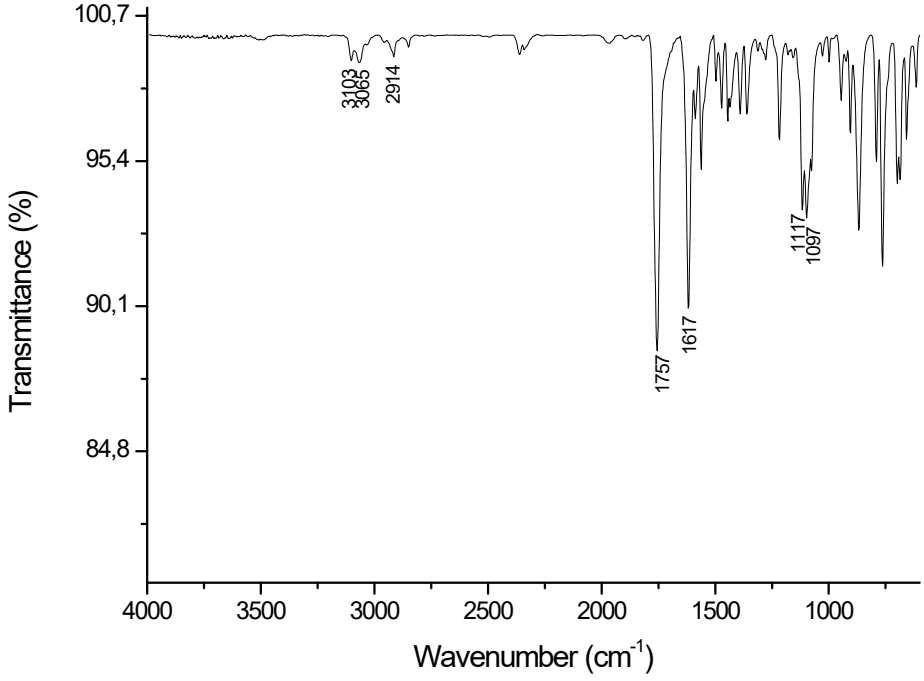


Figure S11. ^{1}H NMR (500 MHz, $CDCl_3$) of *(Z)-4-(3-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

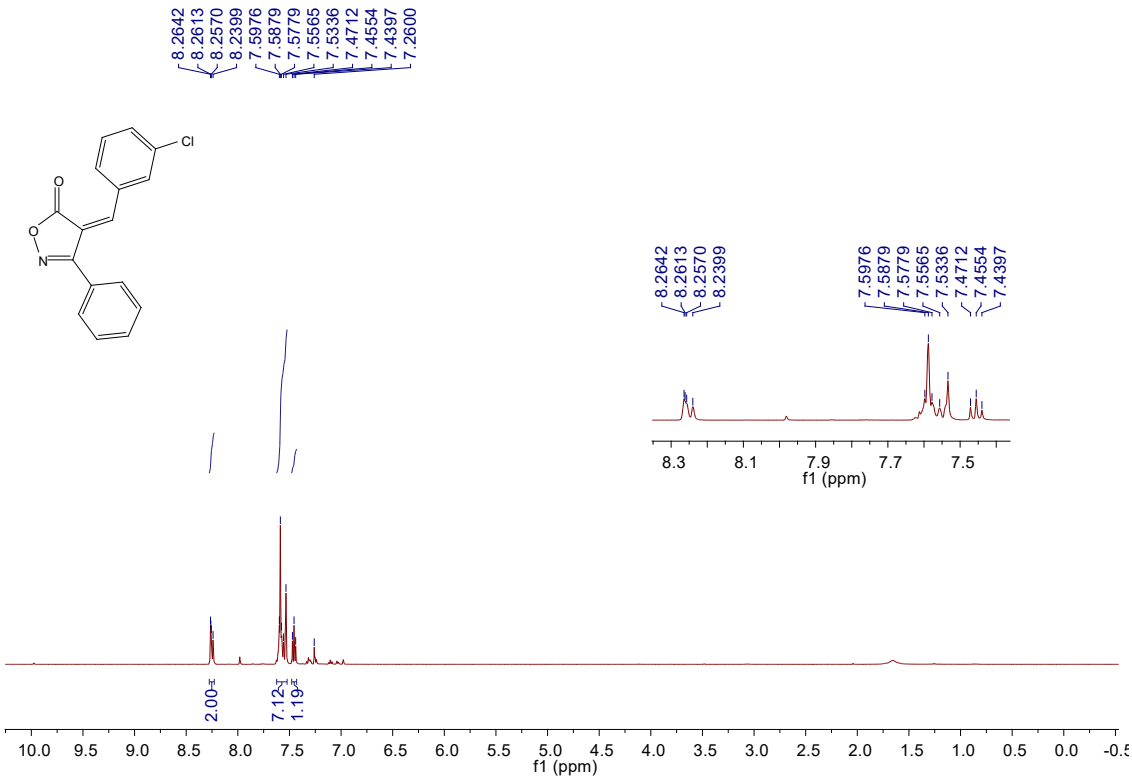


Figure S12. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(Z)-4-(3-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

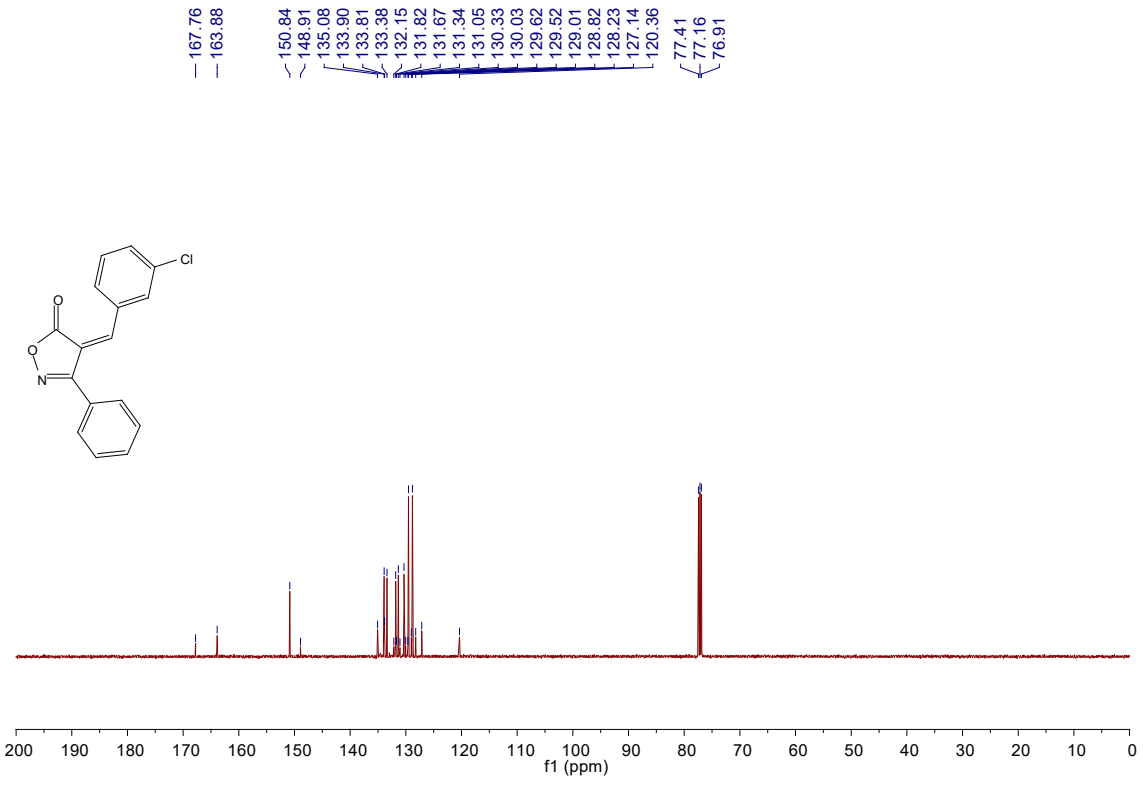


Figure S13. FT-IR (NaCl) of *(Z)-4-(4-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

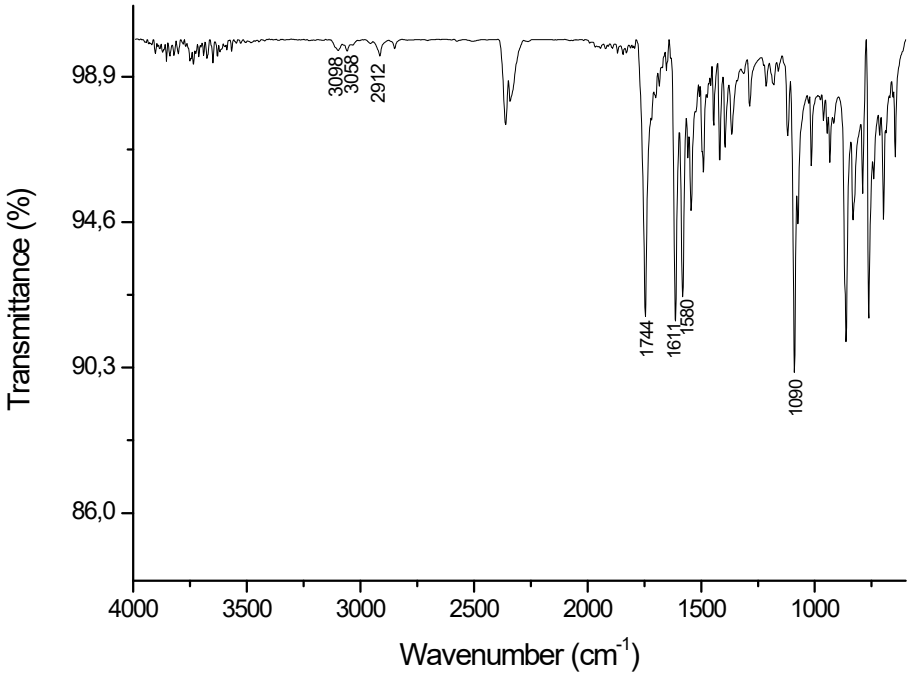


Figure S14. ^{1}H NMR (500 MHz, $CDCl_3$) of *(Z)-4-(4-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

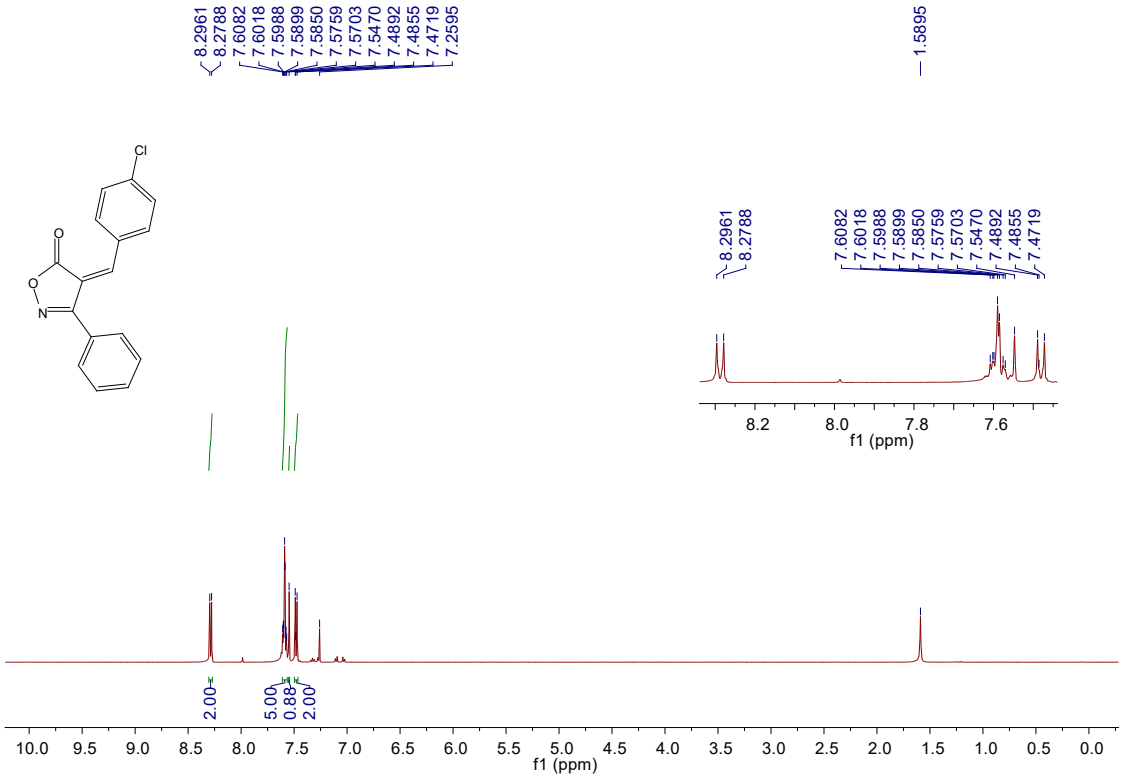


Figure S15. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(Z)-4-(4-chlorobenzylidene)-3-phenylisoxazol-5(4H)-one*

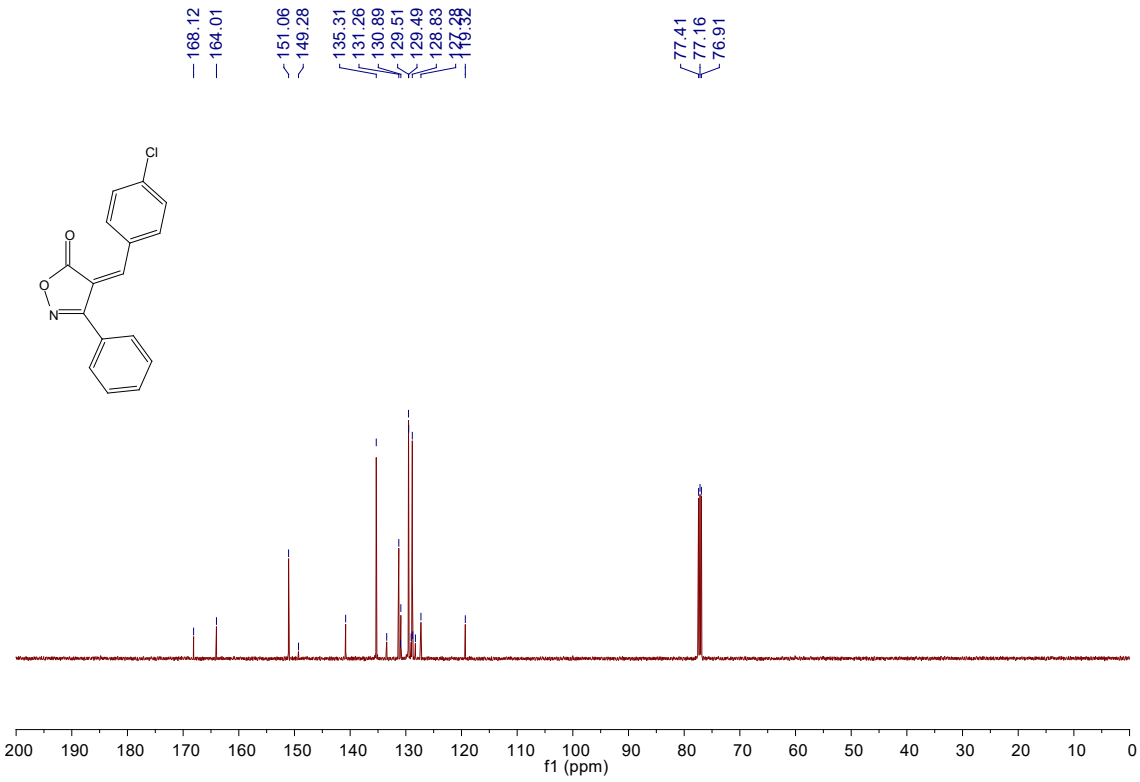


Figure S16. FT-IR (NaCl) of *(Z)-4-(4-methoxybenzylidene)-3-phenylisoxazol-5(4H)-one*

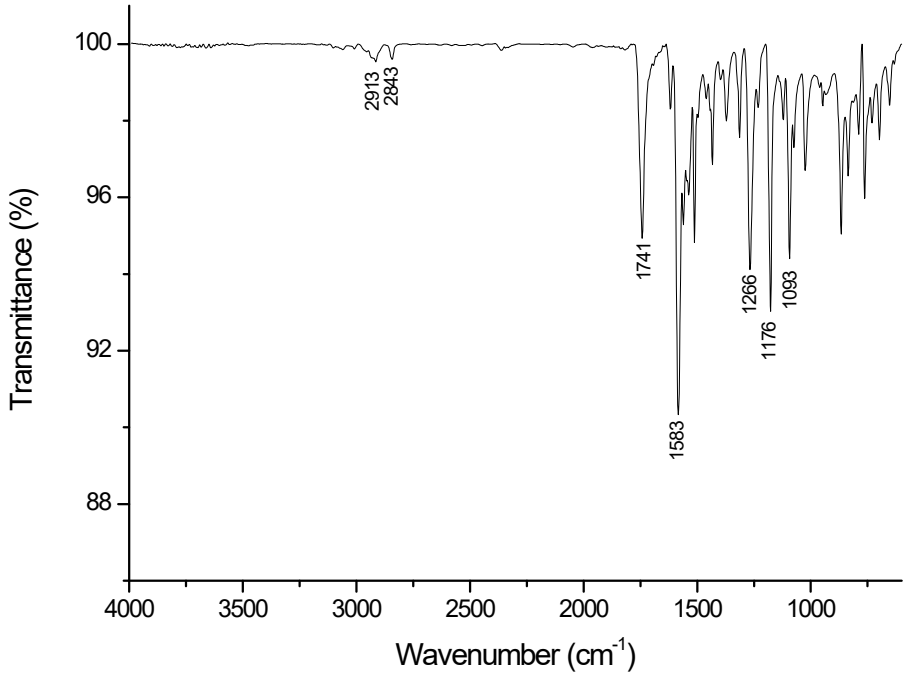


Figure S17. ^{1}H NMR (500 MHz, $CDCl_3$) of *(Z)-4-(4-methoxybenzylidene)-3-phenylisoxazol-5(4H)-one*

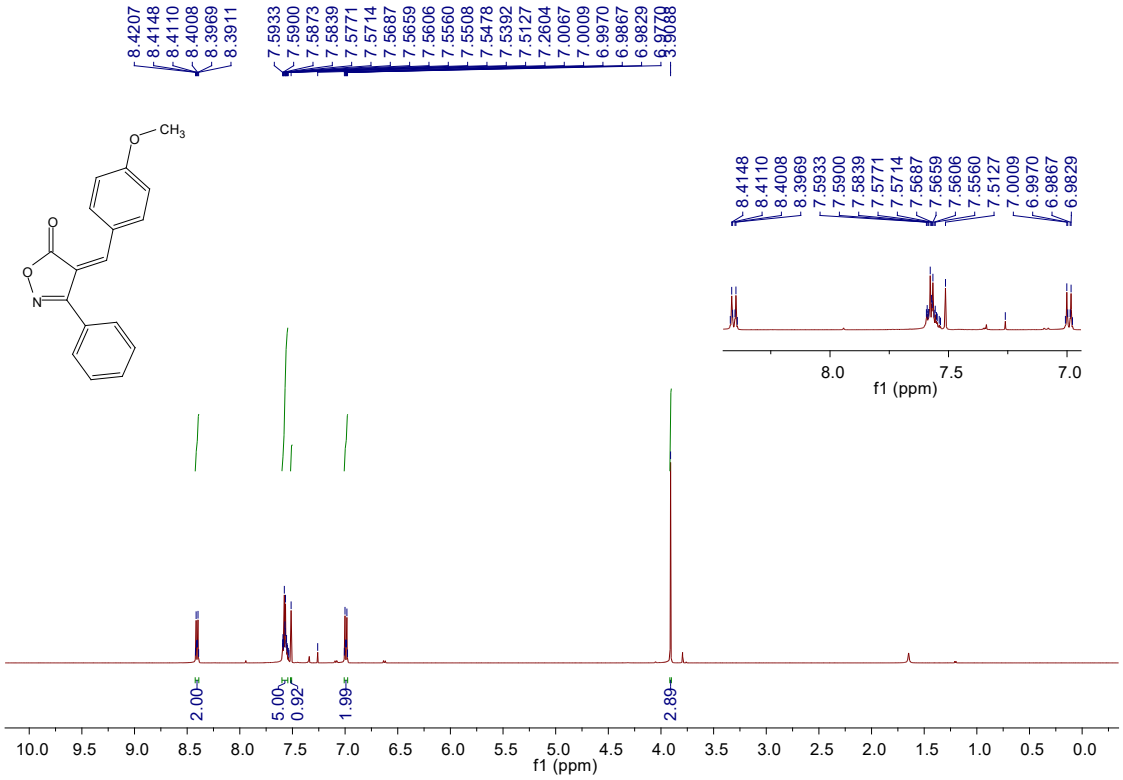


Figure S18. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(Z)-4-(4-methoxybenzylidene)-3-phenylisoxazol-5(4H)-one*

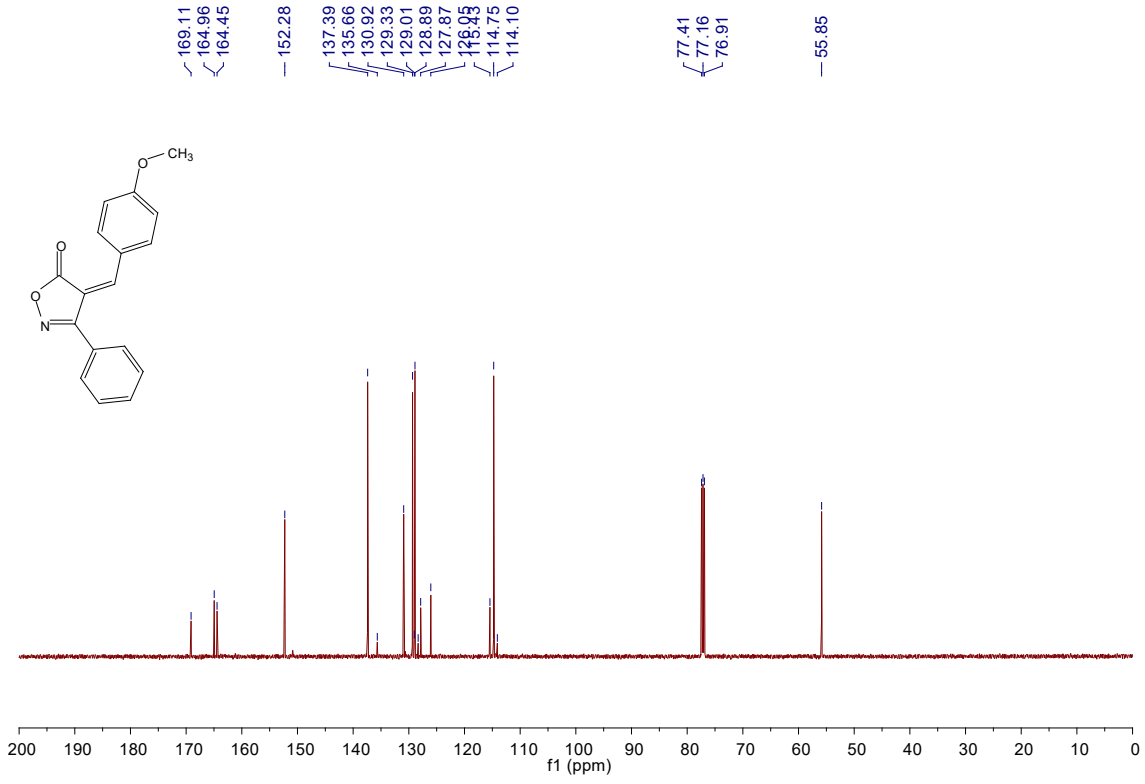


Figure S19. FT-IR (NaCl) of (Z)-4-(furan-2-ylmethylene)-3-phenylisoxazol-5(4H)-one

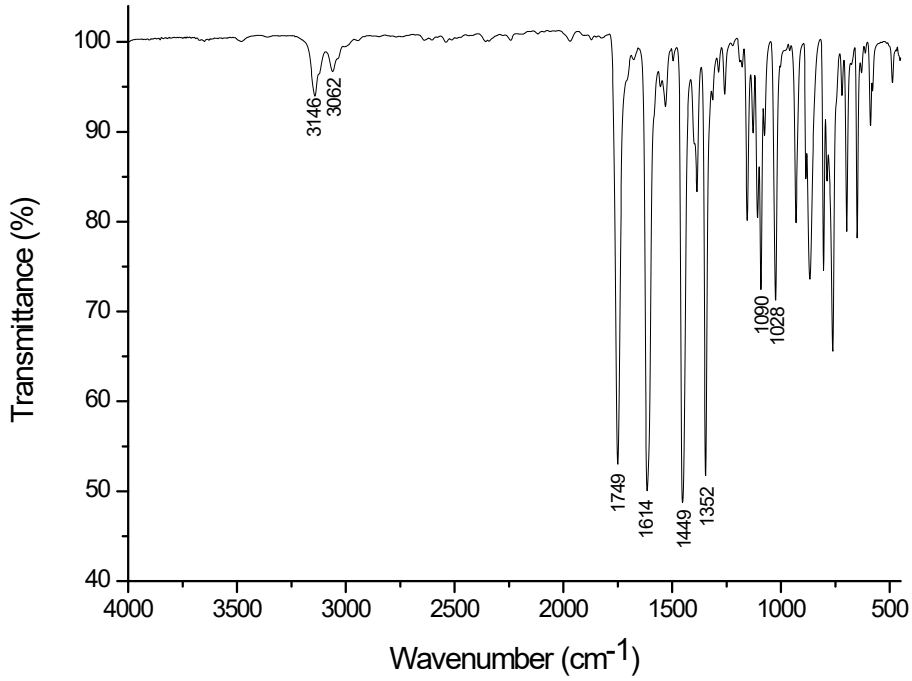


Figure S20. ^{1}H NMR (500 MHz, $CDCl_3$) of (Z)-4-(furan-2-ylmethylene)-3-phenylisoxazol-5(4H)-one

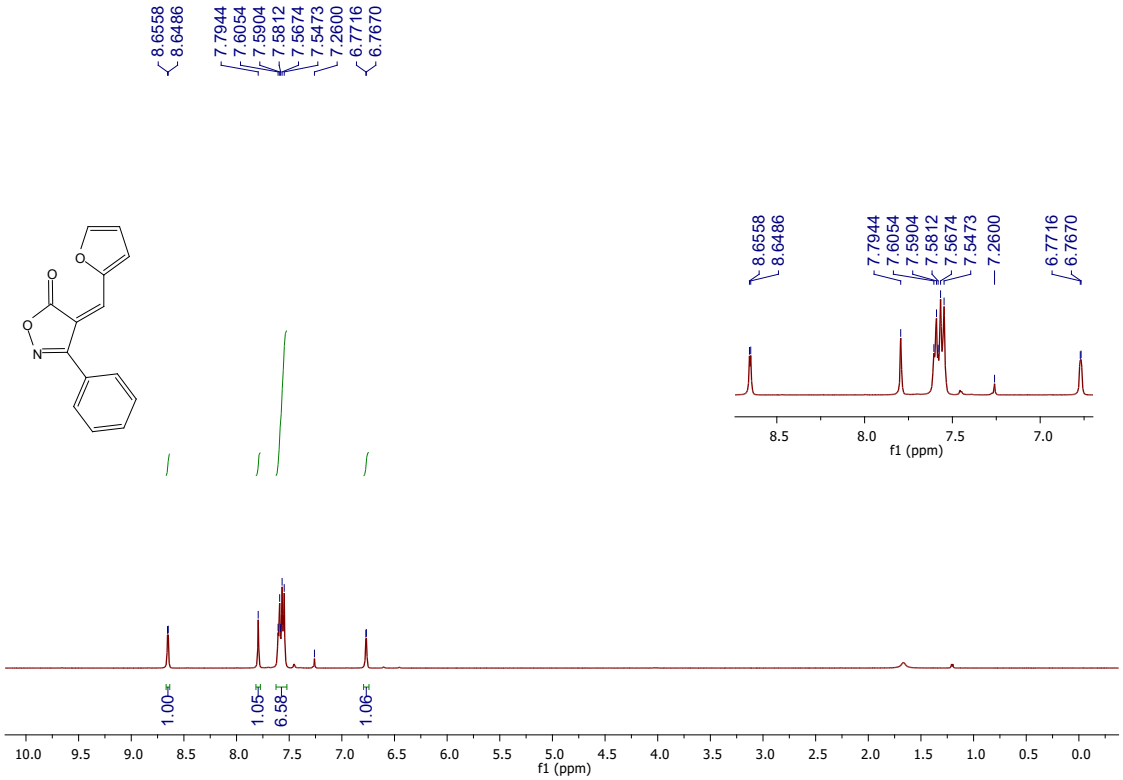


Figure S21. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of (Z)-4-(furan-2-ylmethylene)-3-phenylisoxazol-5(4H)-one

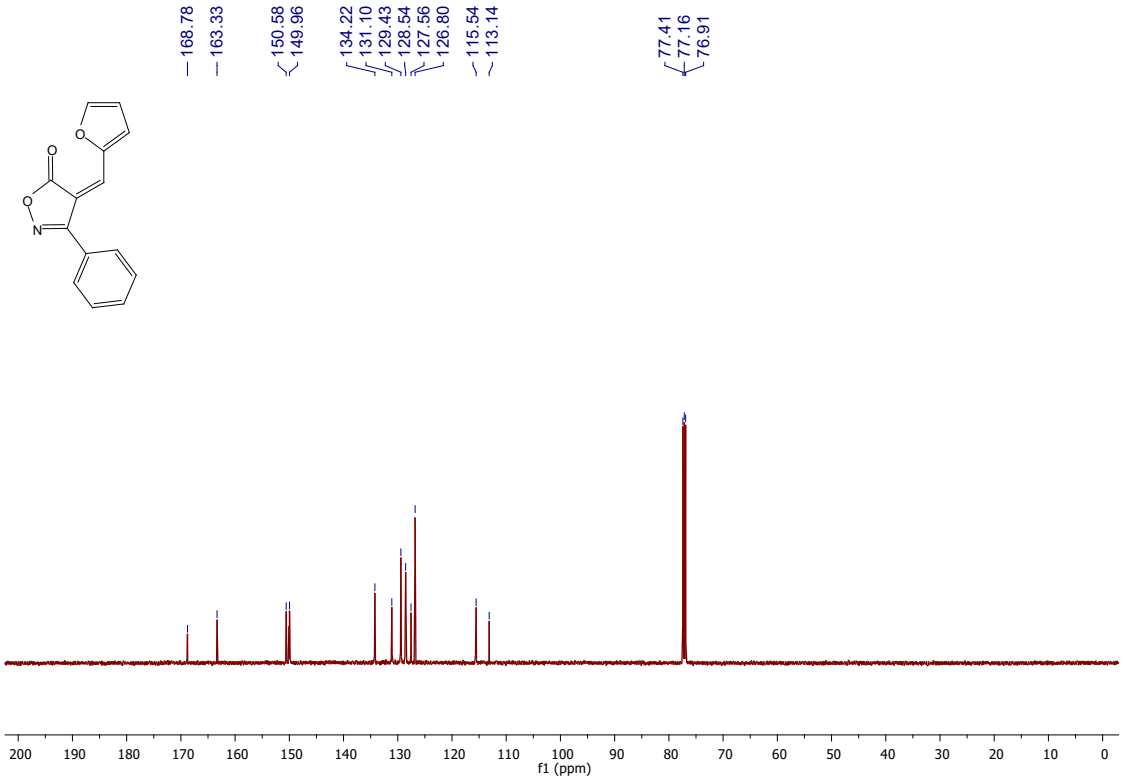


Figure S22. FT-IR (NaCl) of *4-benzyl-3-phenylisoxazol-5(4H)-one*

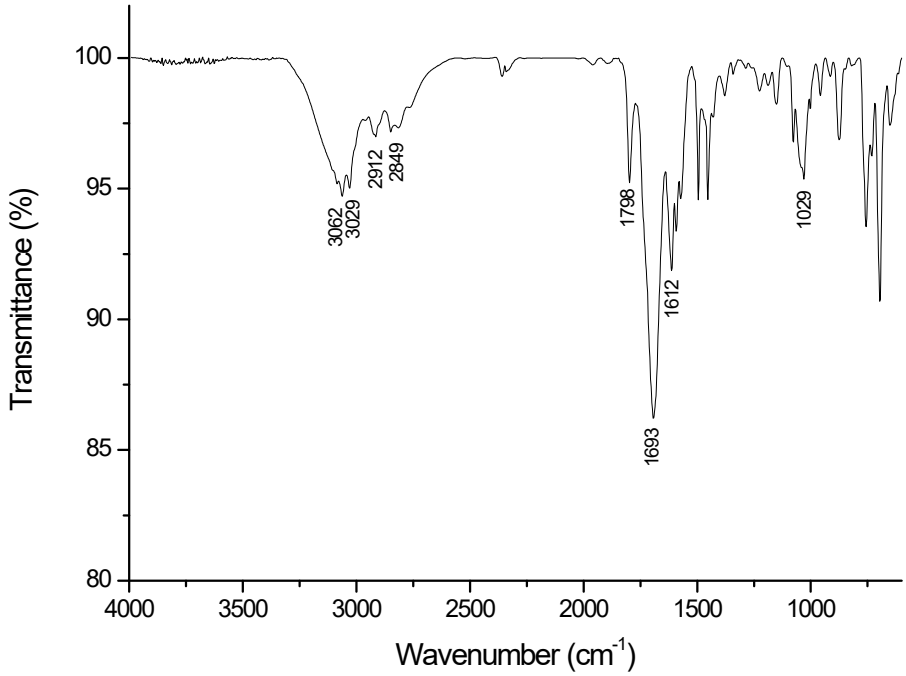


Figure S23. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-3-phenylisoxazol-5(4H)-one*

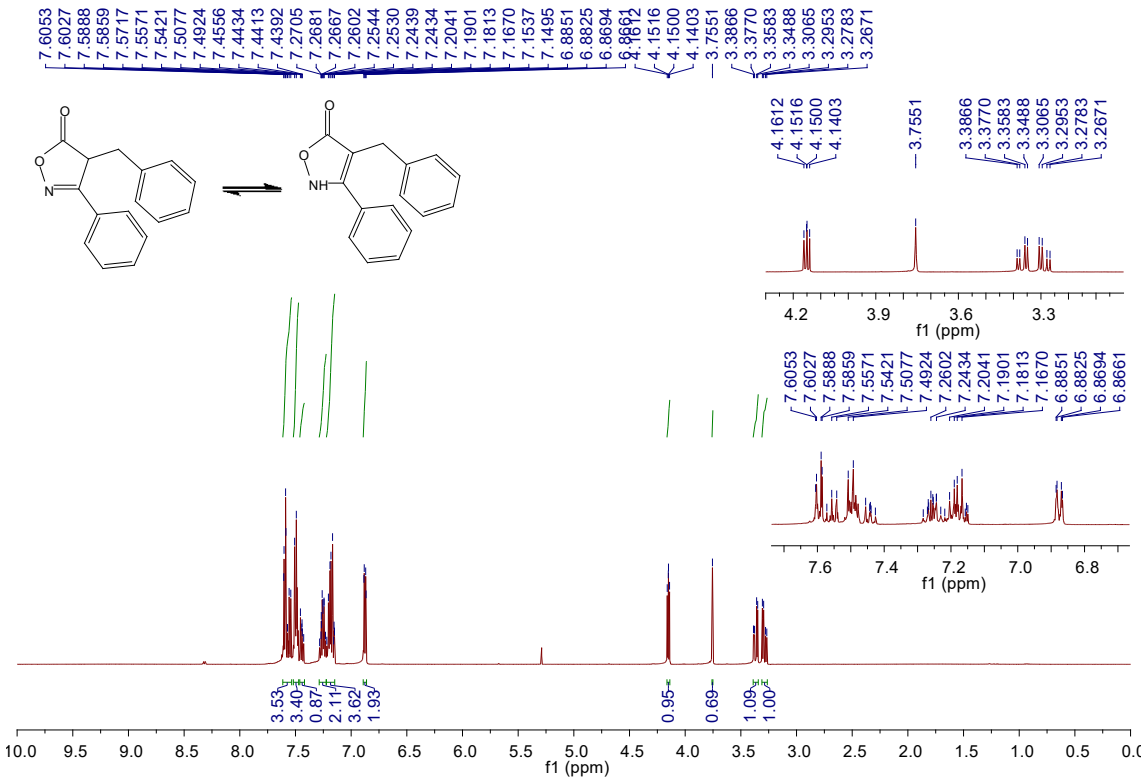


Figure S24. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-3-phenylisoxazol-5(4H)-one*

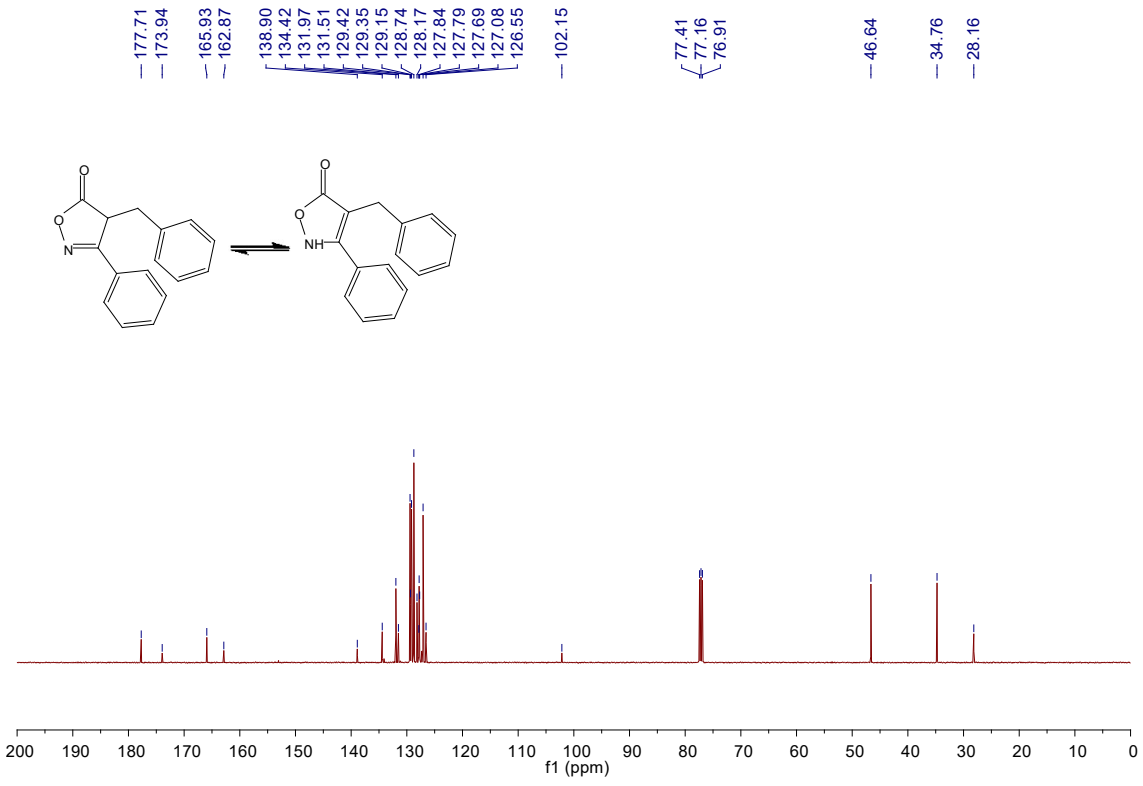


Figure S25. FT-IR (NaCl) of *4-(2-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

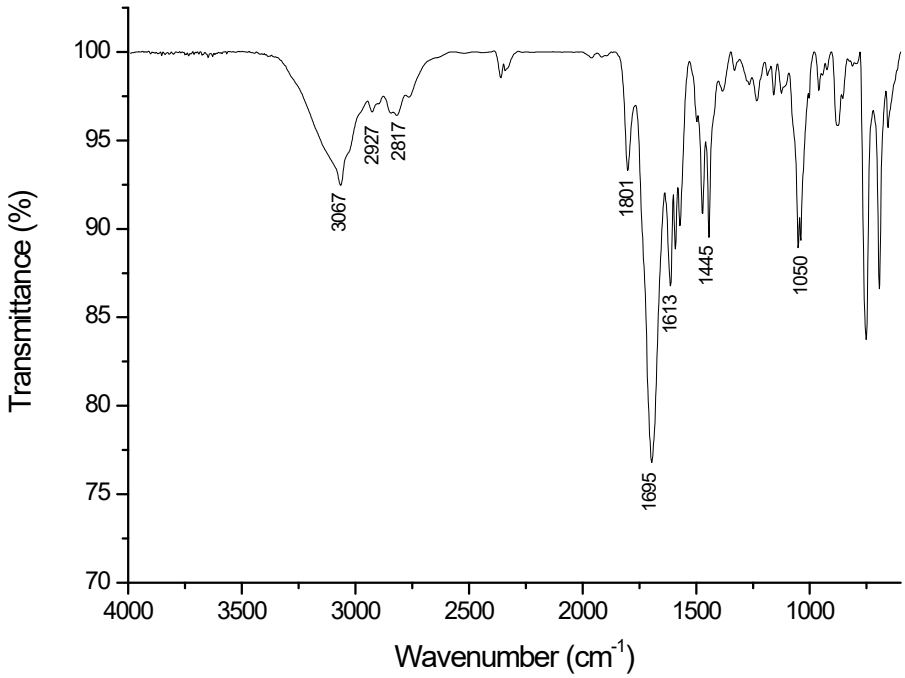


Figure S26. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-(2-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

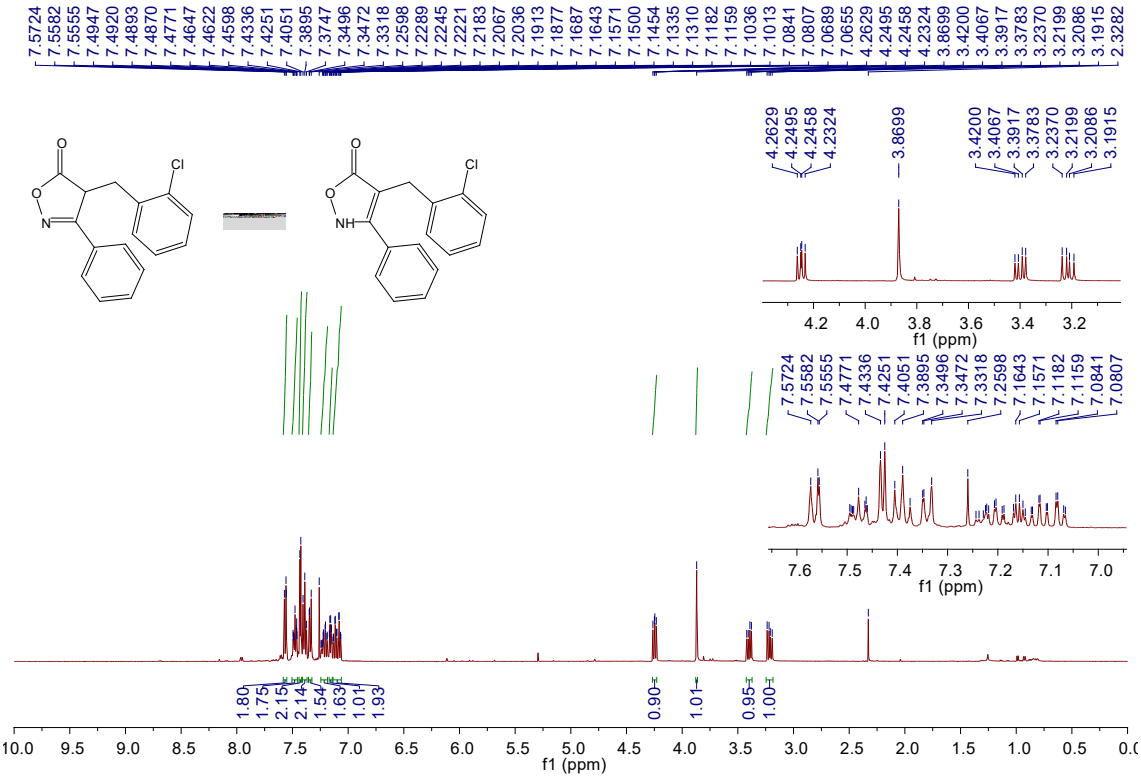


Figure S27. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-(2-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

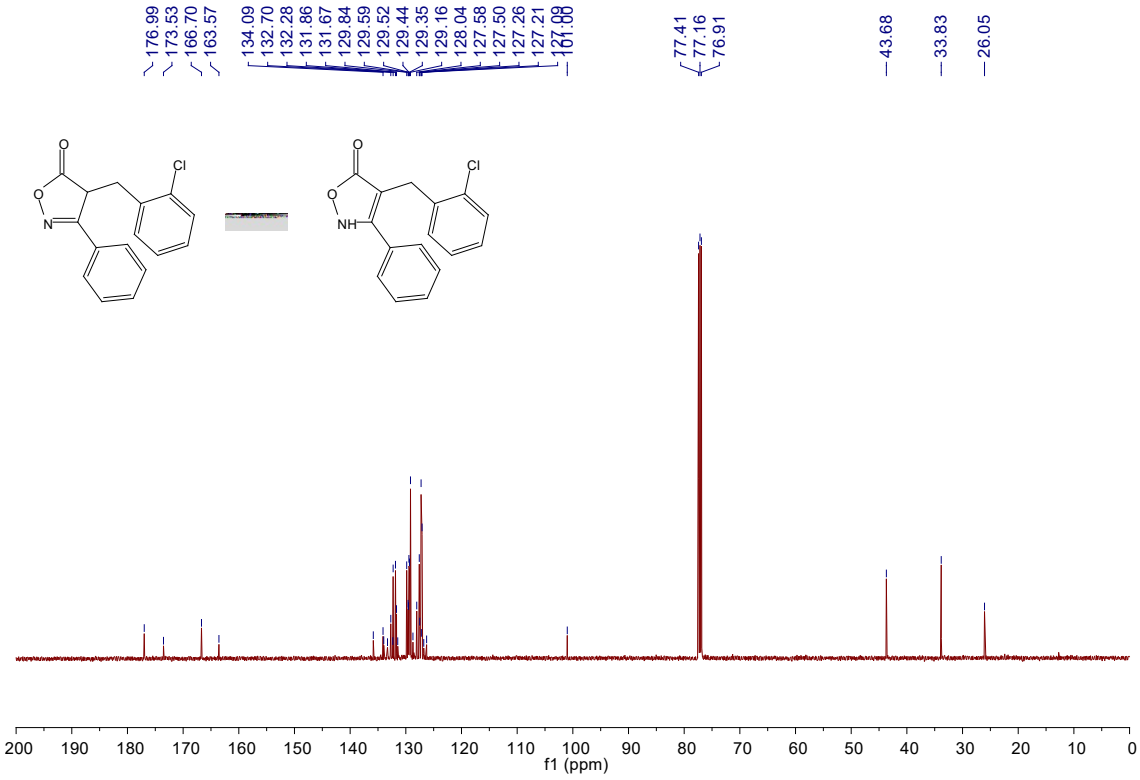


Figure S28. FT-IR (NaCl) of *4-(3-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

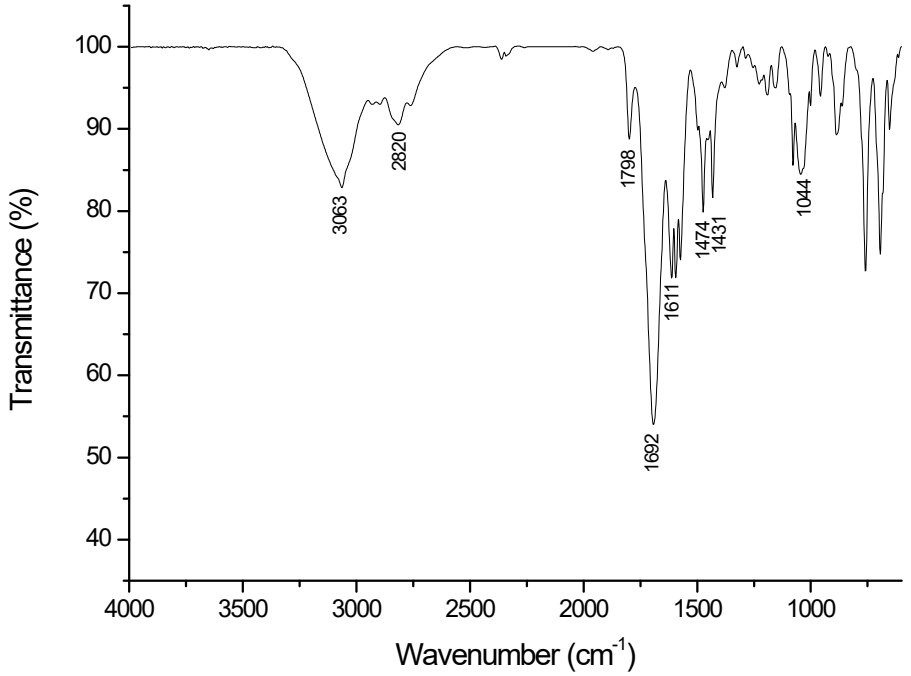


Figure S29. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-(3-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

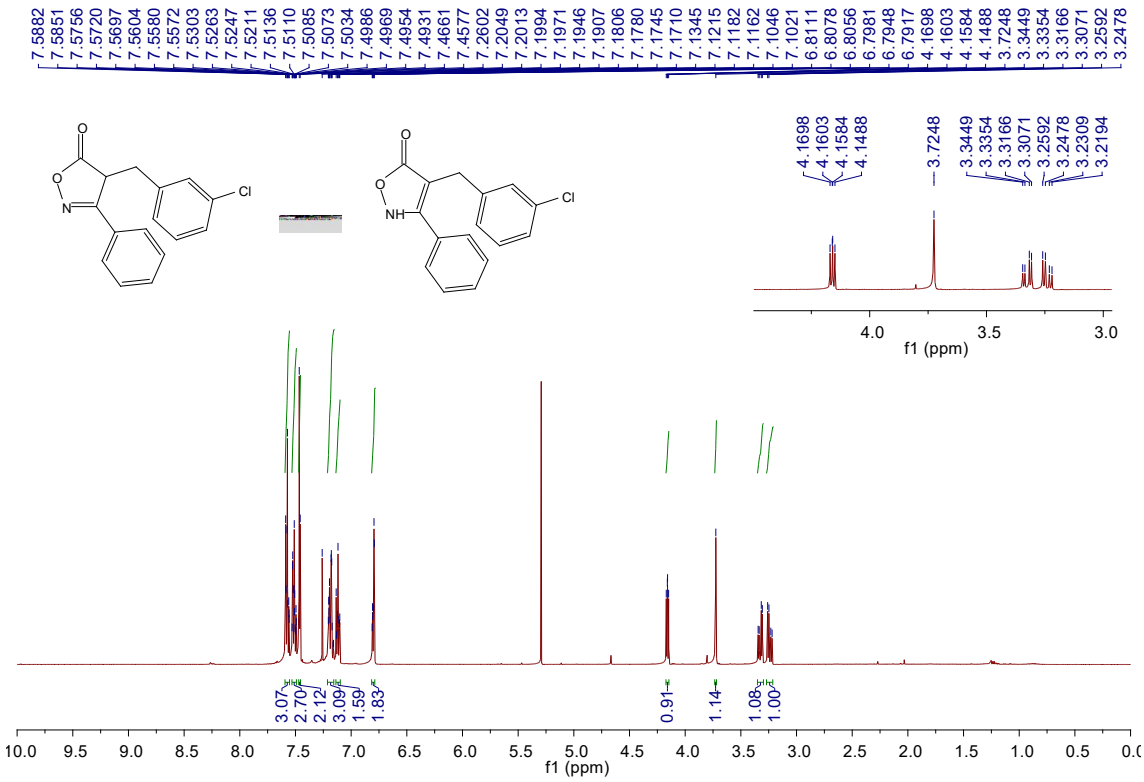


Figure S30. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-(3-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

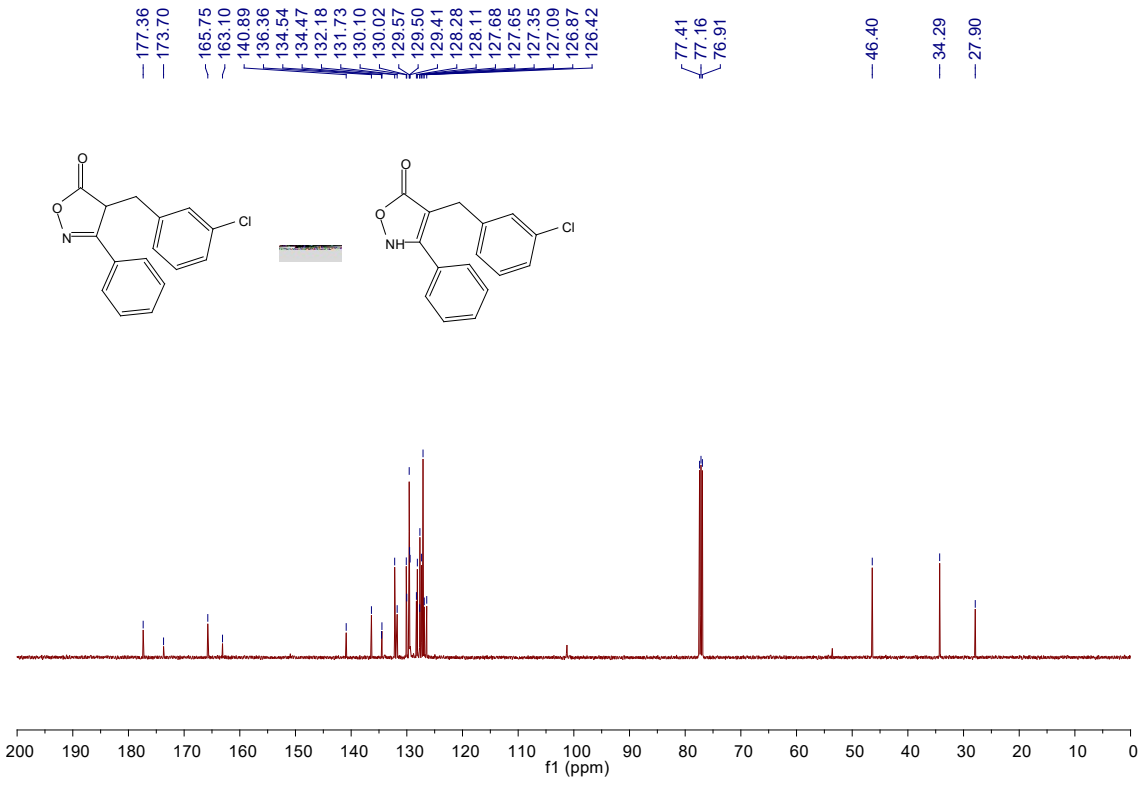


Figure S31. FT-IR (NaCl) of *4-(4-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

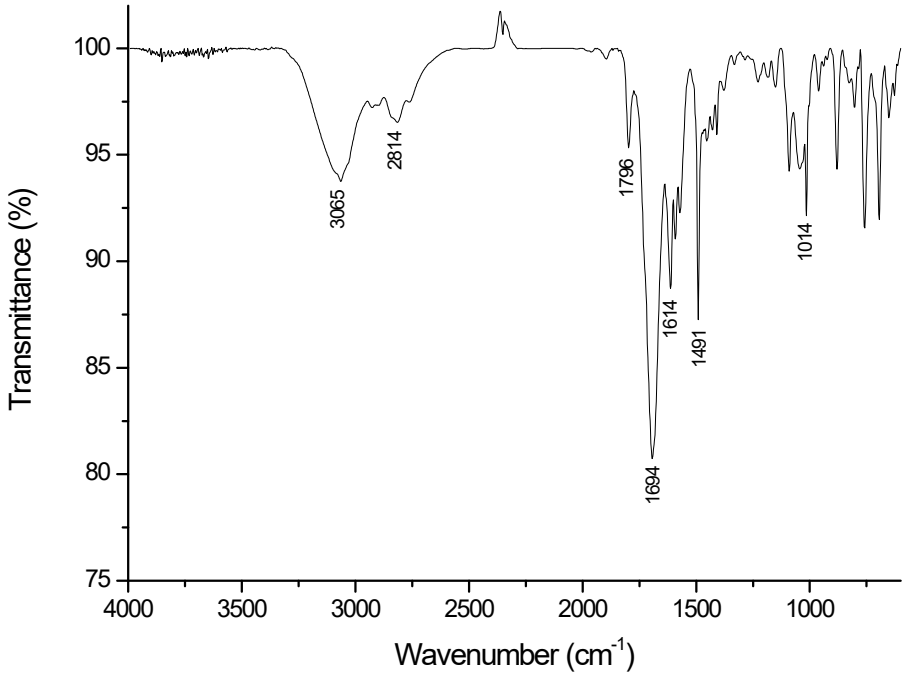


Figure S32. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-(4-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

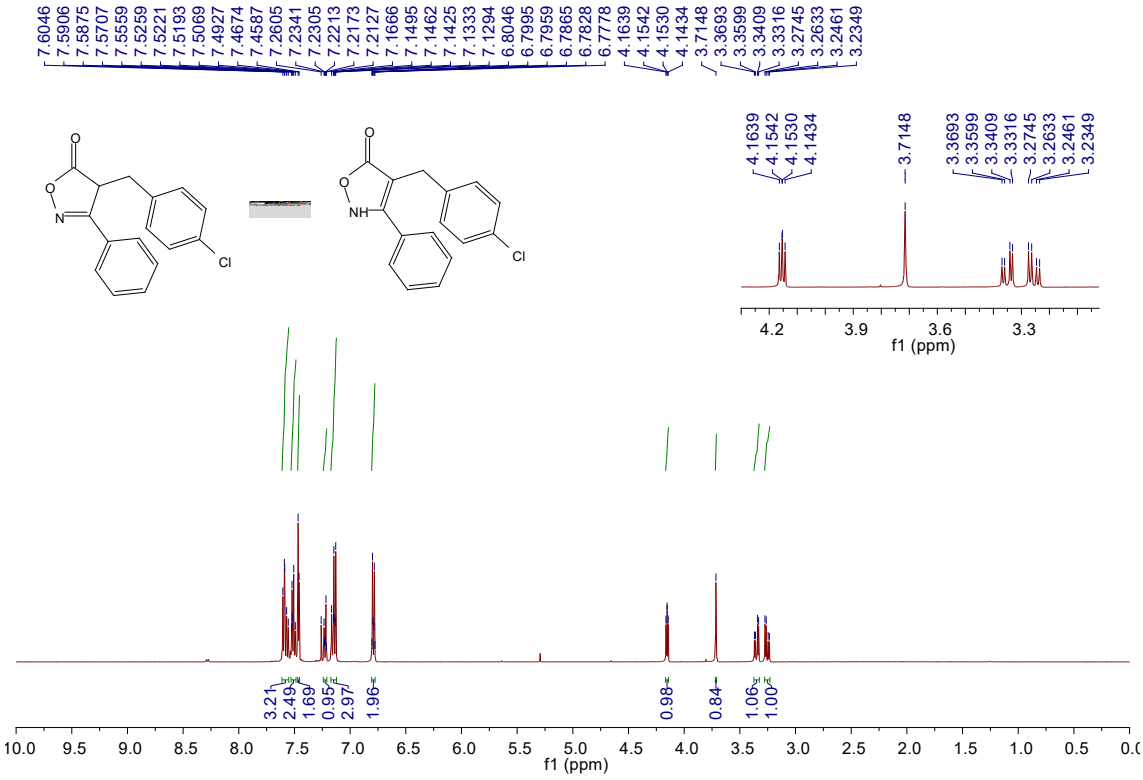


Figure S33. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-(4-chlorobenzyl)-3-phenylisoxazol-5(4H)-one*

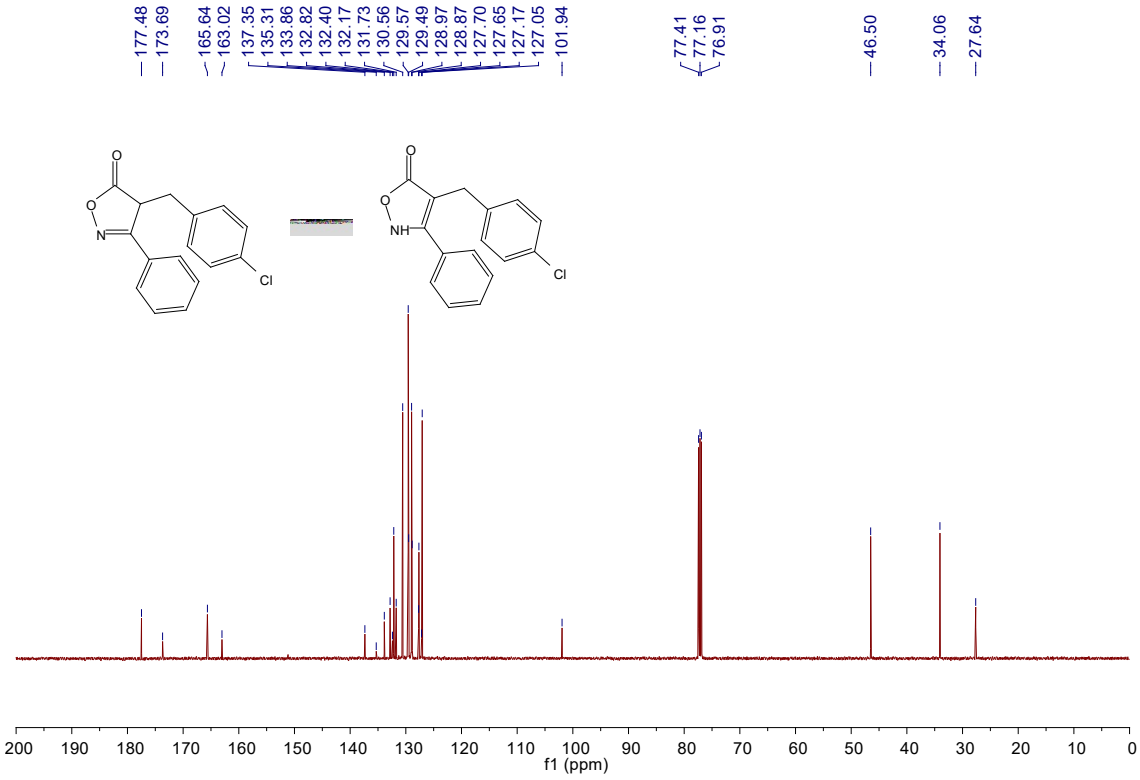


Figure S34. FT-IR (NaCl) of *4-(4-methoxybenzyl)-3-phenylisoxazol-5(4H)-one*

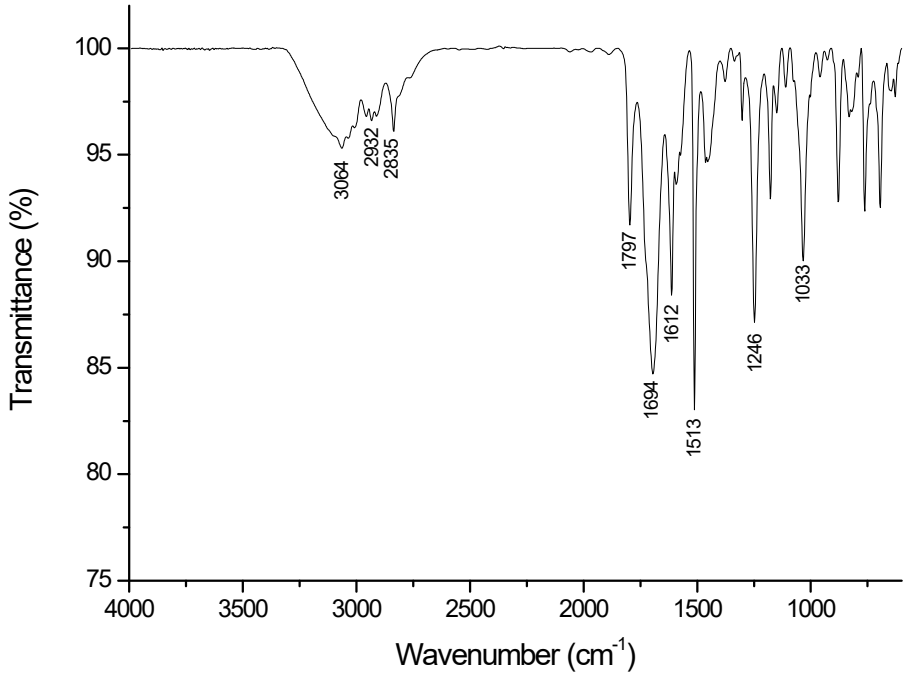


Figure S35. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-(4-methoxybenzyl)-3-phenylisoxazol-5(4H)-one*

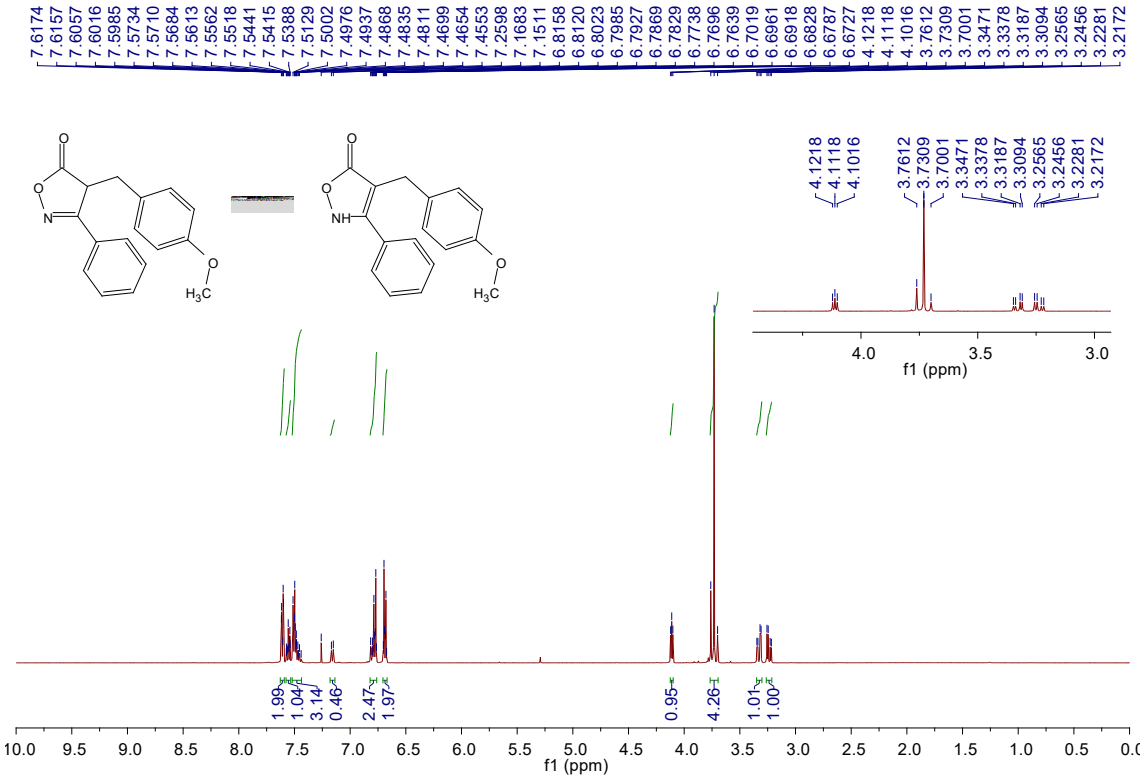


Figure S36. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-(4-methoxybenzyl)-3-phenylisoxazol-5(4H)-one*

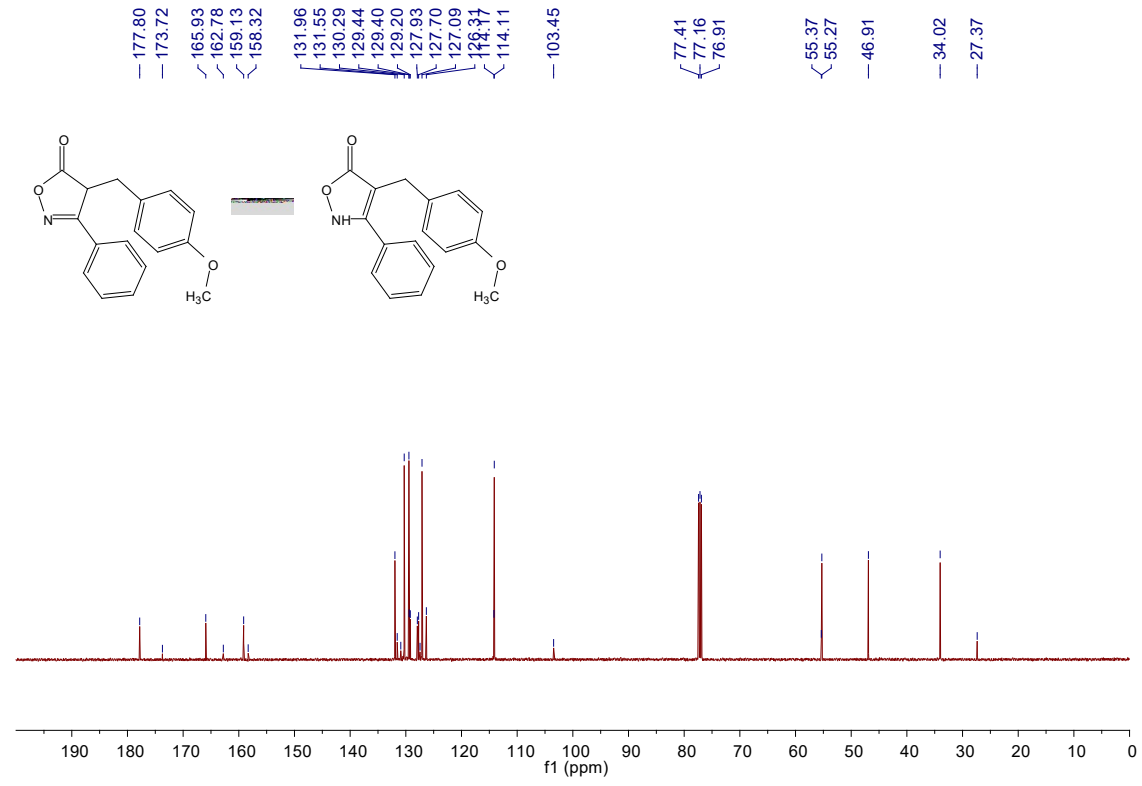


Figure S37. FT-IR (NaCl) of *4-(furan-2-ylmethyl)-3-phenylisoxazol-5(4H)-one*

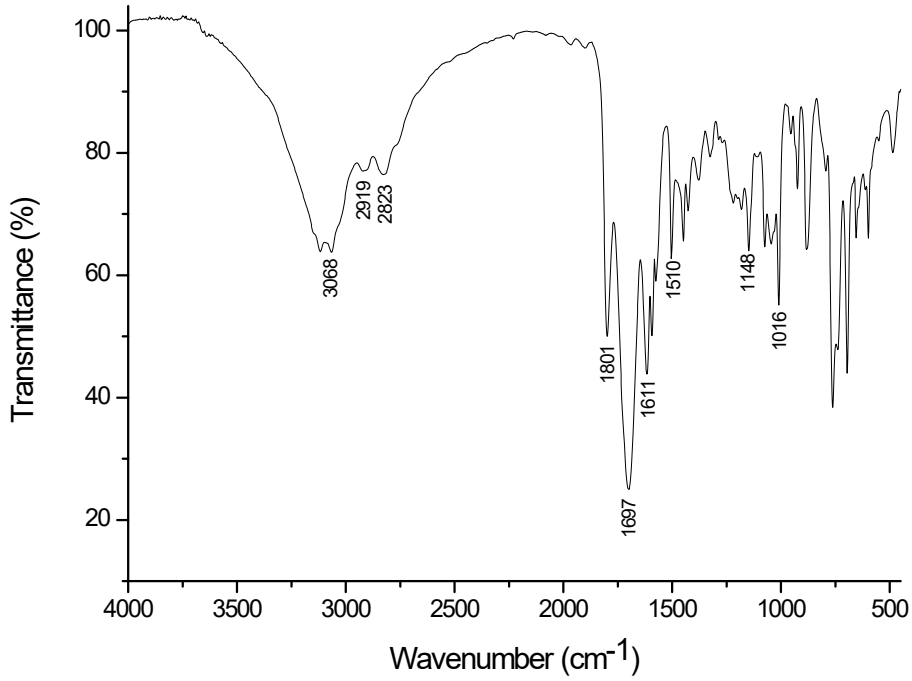


Figure S38. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-(furan-2-ylmethyl)-3-phenylisoxazol-5(4H)-one*

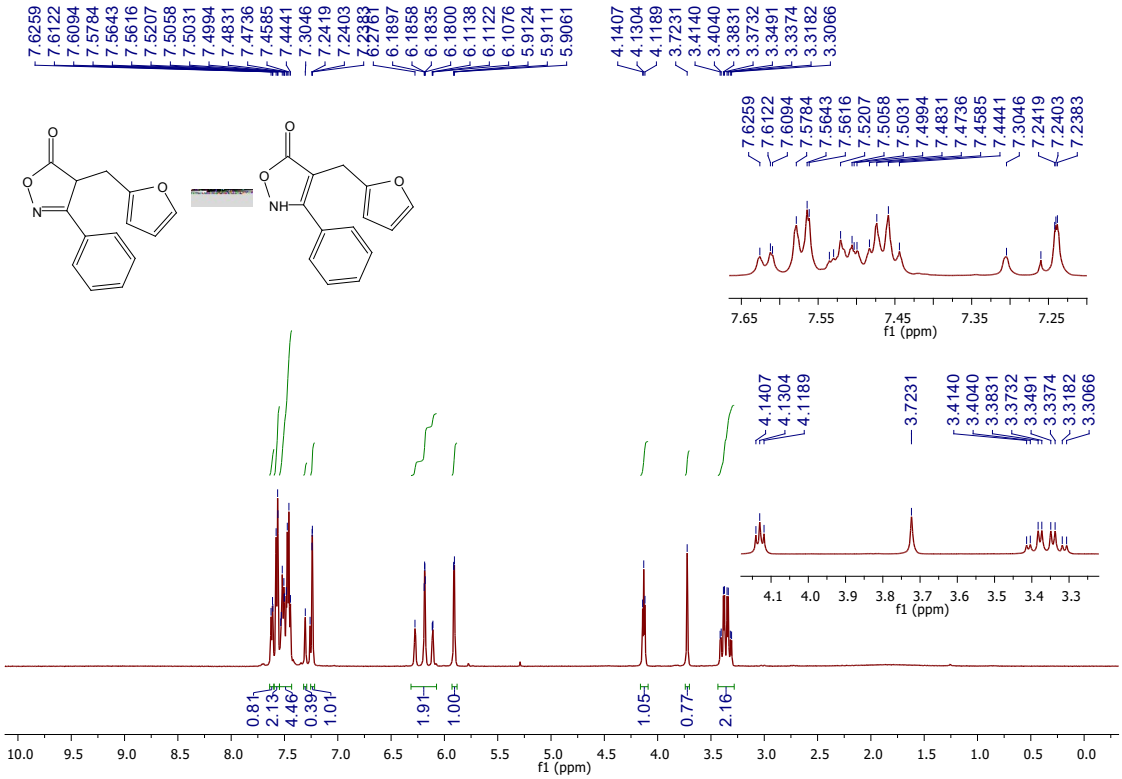
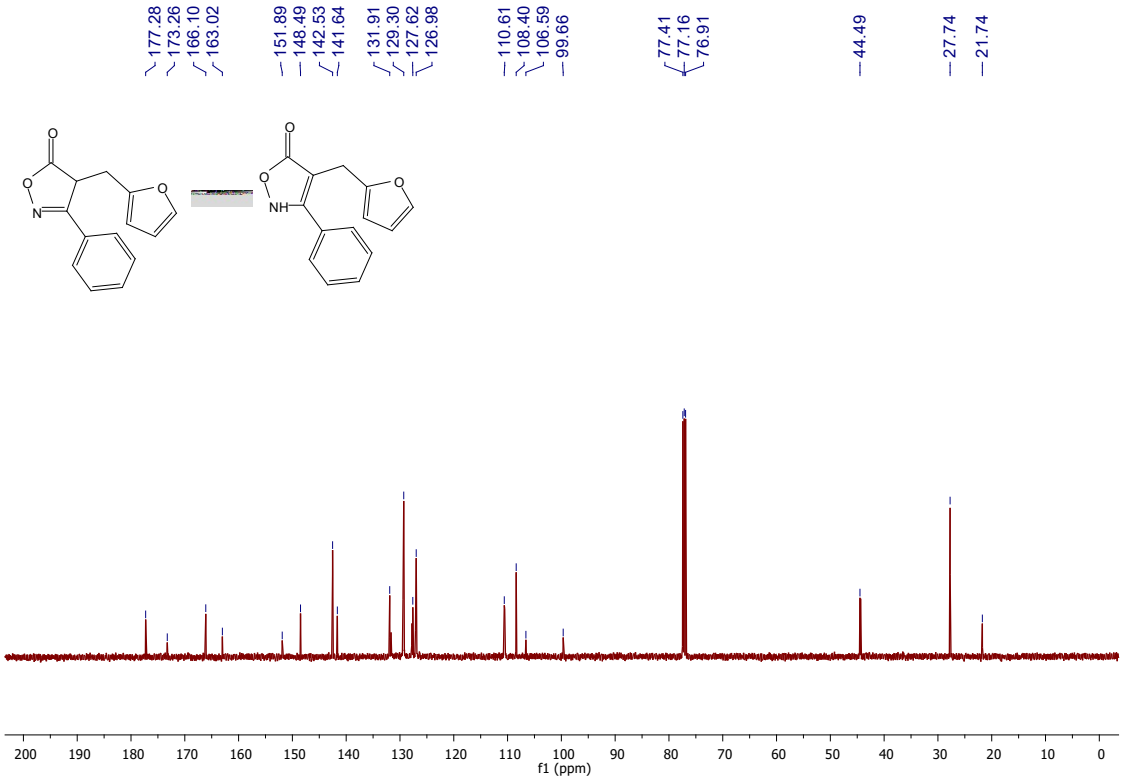


Figure S39. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-(furan-2-ylmethyl)-3-phenylisoxazol-5(4H)-one*



2. NMR and IR spectra of compounds 3a-3u and 4a

Figure S40. FT-IR (NaCl) of *(E)-4-benzyl-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3a).

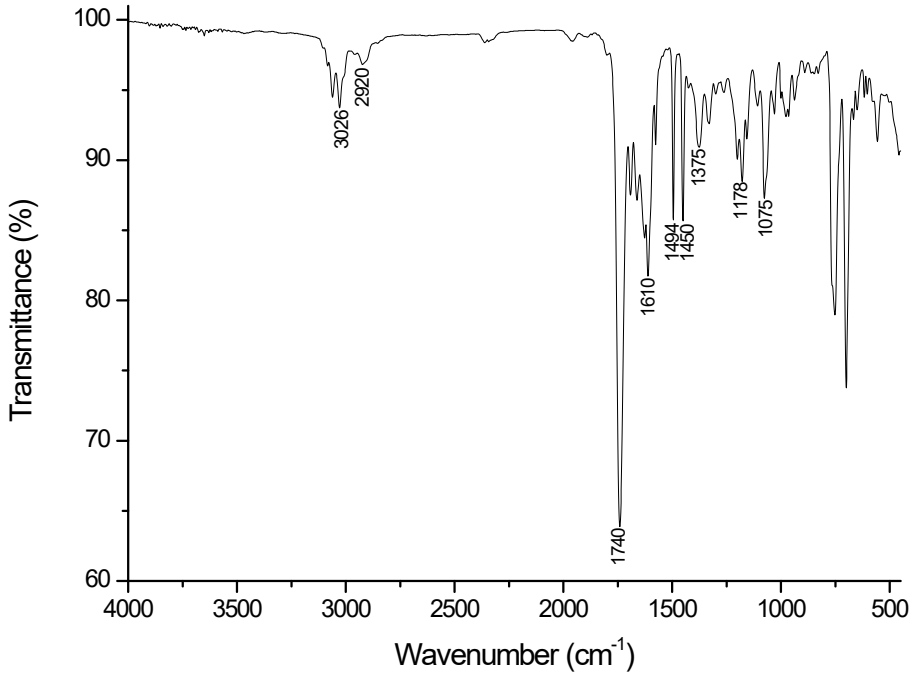


Figure S41. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3a).

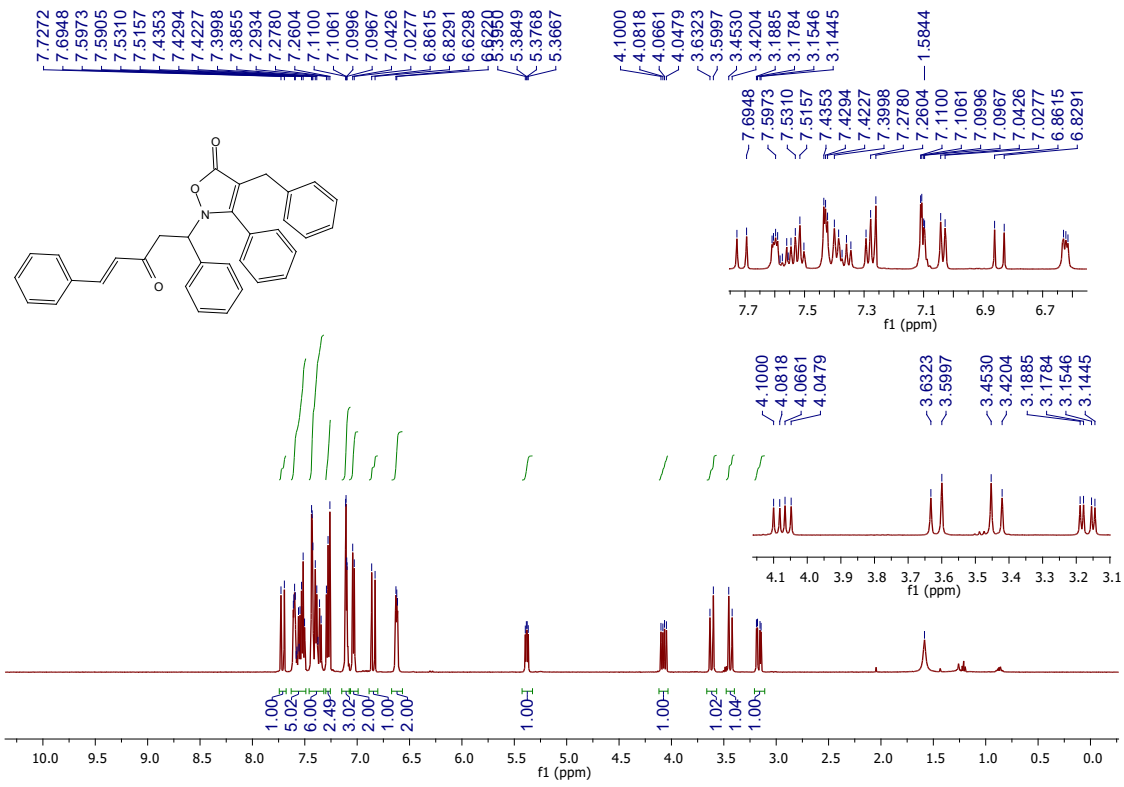


Figure S42. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3a).

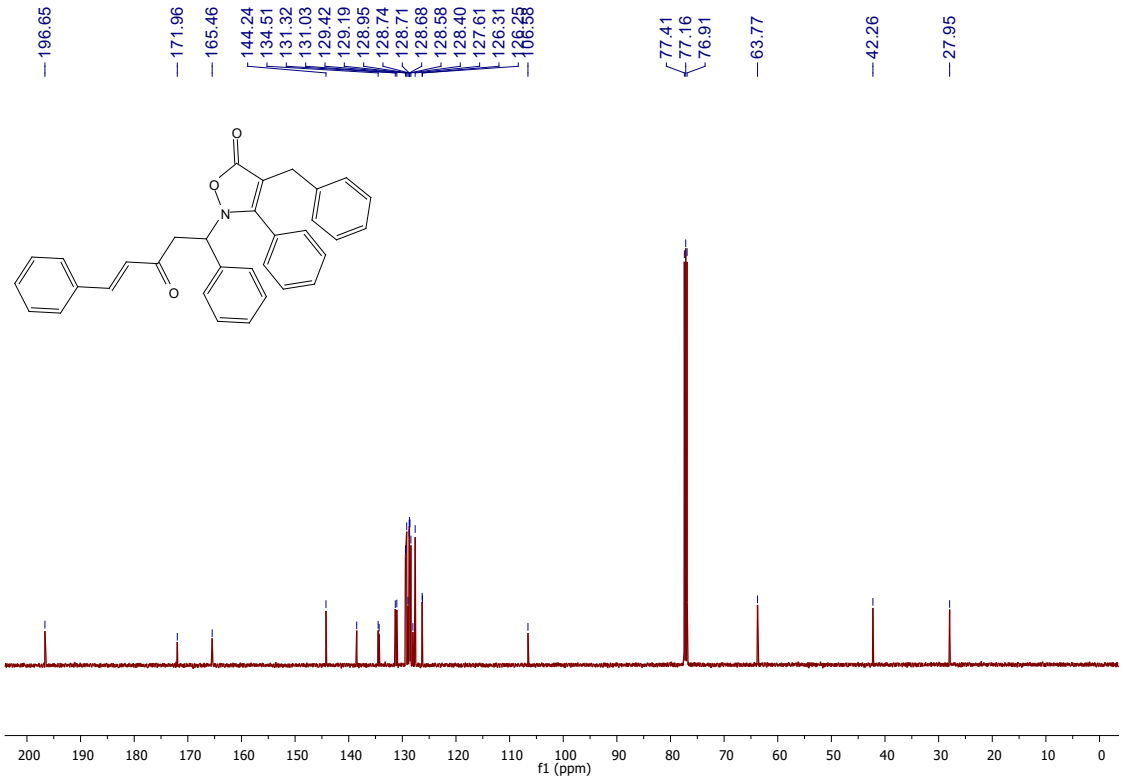


Figure S43. FT-IR (NaCl) of *(E)-4-(4-methoxybenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3b).

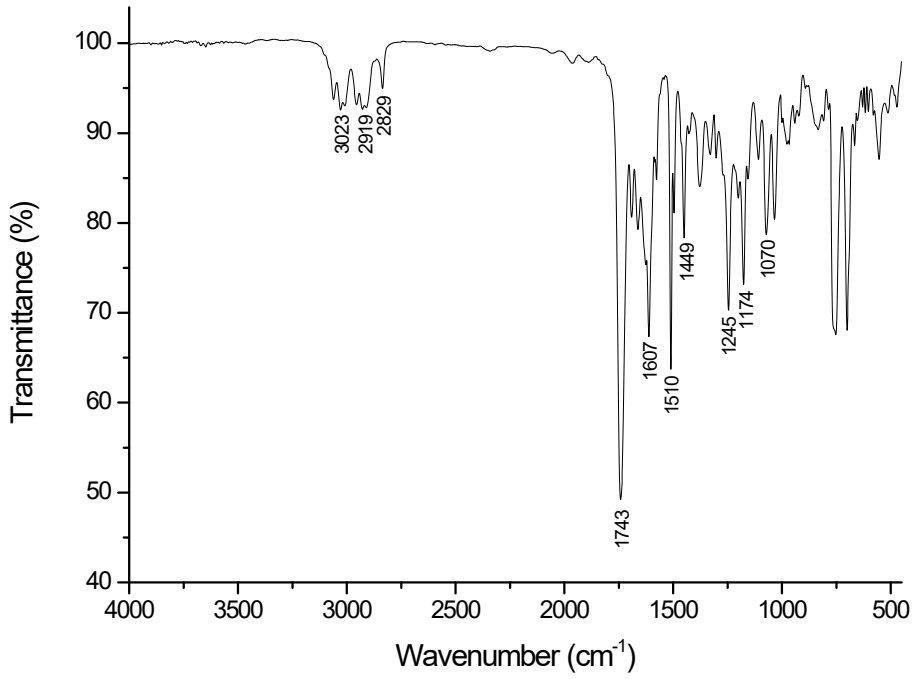


Figure S44. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(4-methoxybenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3b).

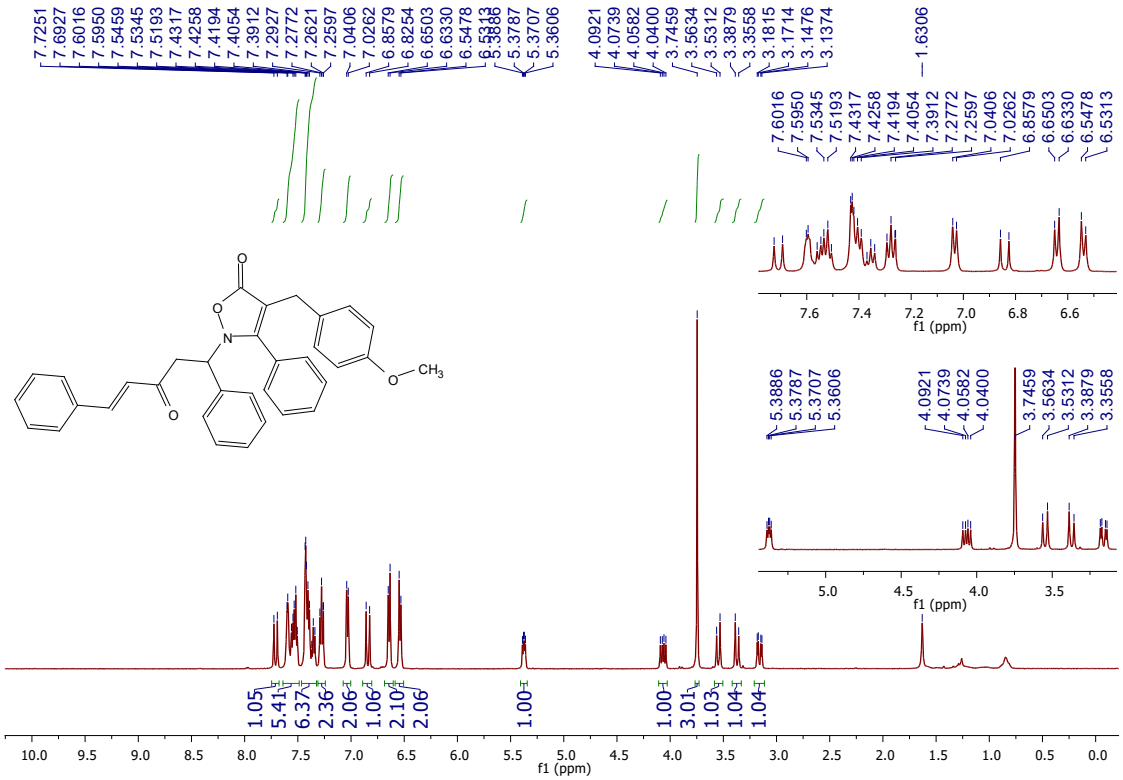


Figure S45. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(4-methoxybenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3b).

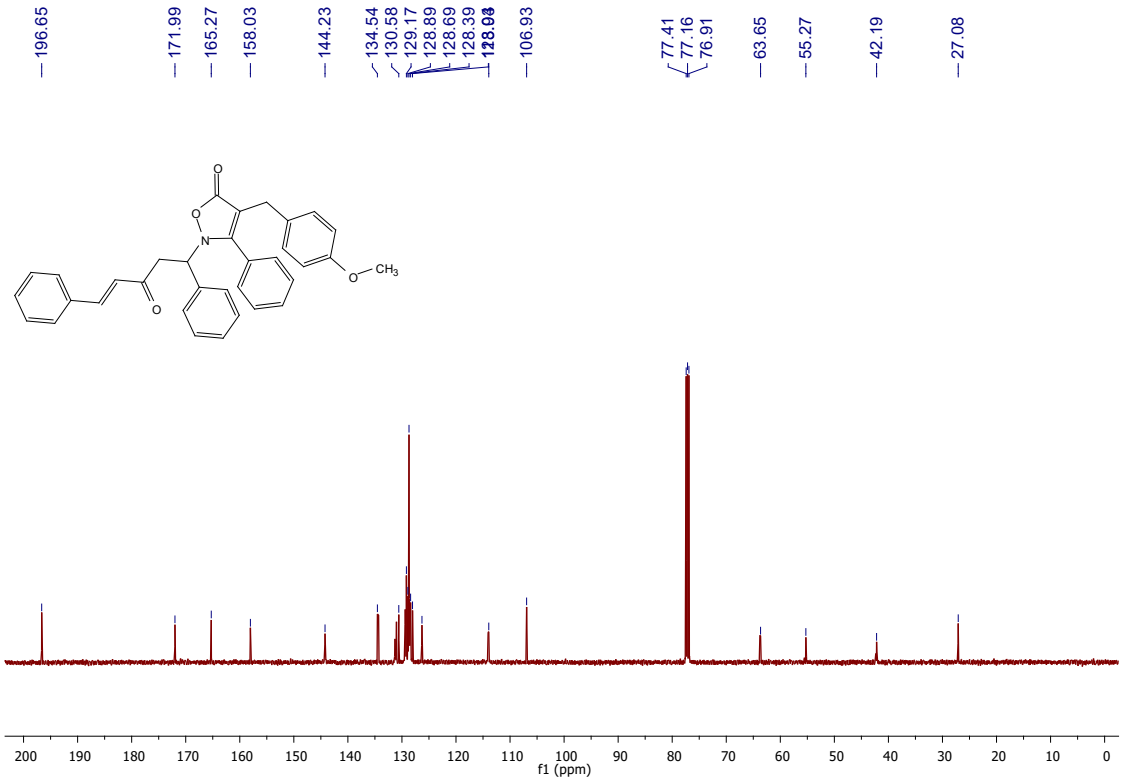
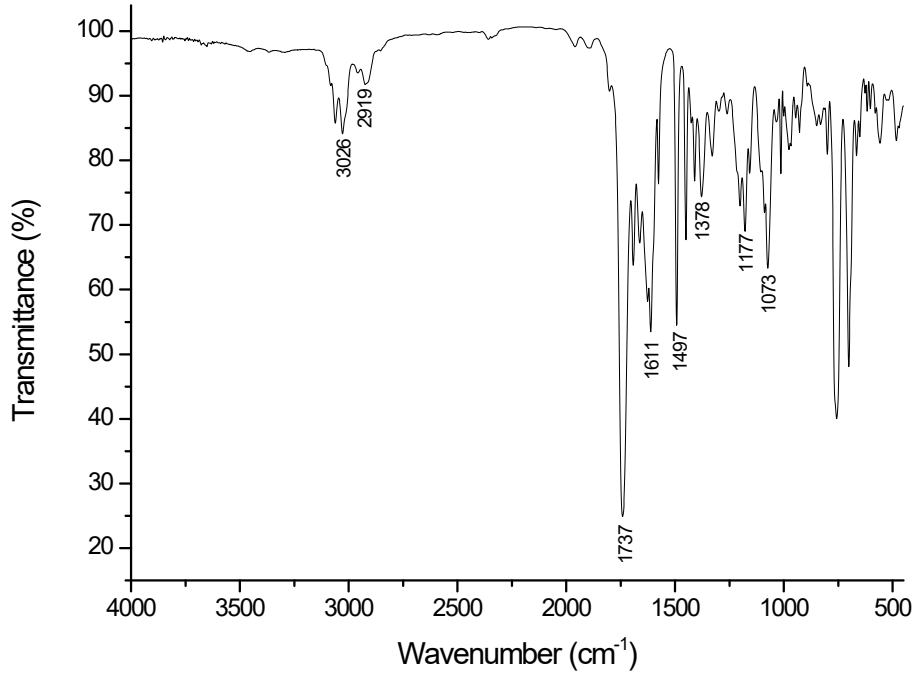


Figure S46. FT-IR (NaCl) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3c).



Figure

S47. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3c).

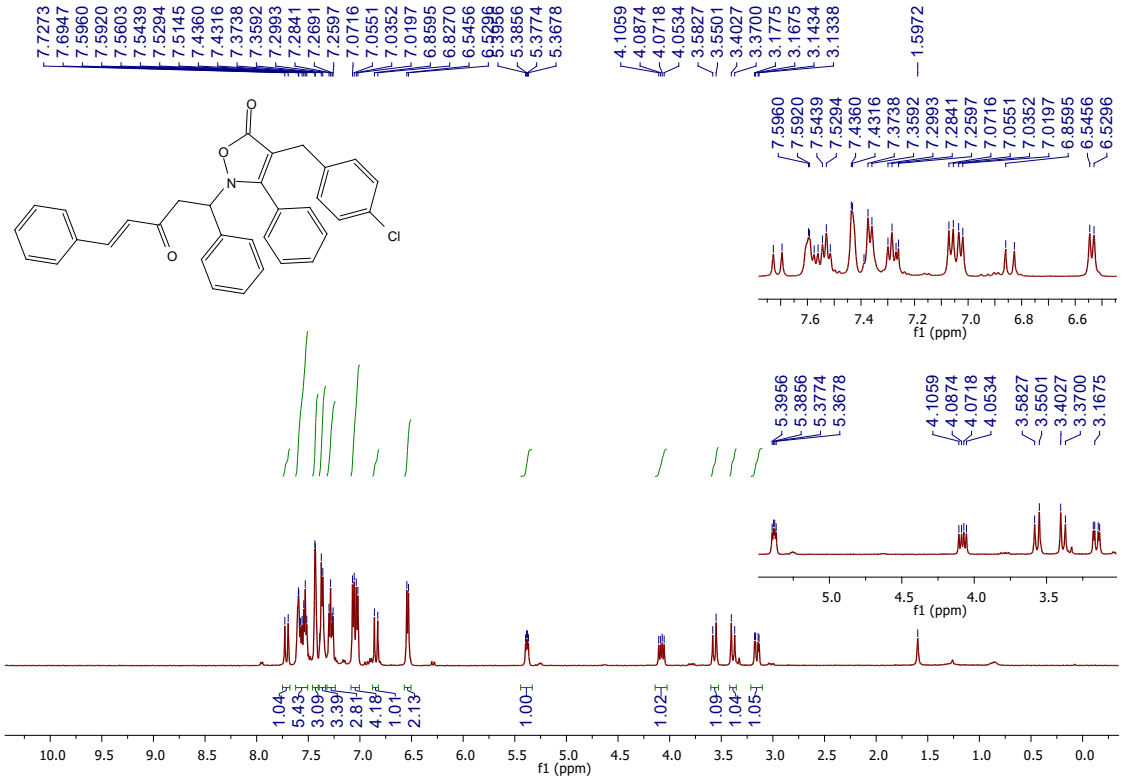


Figure S48. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3c).

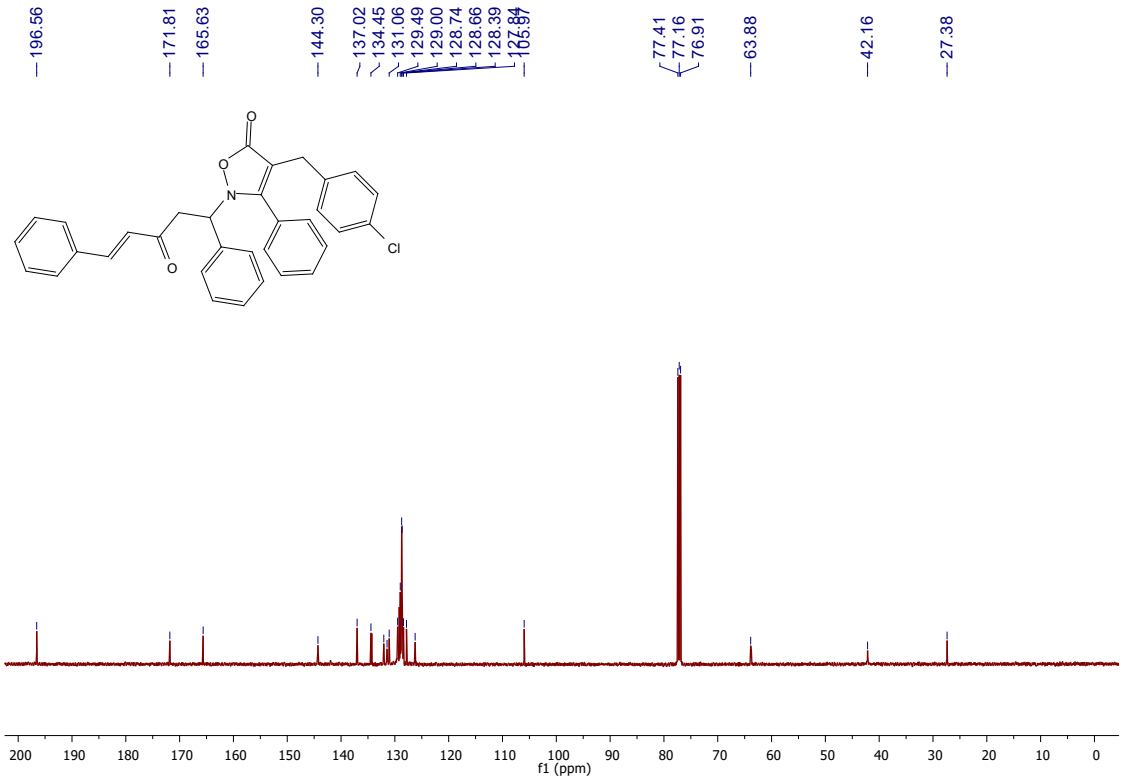


Figure S49. FT-IR (NaCl) of *(E)-4-(3-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3d).

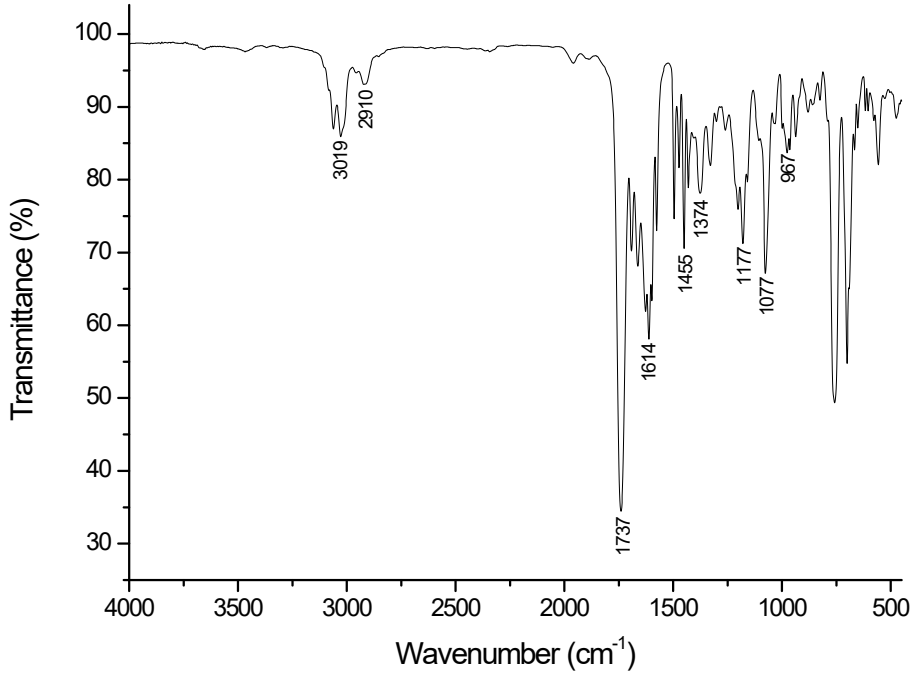


Figure S50. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(3-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3d).

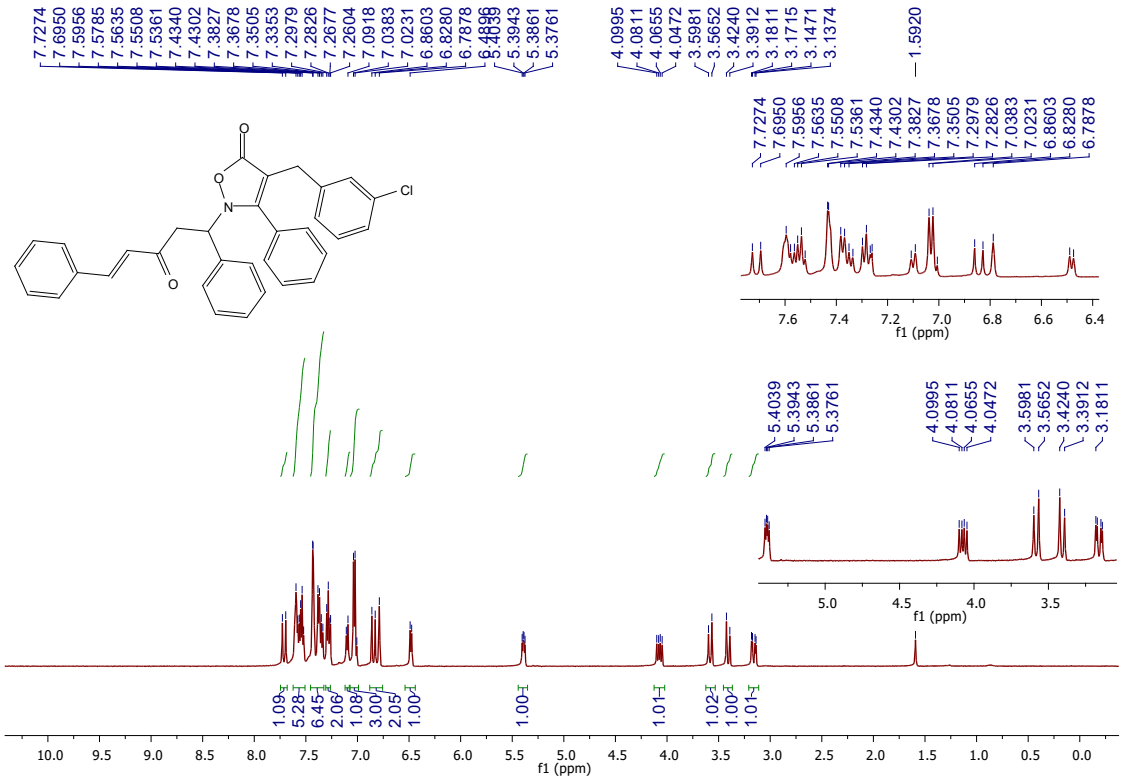


Figure S51. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(3-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3d).

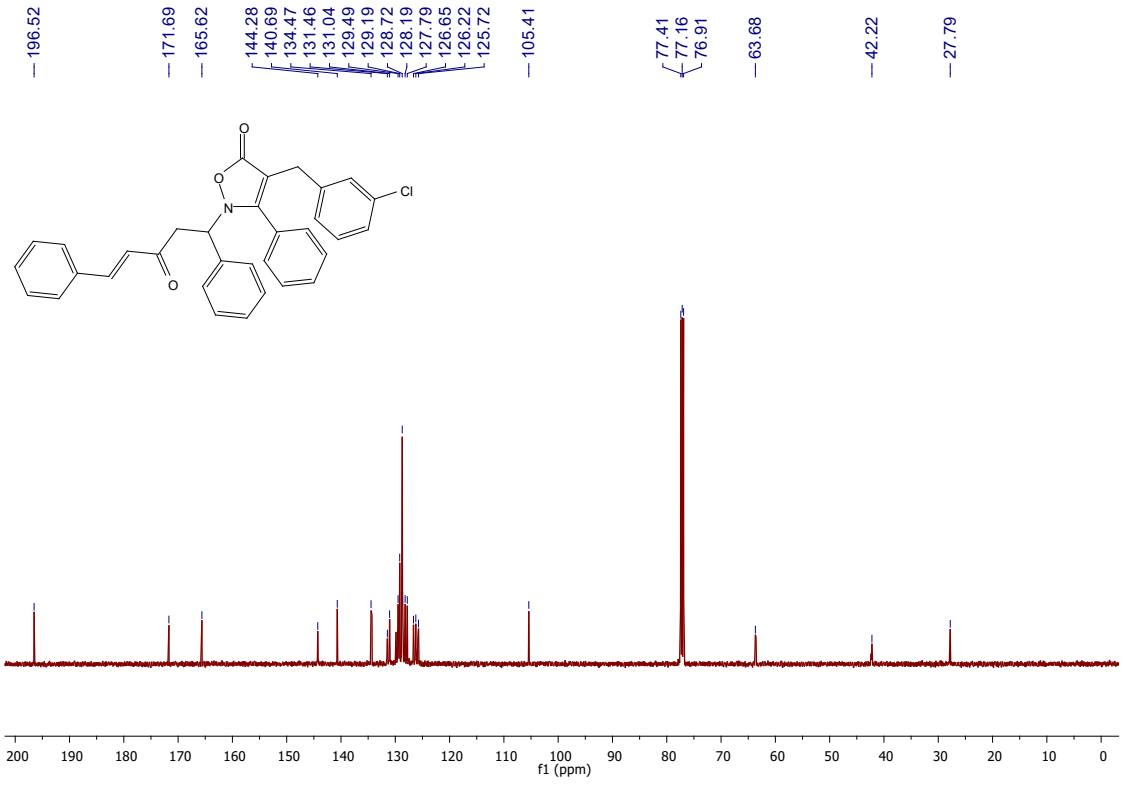


Figure S52. FT-IR (NaCl) of *(E)-4-(2-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3e).

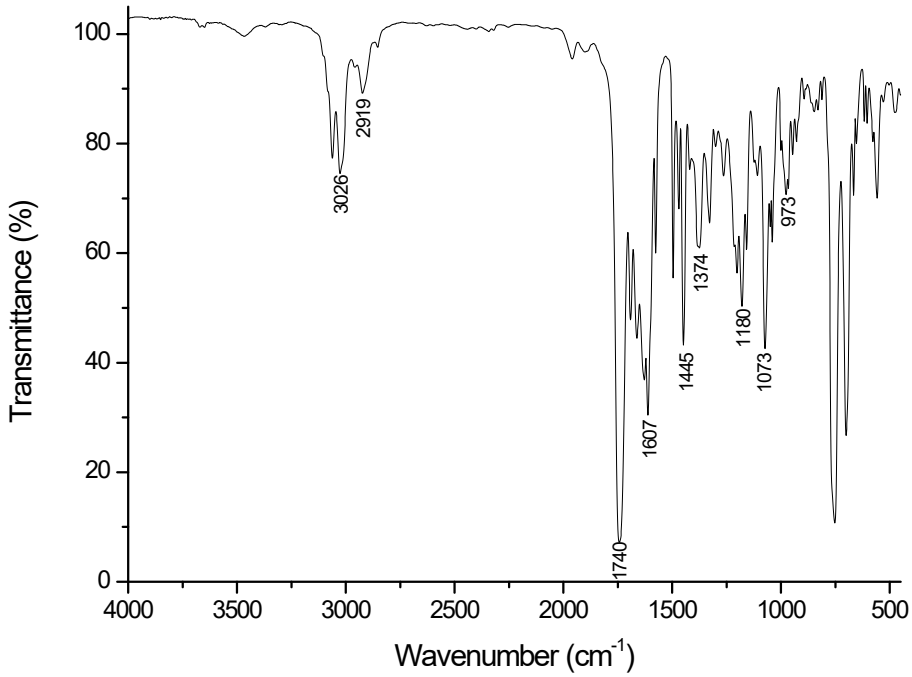


Figure S53. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(2-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3e).

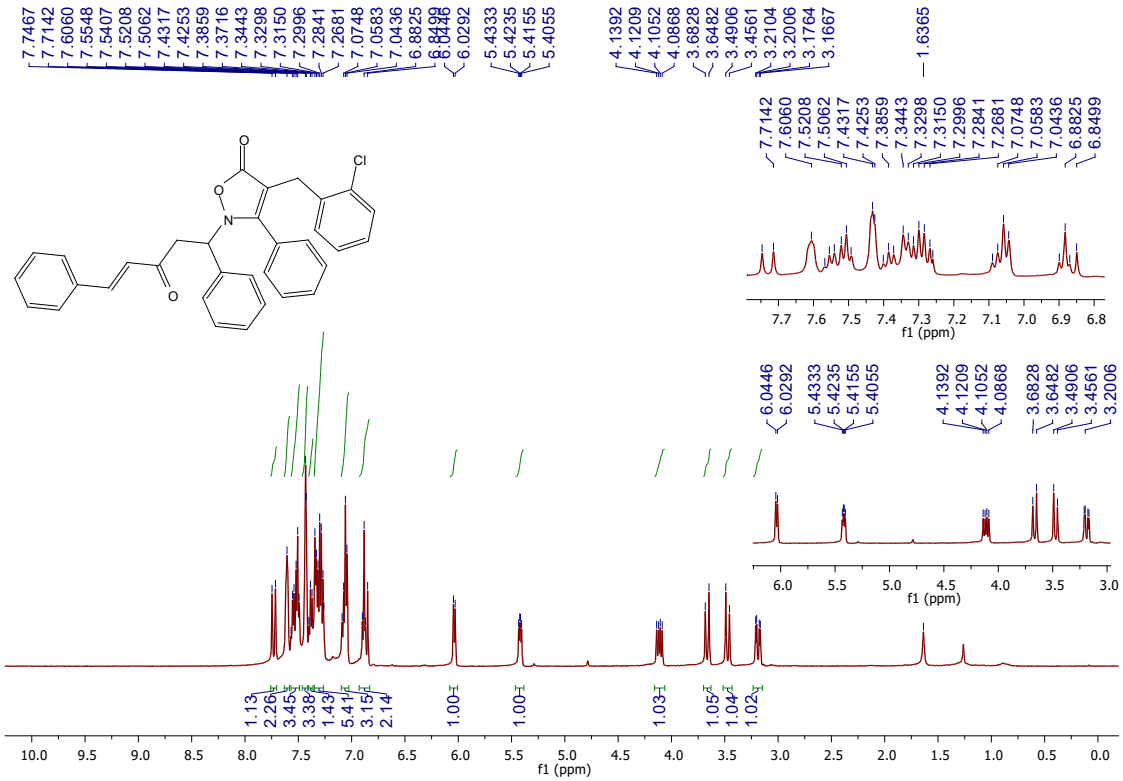


Figure S54. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(2-chlorobenzyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3e).

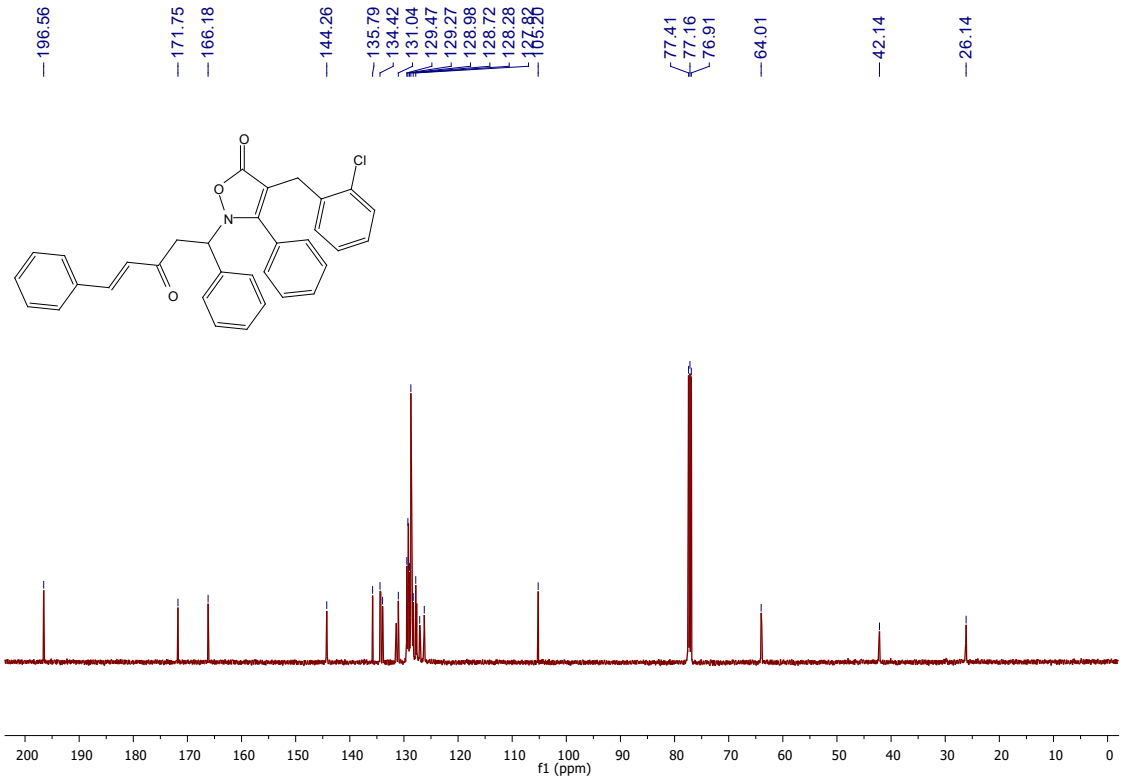


Figure S55. FT-IR (NaCl) of *(E)-4-benzyl-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3f).

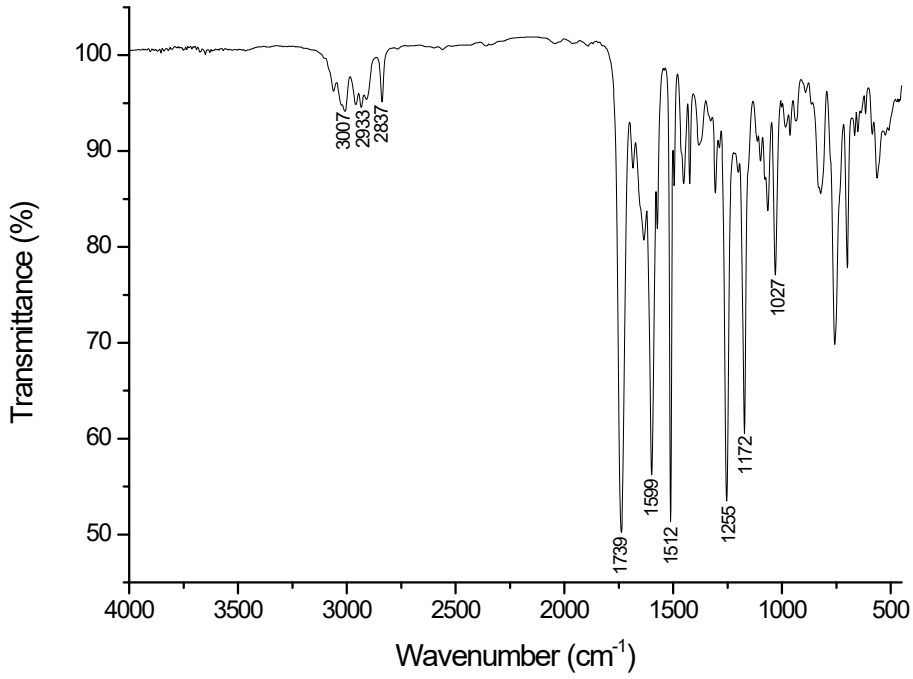


Figure S56. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3f).

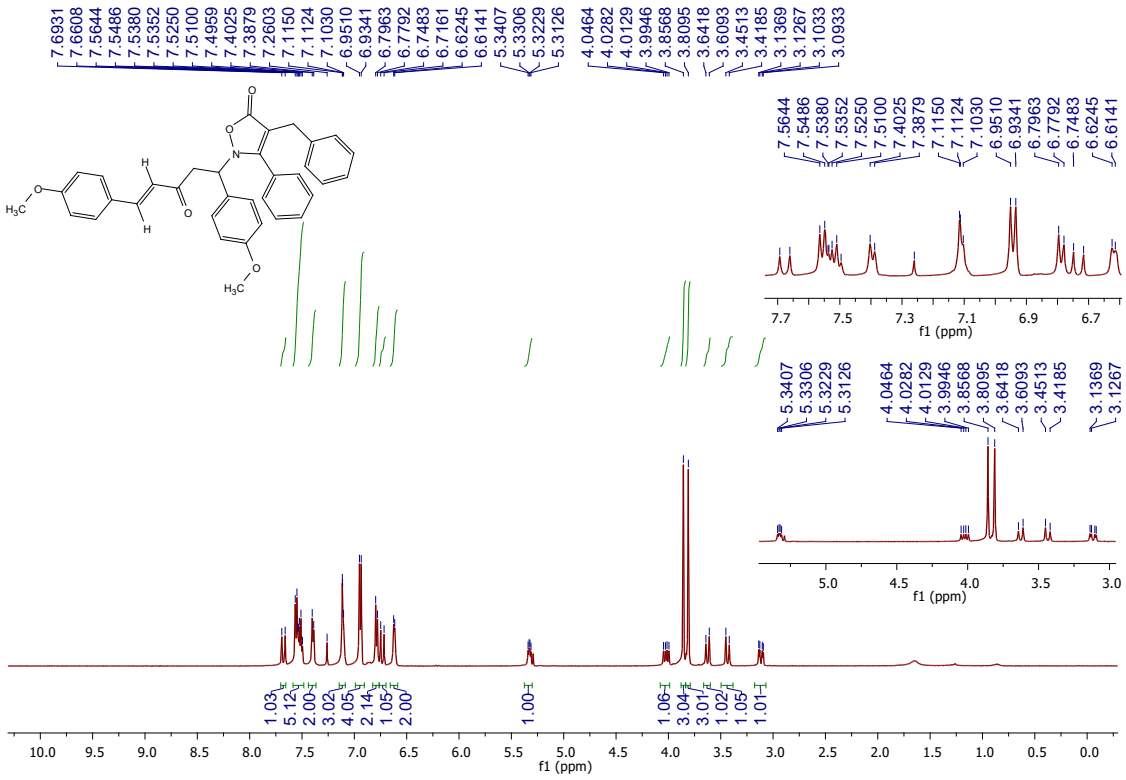


Figure S57. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3f).

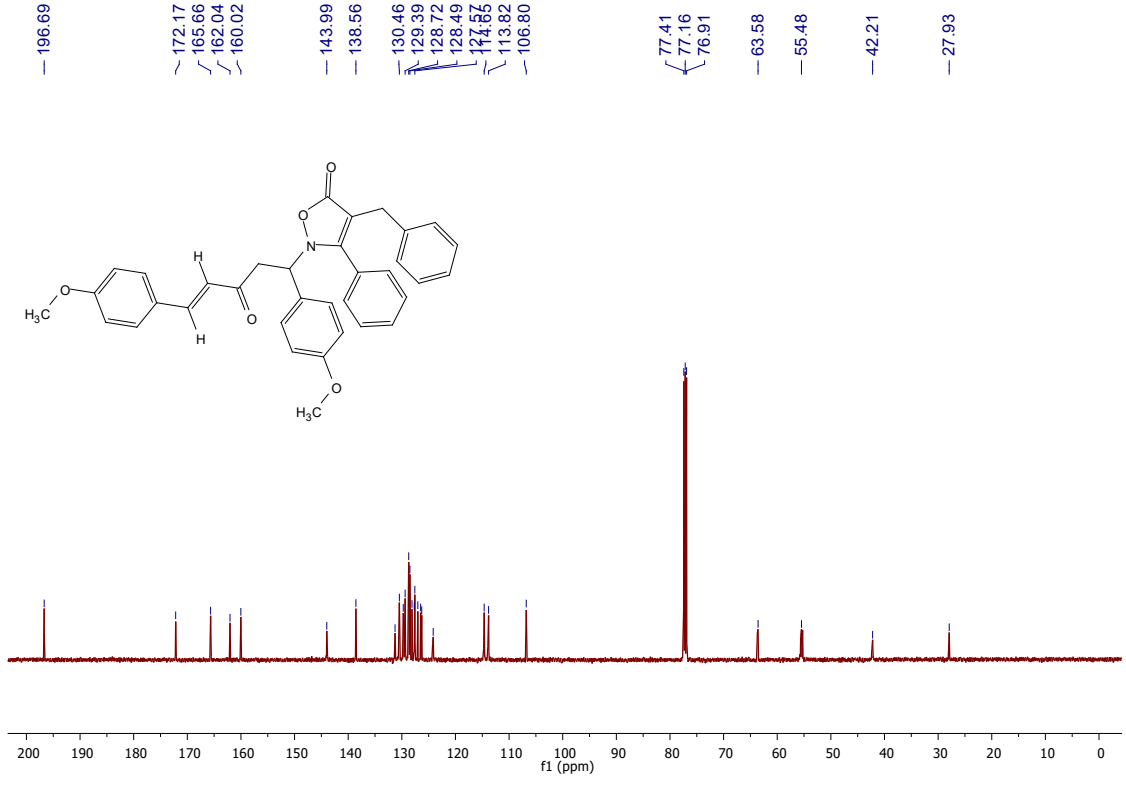


Figure S58. FT-IR (NaCl) of *(E)-4-benzyl-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3g).

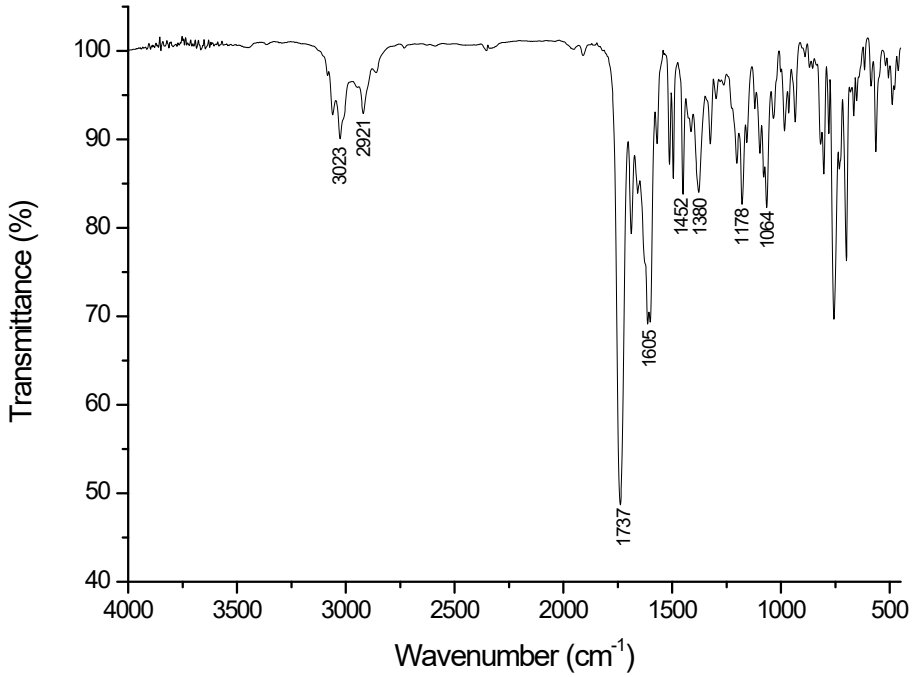


Figure S59. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3g).

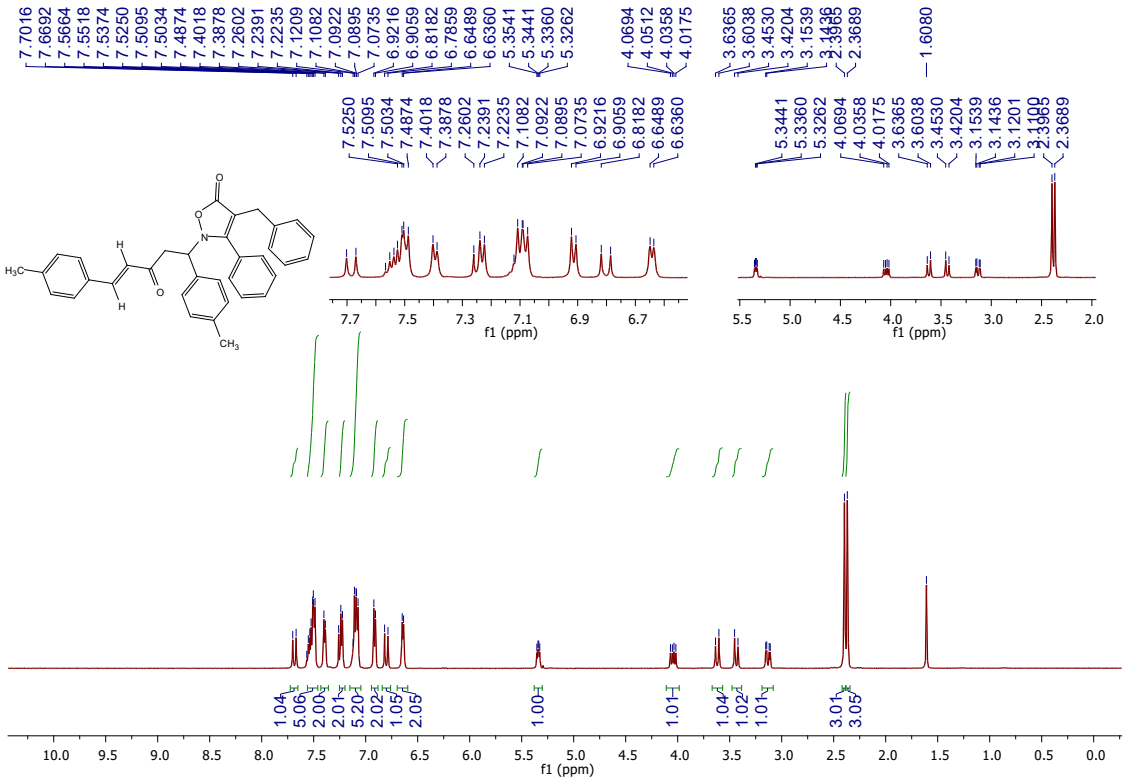


Figure S60. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3g).

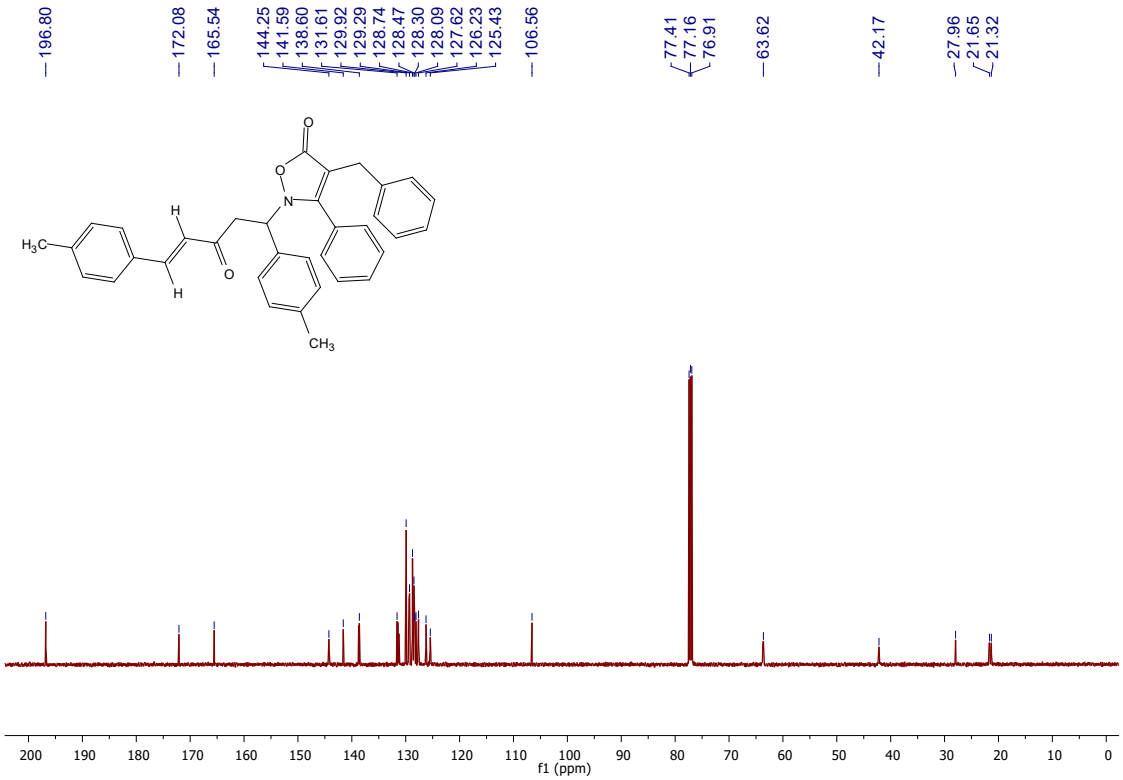


Figure S61. IR (ATR) of *(E)-4-benzyl-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3h).

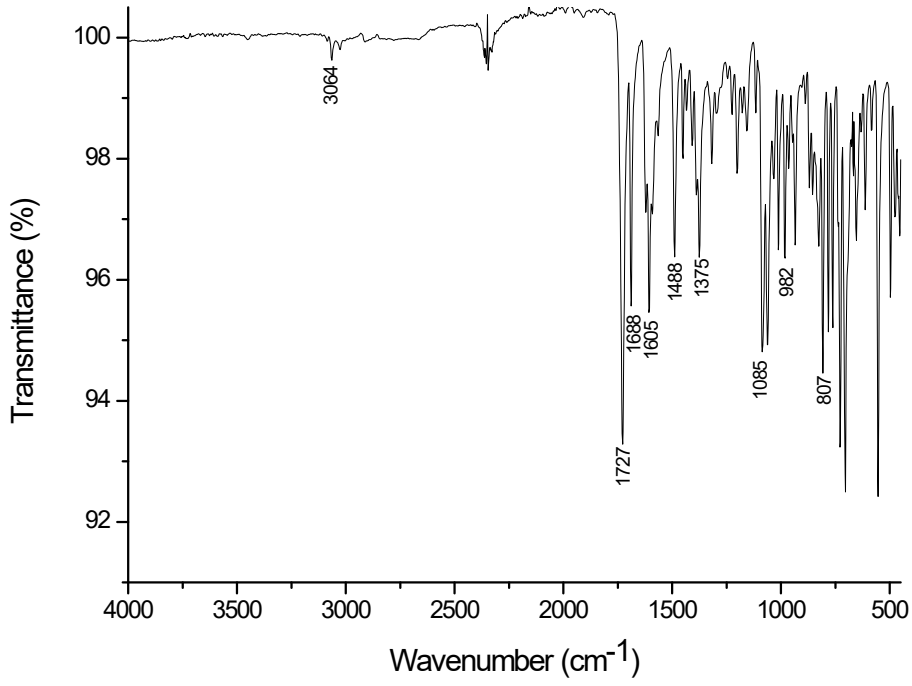


Figure S62. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3h).

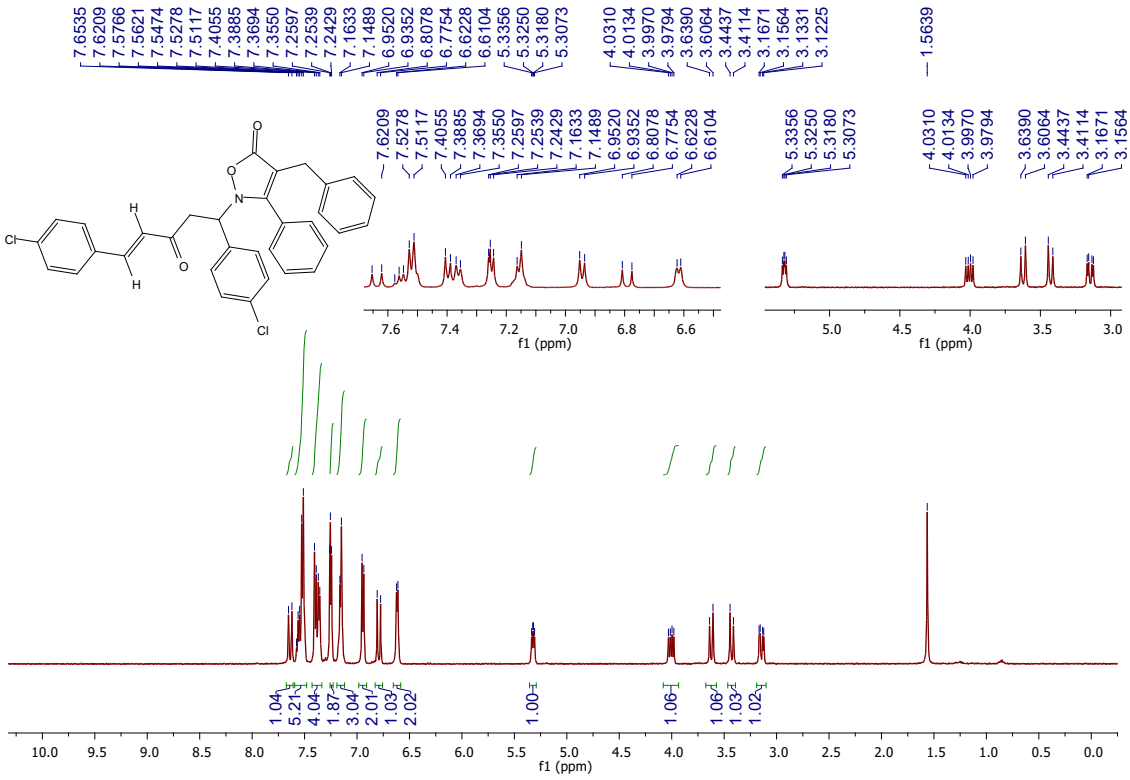


Figure S63. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3h).

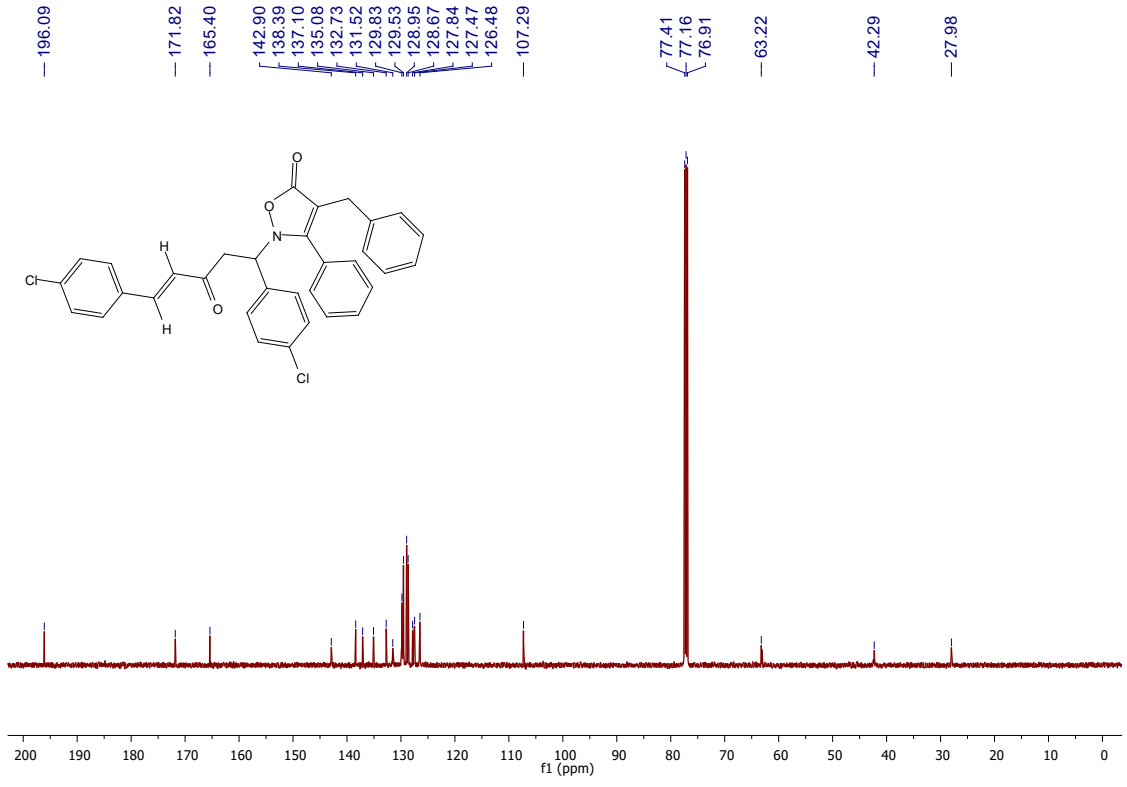


Figure S64. FT-IR (NaCl) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3i).

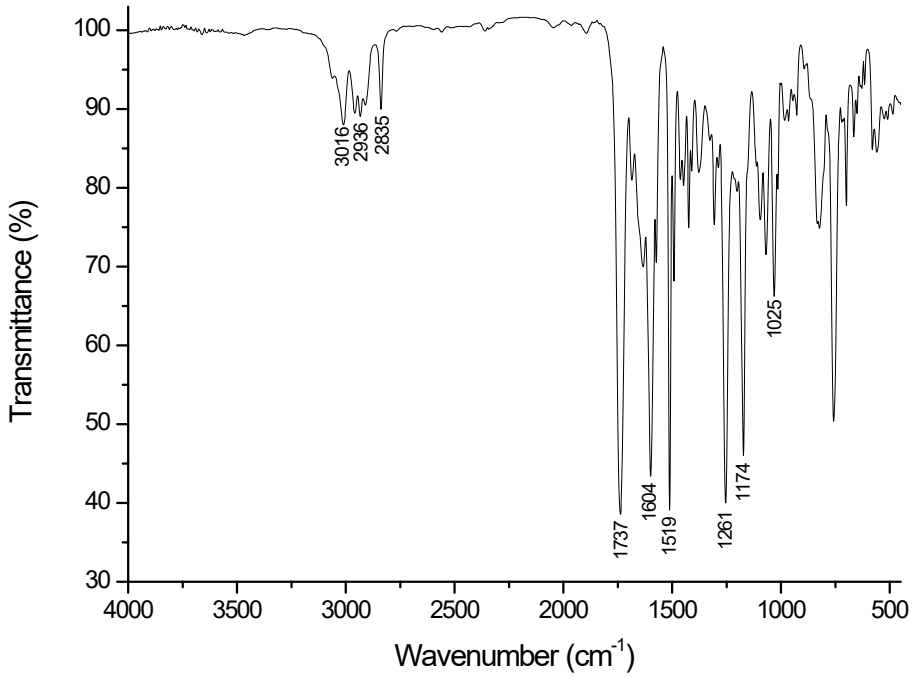


Figure S65. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3i).

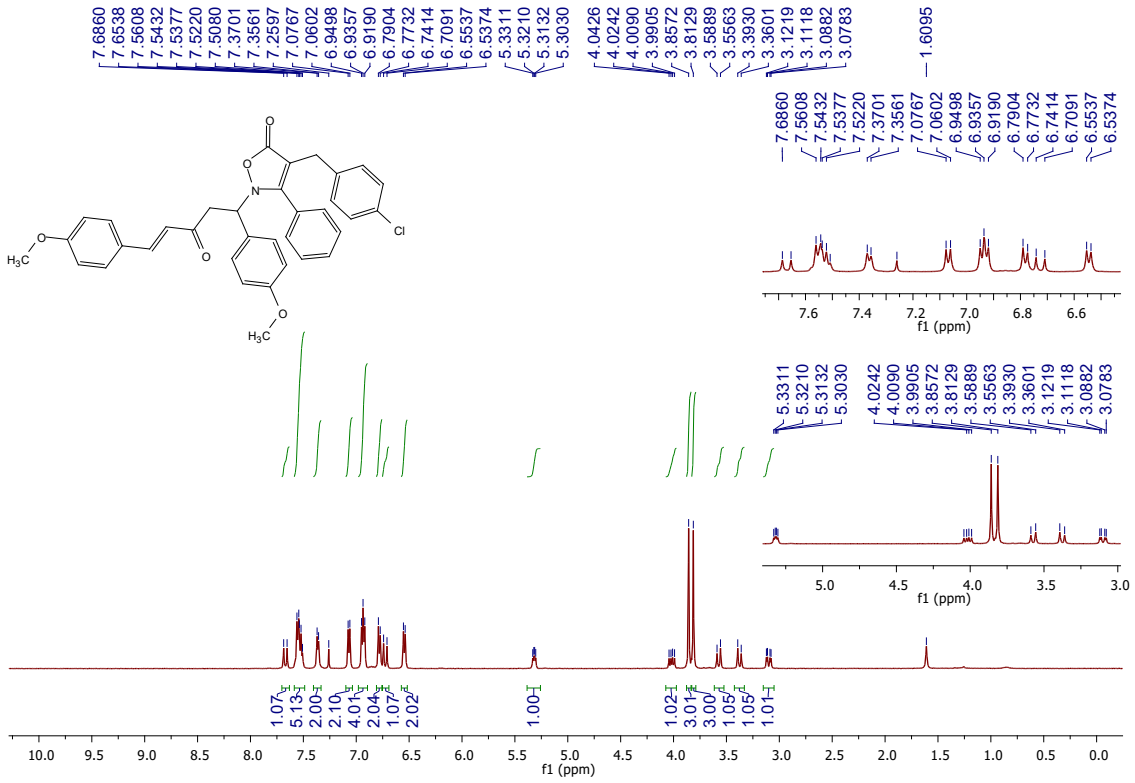


Figure S66. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3i).

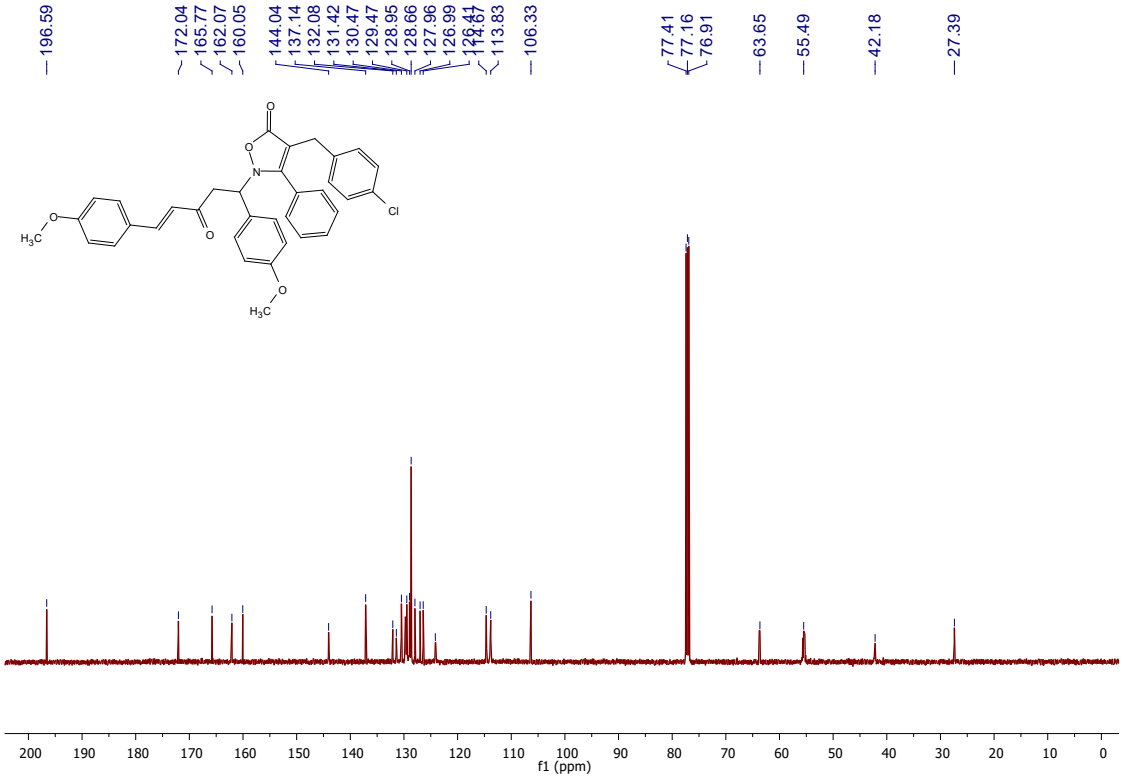


Figure S67. IR (ATR) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3j).

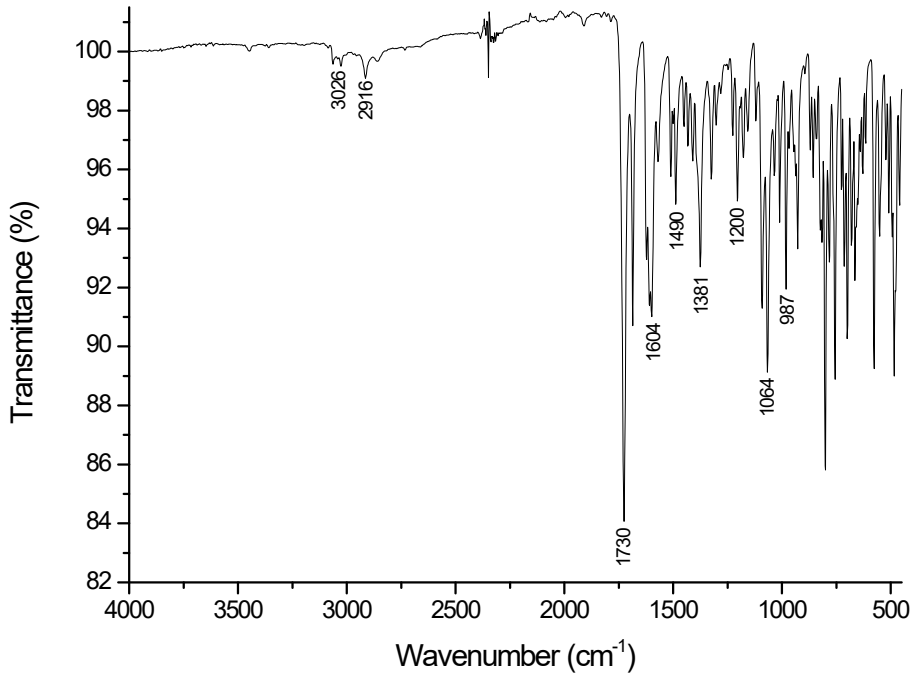


Figure S68. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3j).

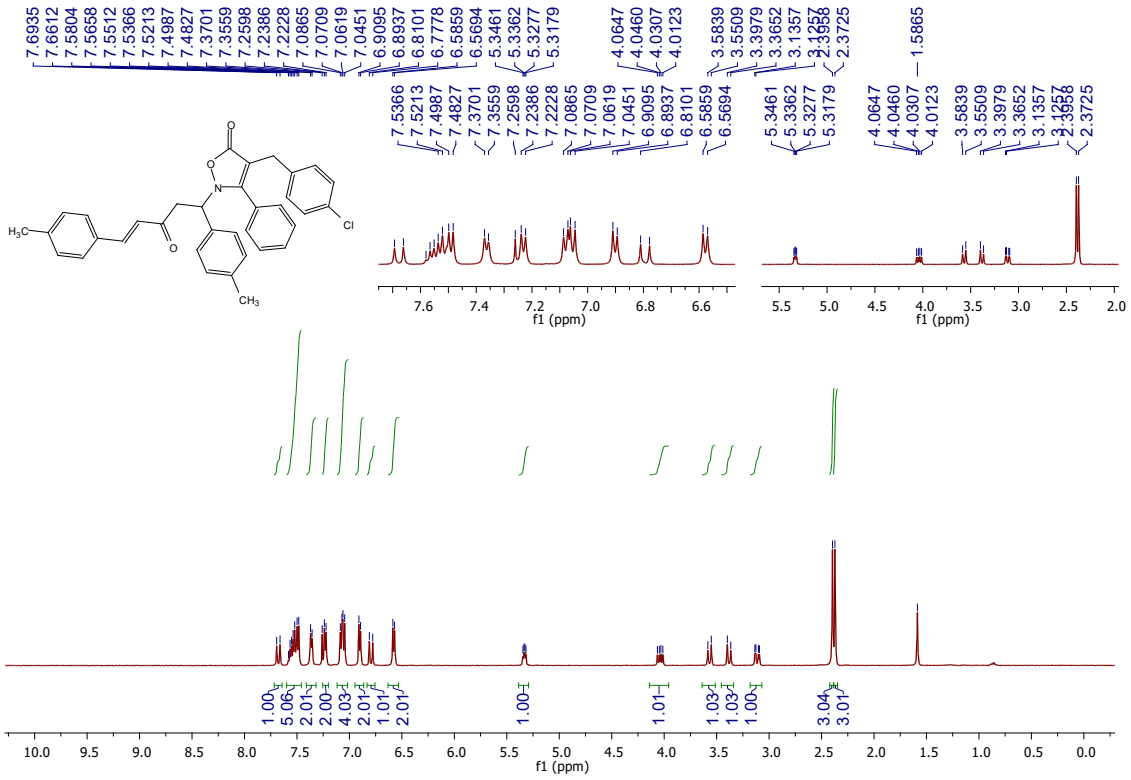


Figure S69. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(4-chlorobenzyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3j).

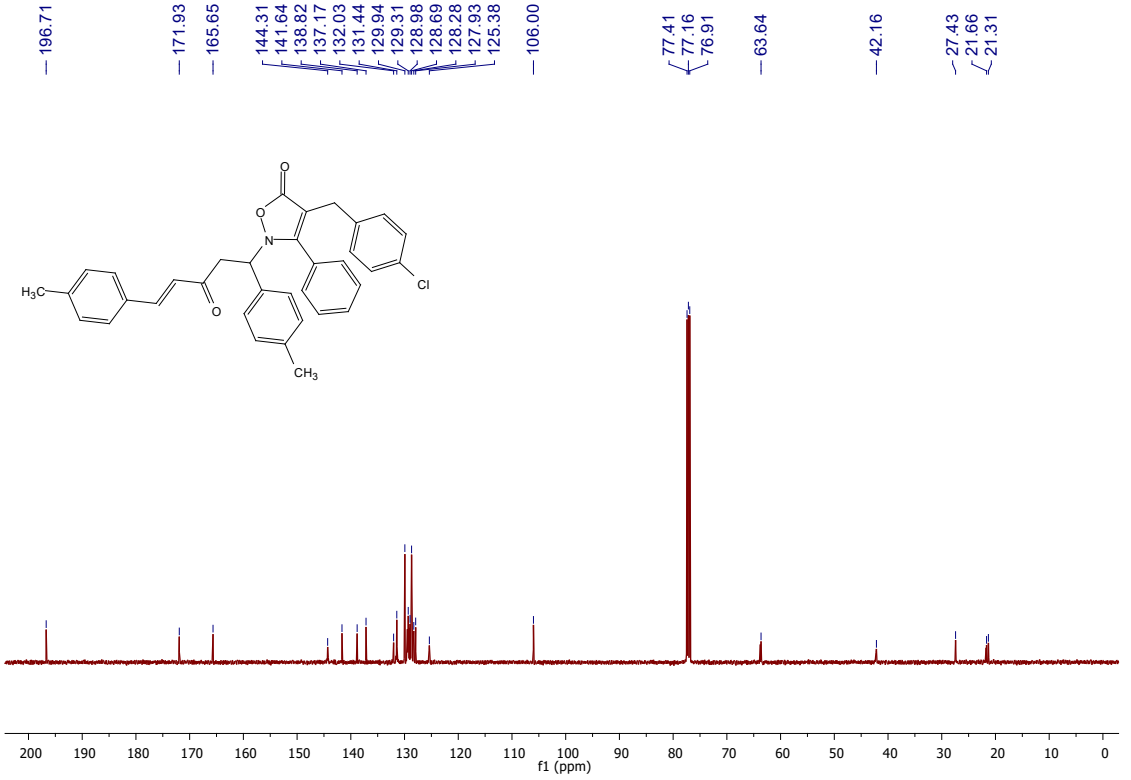


Figure S70. IR (ATR) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3k).

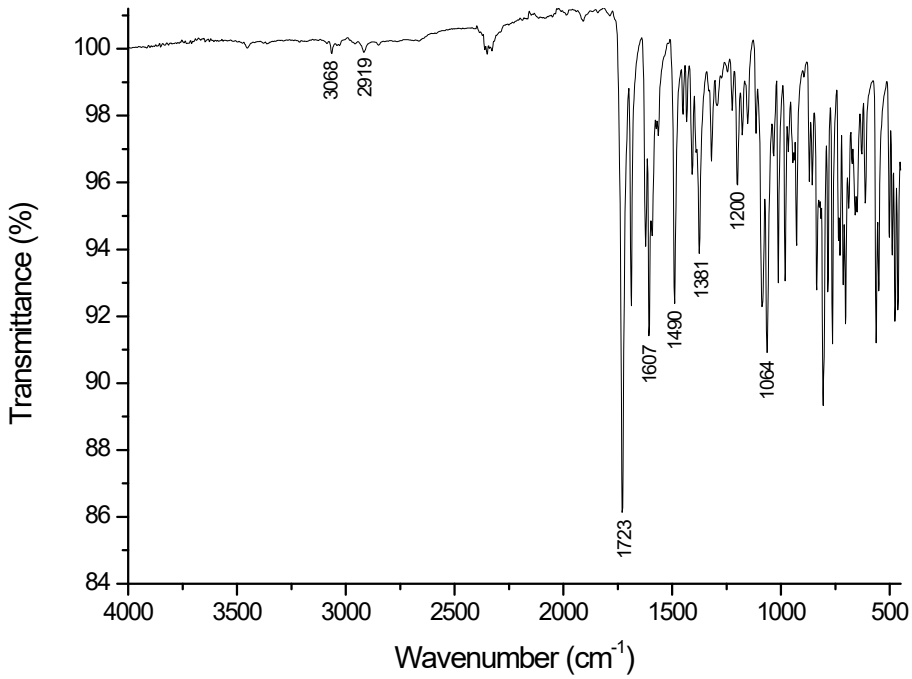


Figure S71. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3k).

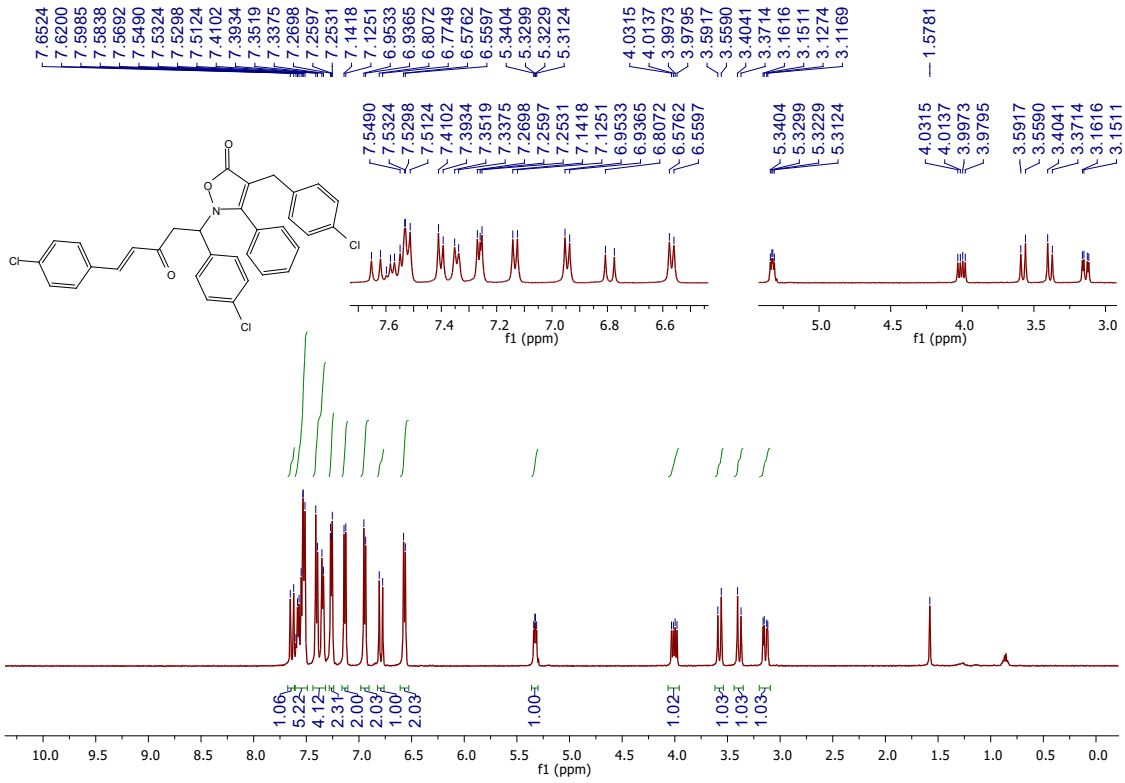


Figure S72. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(4-chlorobenzyl)-3-phenylisoxazol-5(2H)-one* (3k).

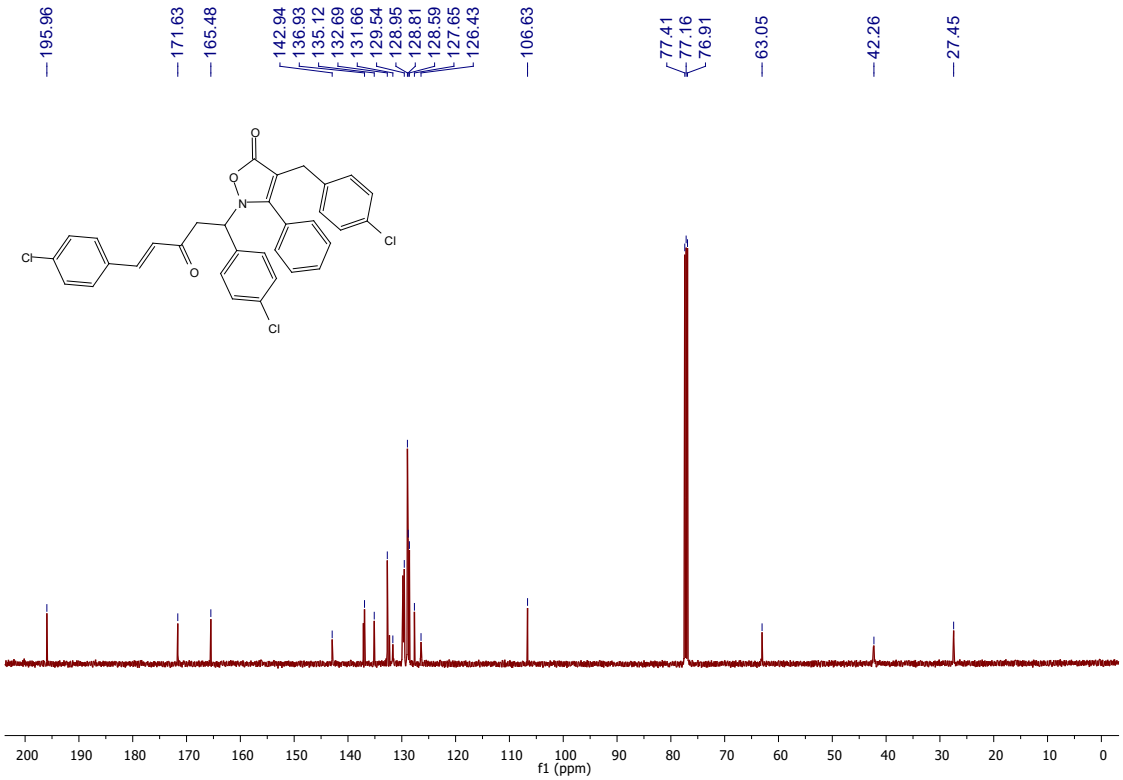


Figure S73. FT-IR (NaCl) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3l).

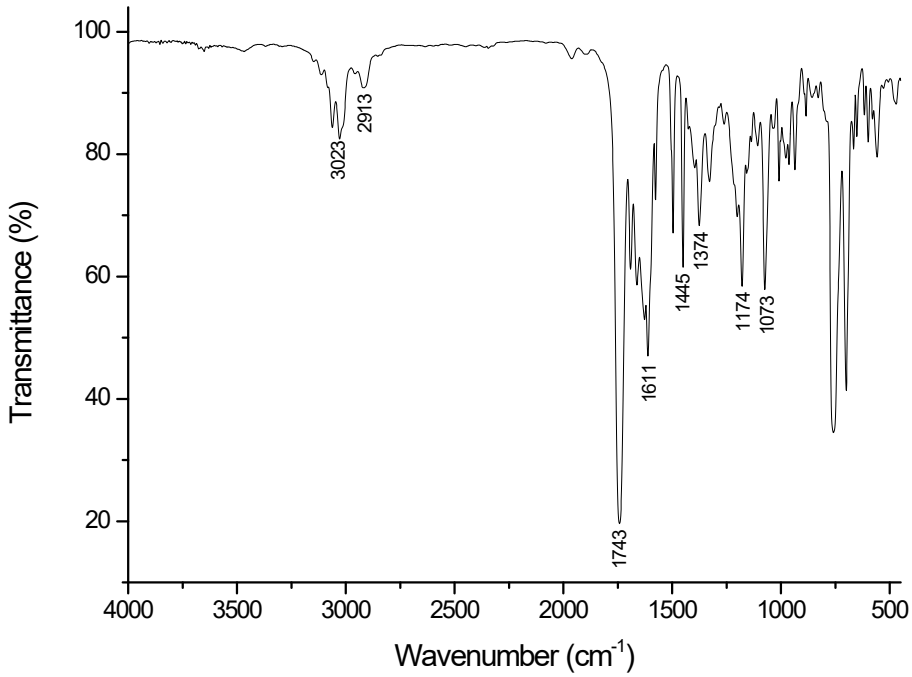


Figure S74. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3l).

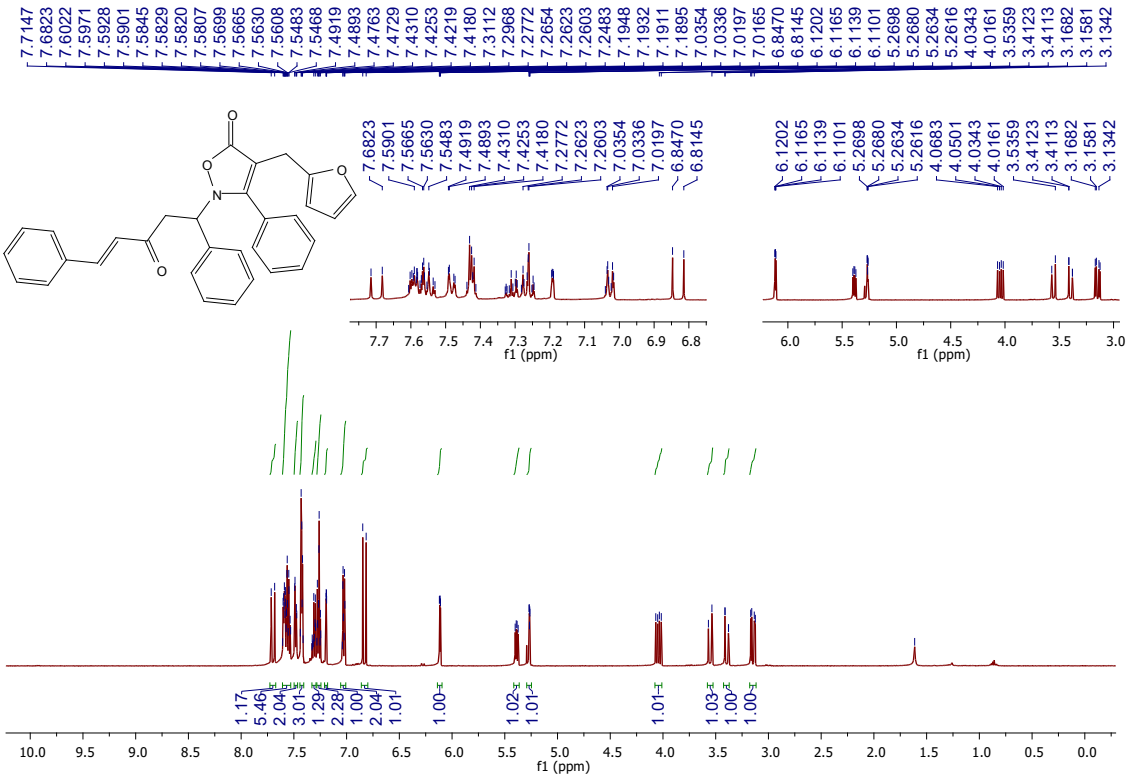


Figure S75. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3l).

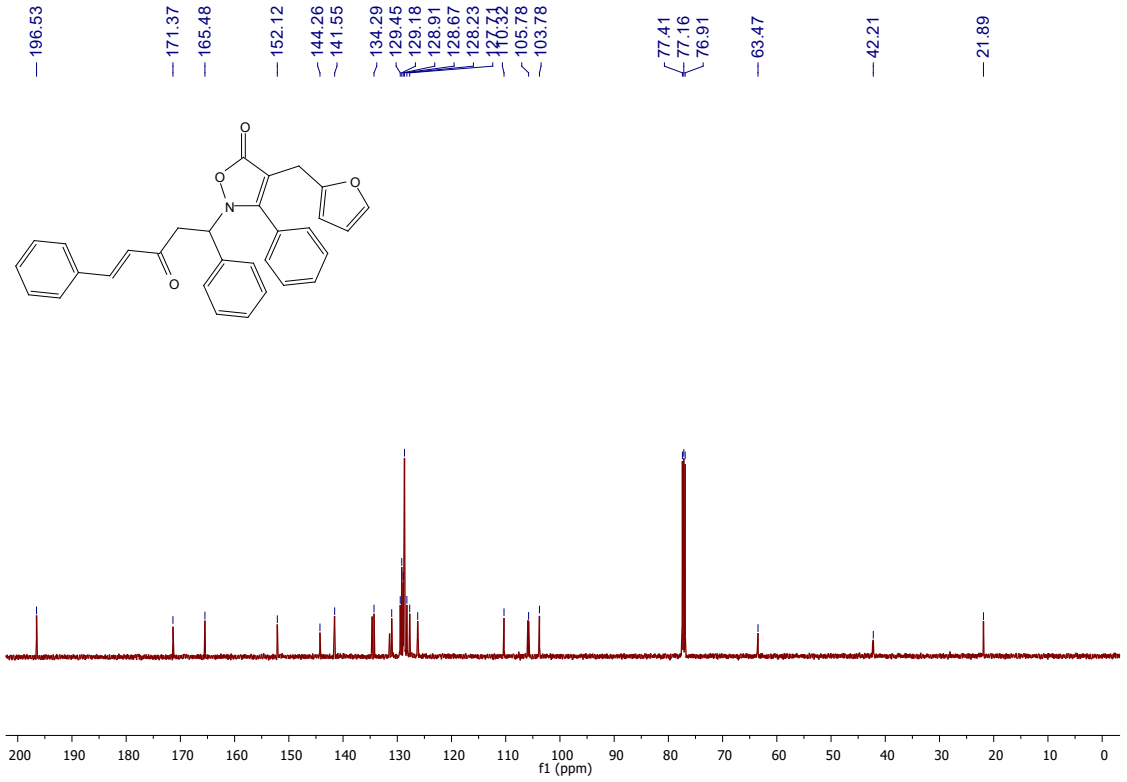


Figure S76. FT-IR (NaCl) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3m).

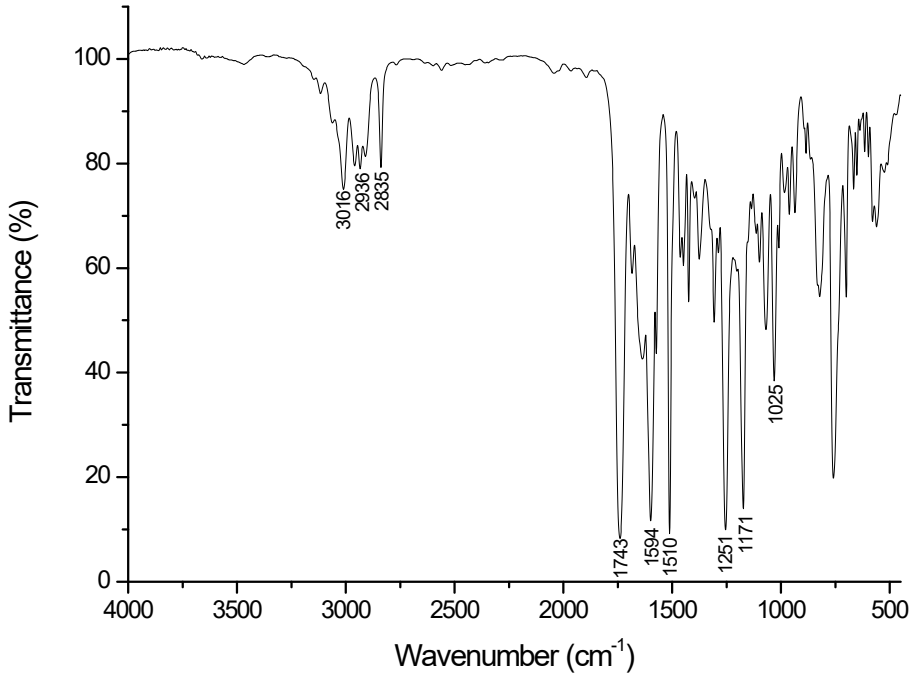


Figure S77. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3m).

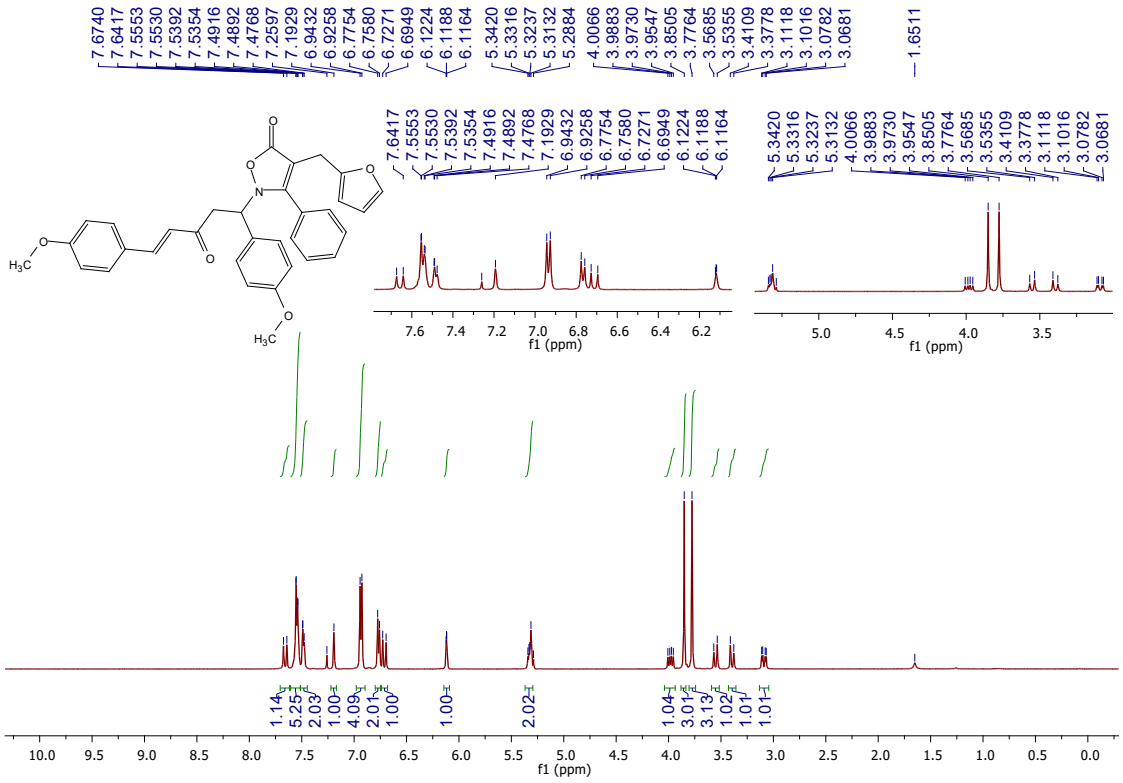


Figure S78. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-methoxyphenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3m).

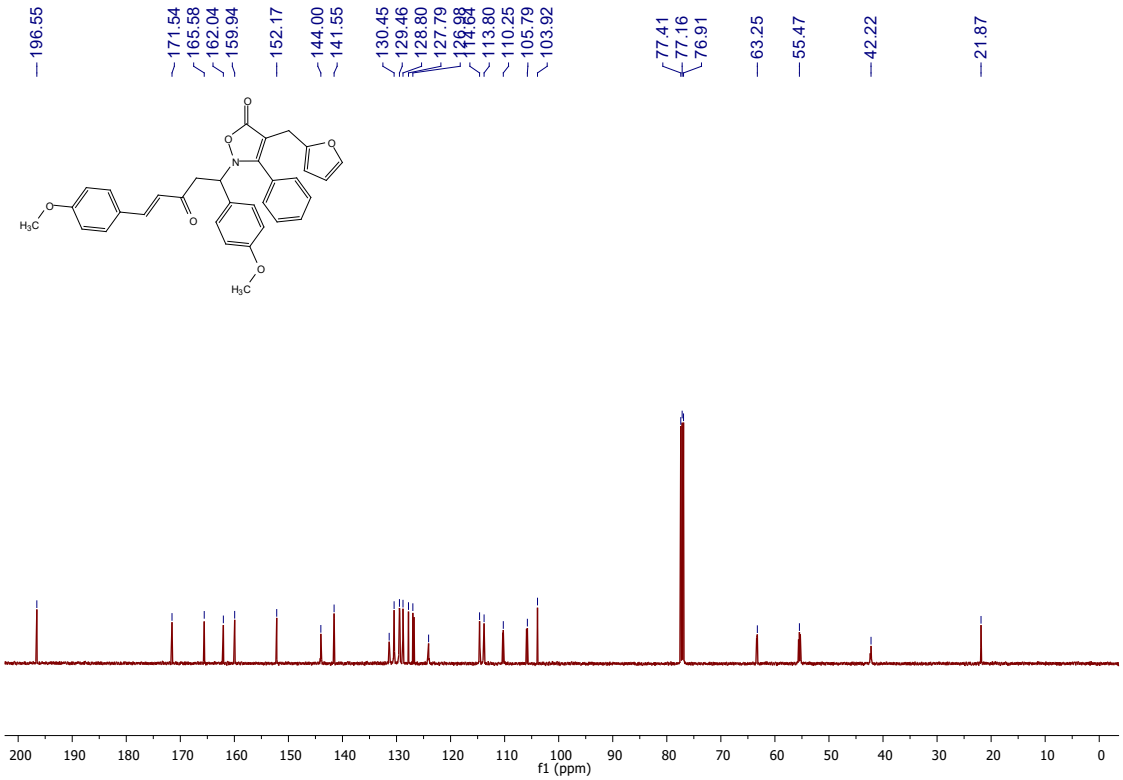


Figure S79. FT-IR (NaCl) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3n).

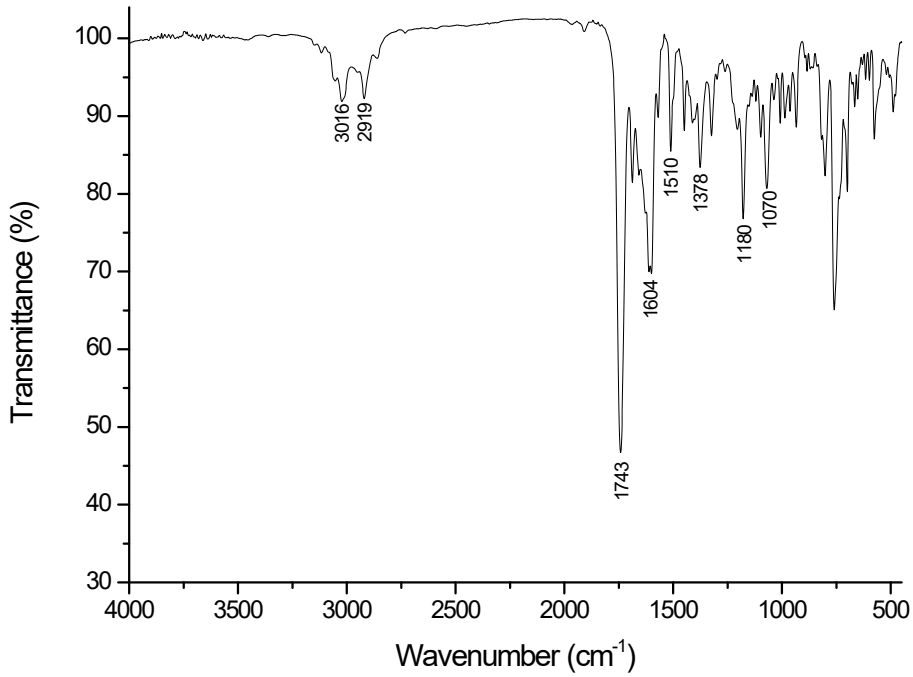


Figure S80. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3n).

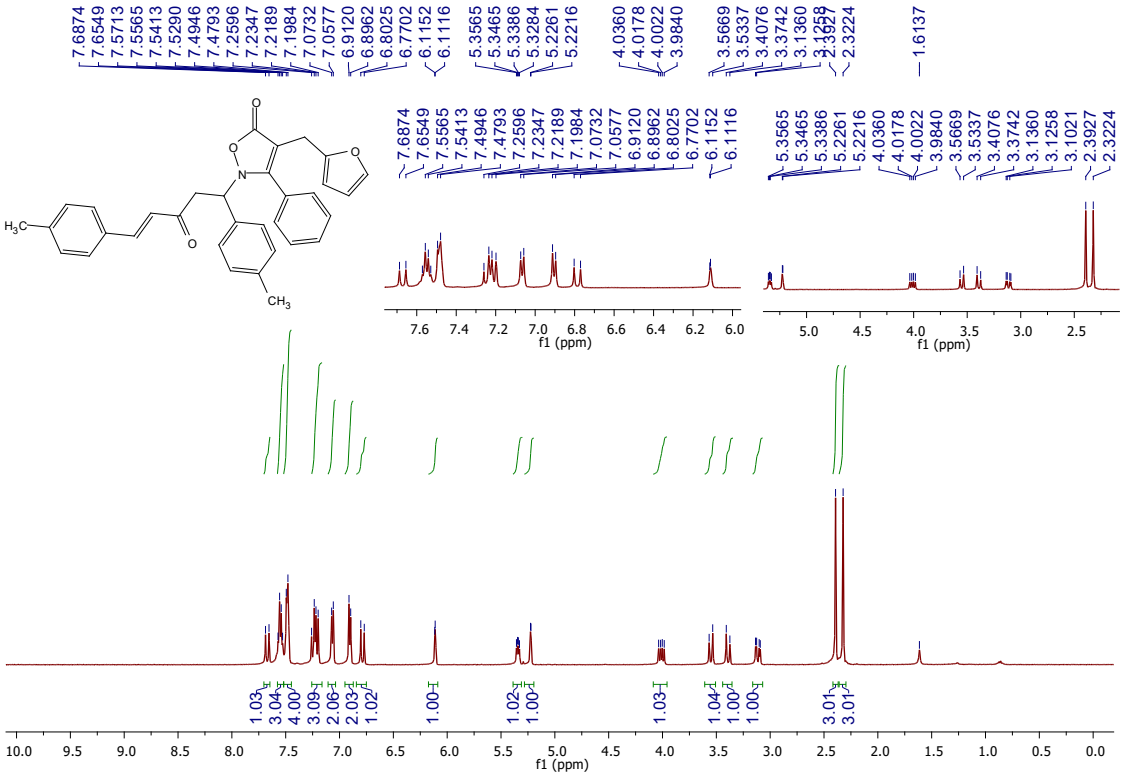


Figure S81. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-(furan-2-ylmethyl)-2-(3-oxo-1,5-di-p-tolylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one* (3n).

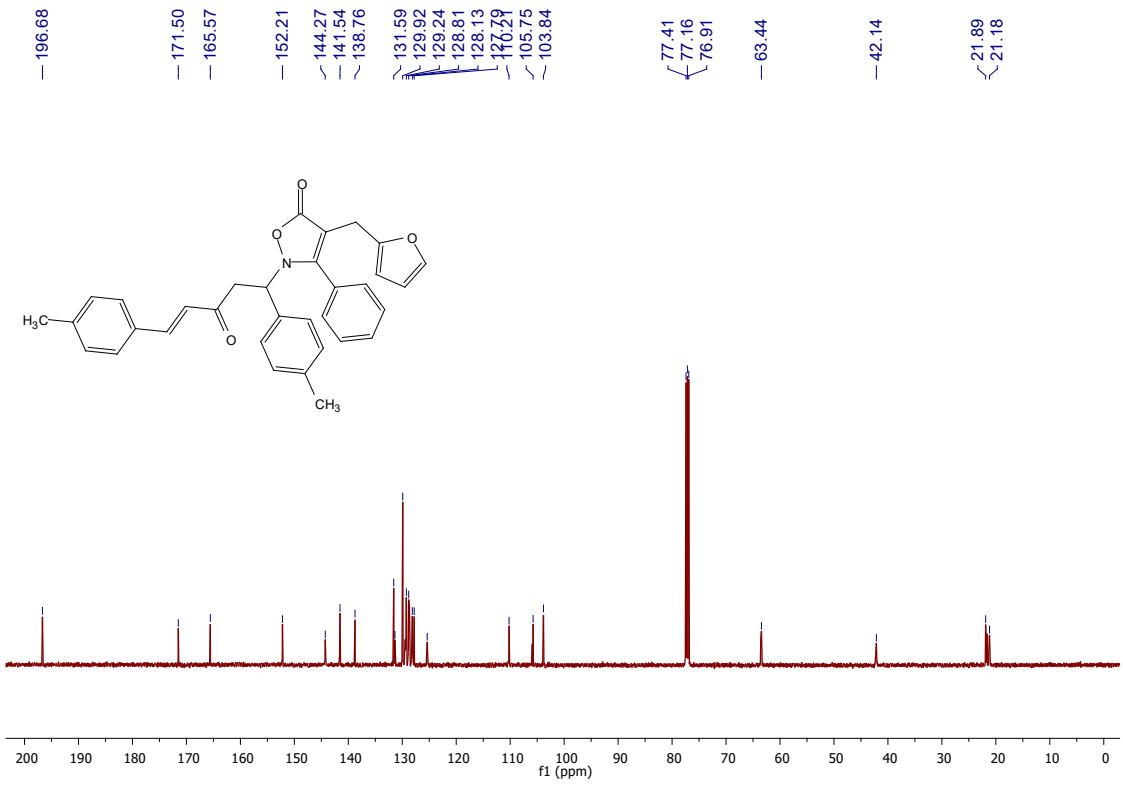


Figure S82. IR (ATR) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3o).

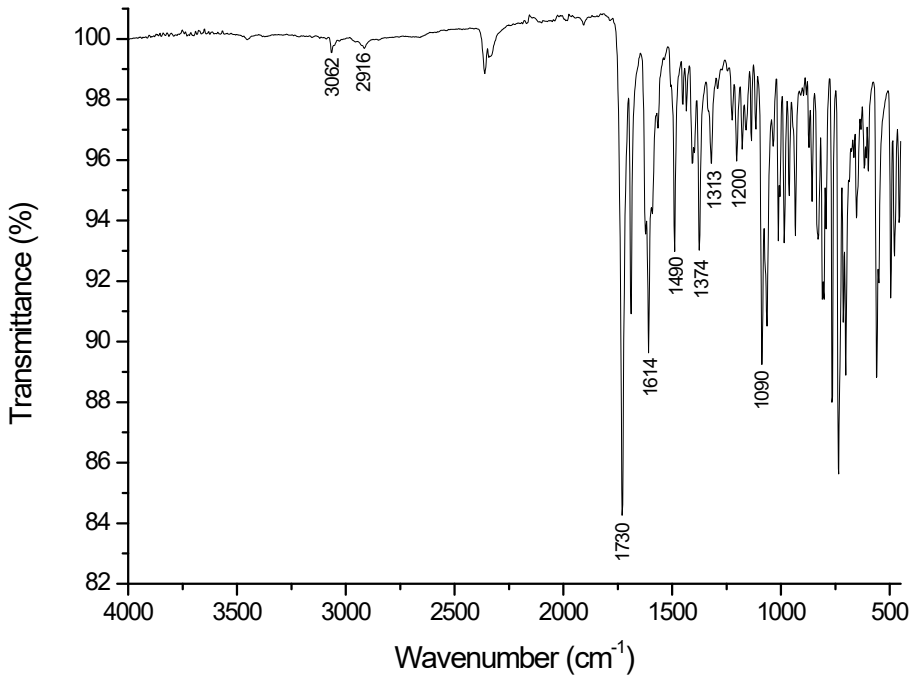


Figure S83. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3o).

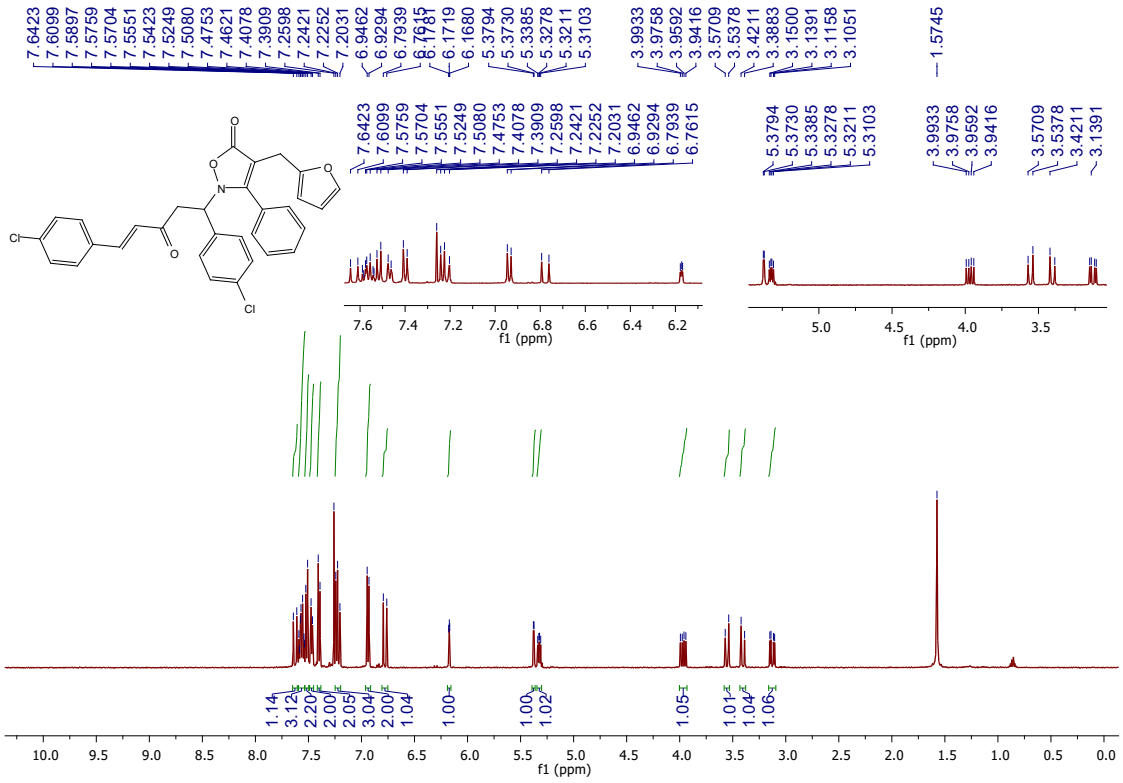


Figure S84. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-2-(1,5-bis(4-chlorophenyl)-3-oxopent-4-en-1-yl)-4-(furan-2-ylmethyl)-3-phenylisoxazol-5(2H)-one* (3o).

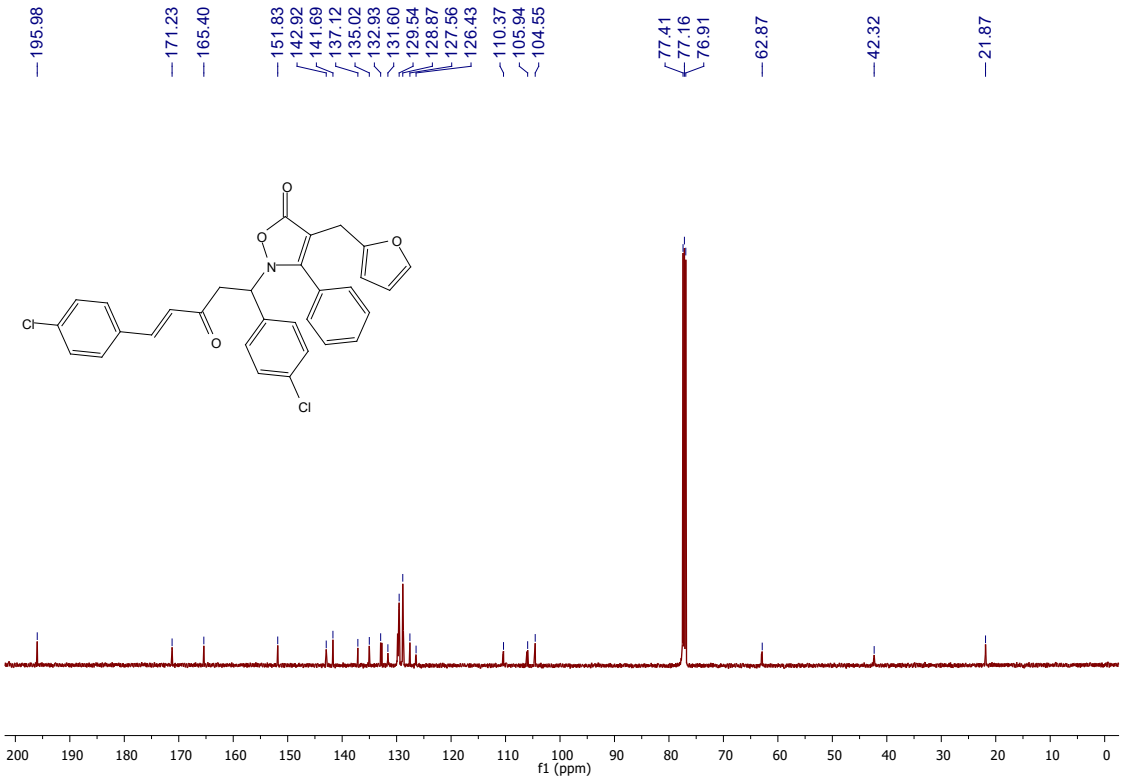


Figure S85. IR (ATR) of *4-benzyl-2-(3-oxocyclohexyl)-3-phenylisoxazol-5(2H)-one* (3p).

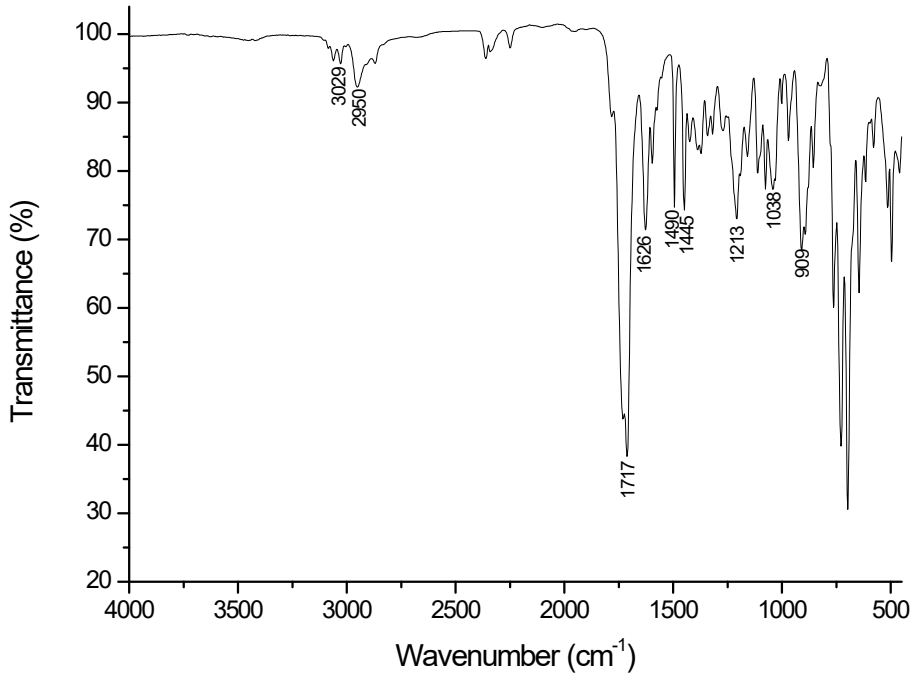


Figure S86. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxocyclohexyl)-3-phenylisoxazol-5(2H)-one* (3p).

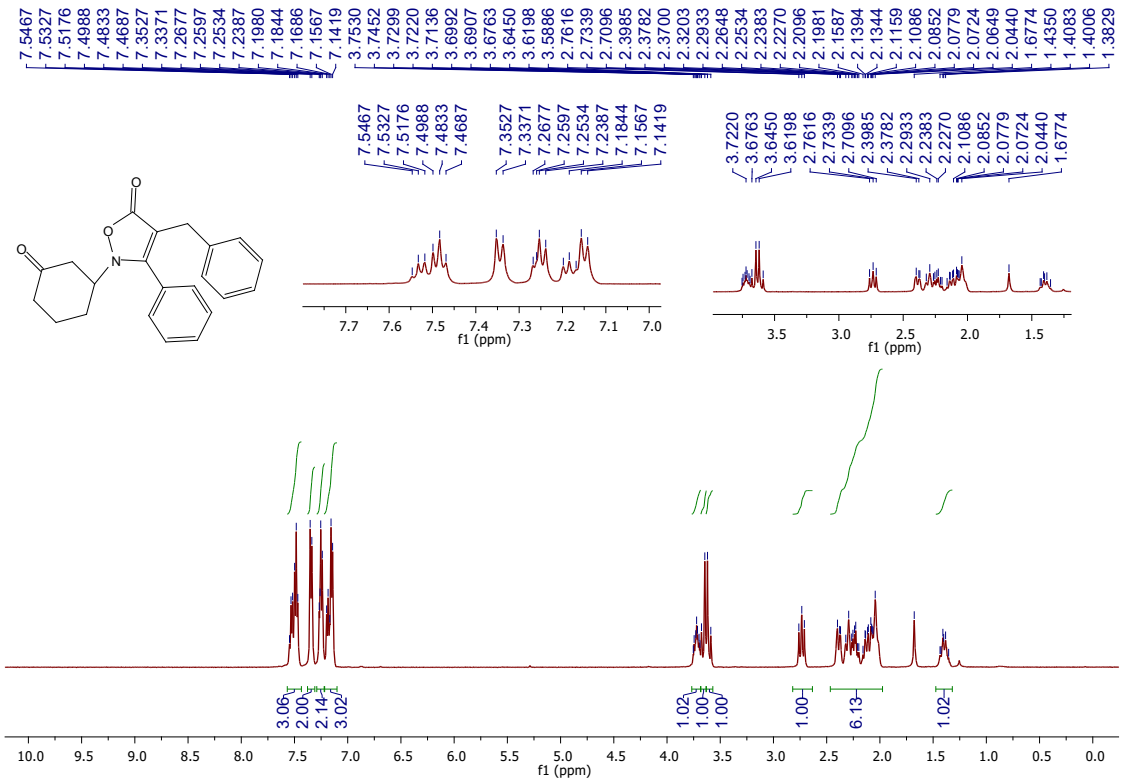


Figure S87. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxocyclohexyl)-3-phenylisoxazol-5(2H)-one* (3p).

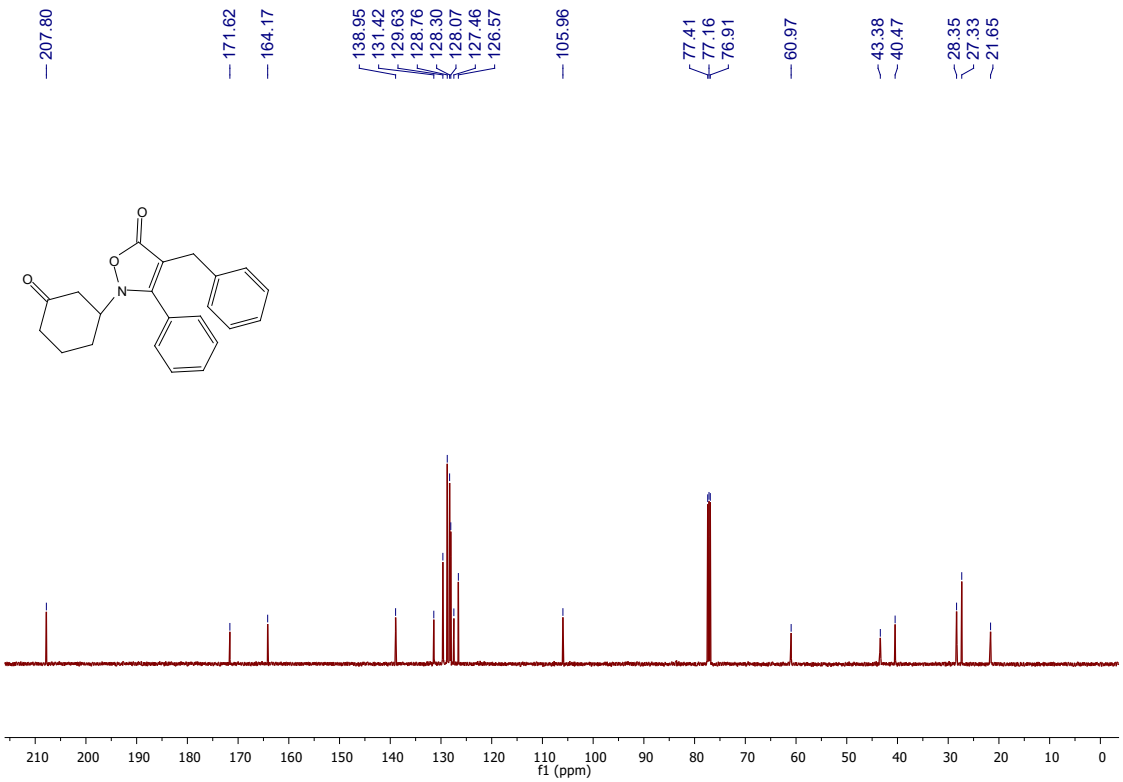


Figure S88. IR (ATR) of *4-benzyl-2-(3-oxobutyl)-3-phenylisoxazol-5(2H)-one* (3q).

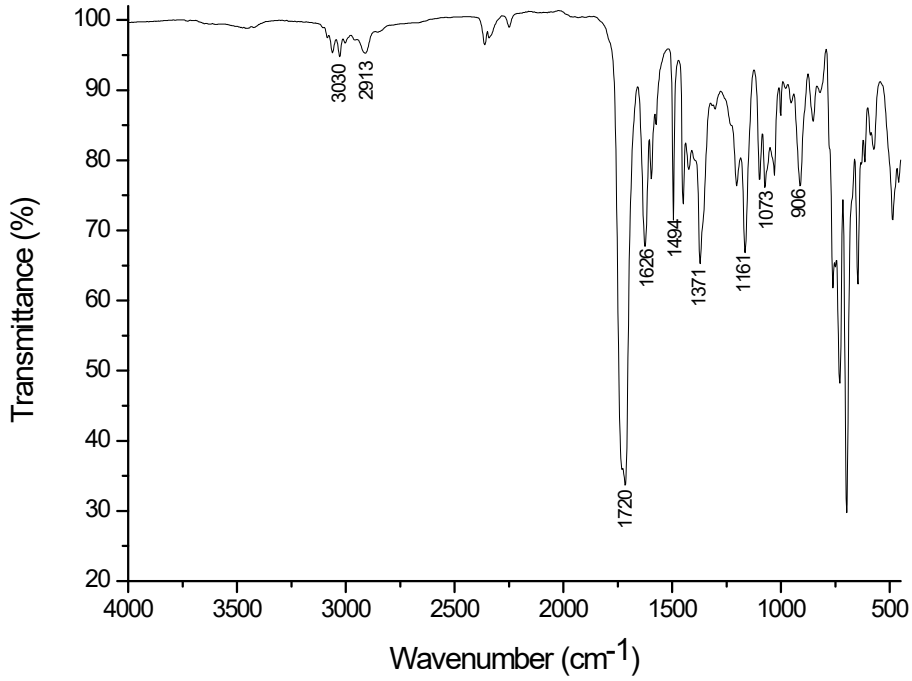


Figure S89. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxobutyl)-3-phenylisoxazol-5(2H)-one* (3q).

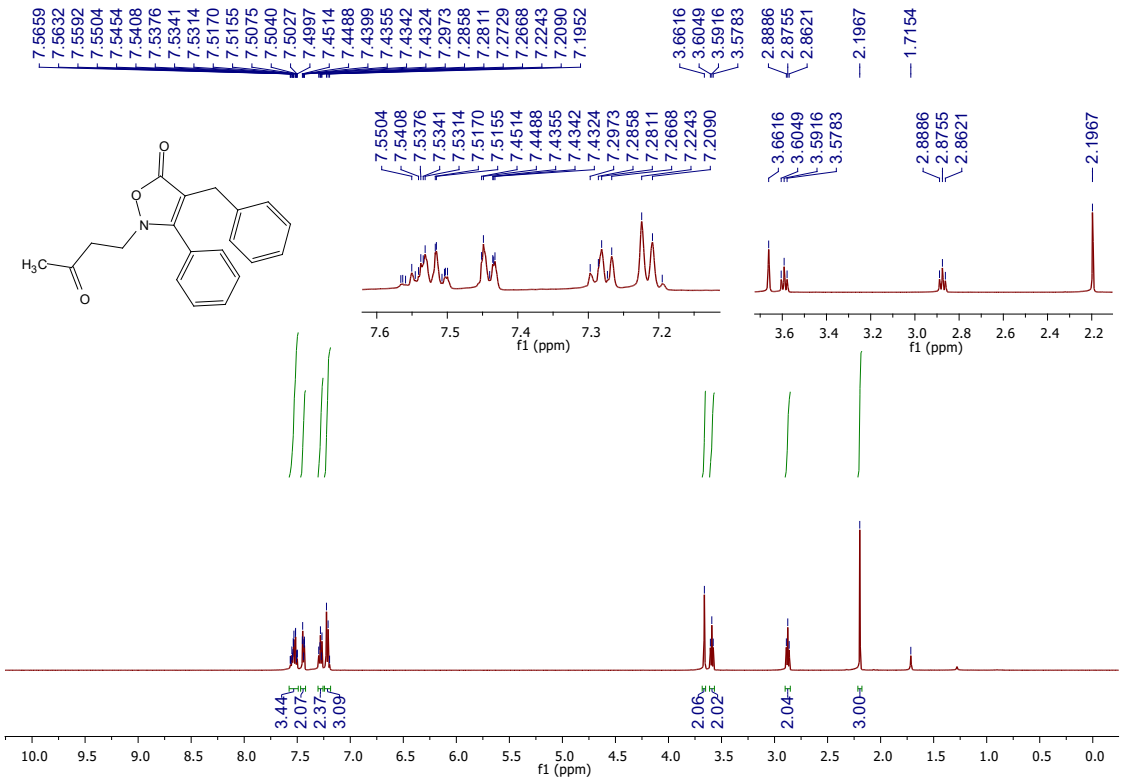


Figure S90. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxobutyl)-3-phenylisoxazol-5(2H)-one* (3q).

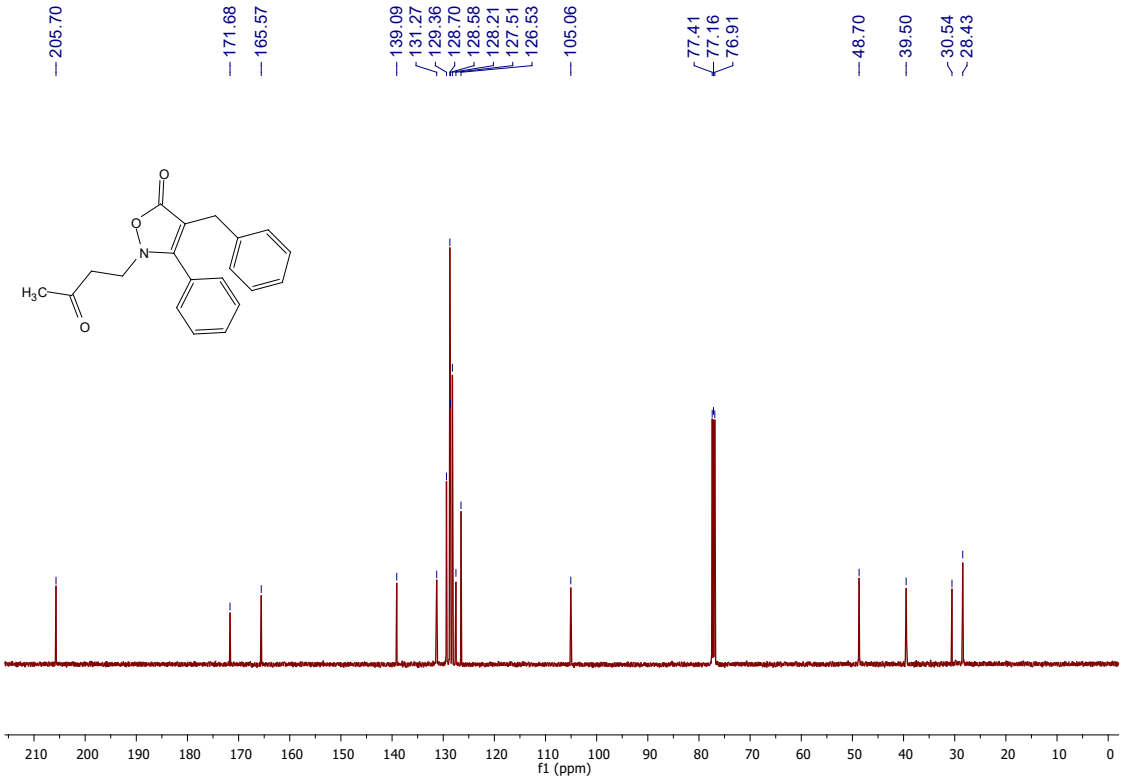


Figure S91. IR (ATR) of *4-benzyl-2-(3-oxo-1,3-diphenylpropyl)-3-phenylisoxazol-5(2H)-one* (3r).

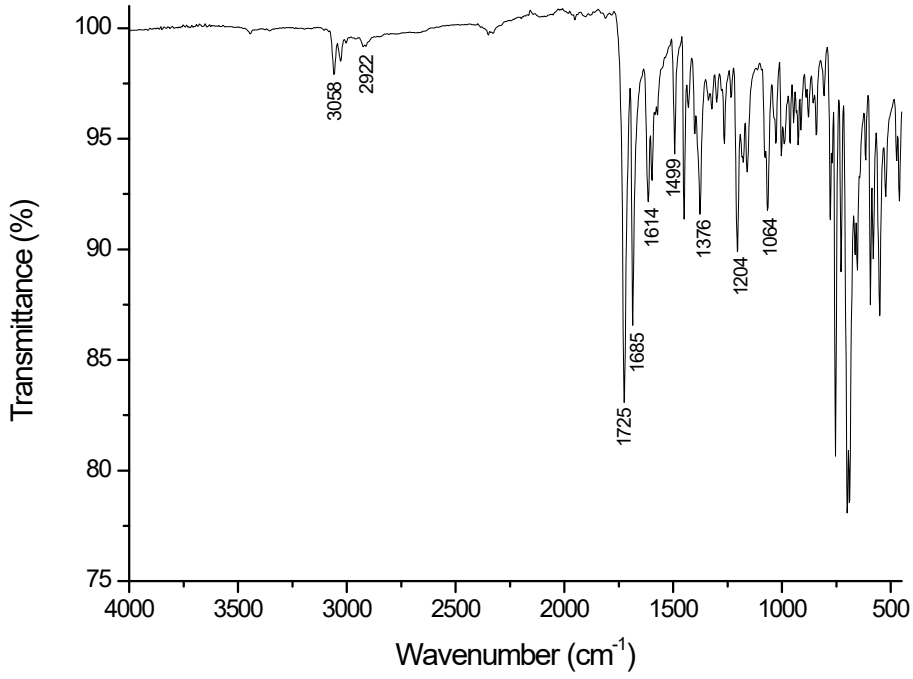


Figure S92. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxo-1,3-diphenylpropyl)-3-phenylisoxazol-5(2H)-one* (3r).

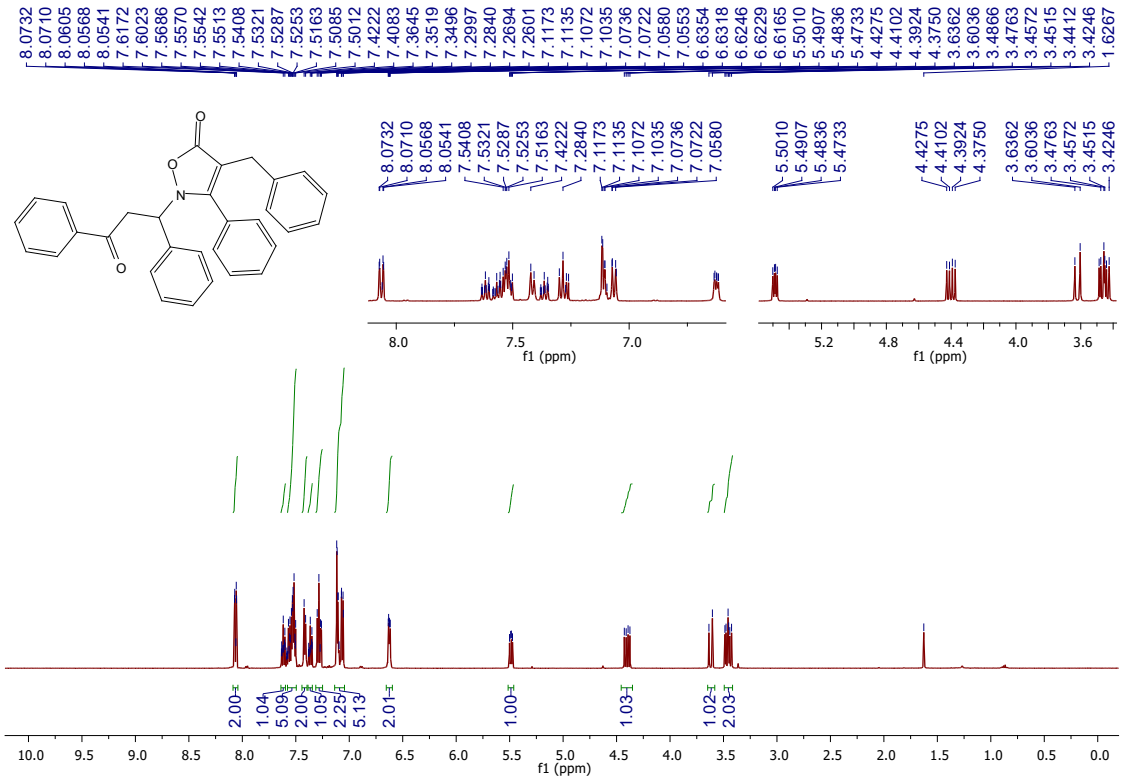


Figure S93. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxo-1,3-diphenylpropyl)-3-phenylisoxazol-5(2H)-one* (3r).

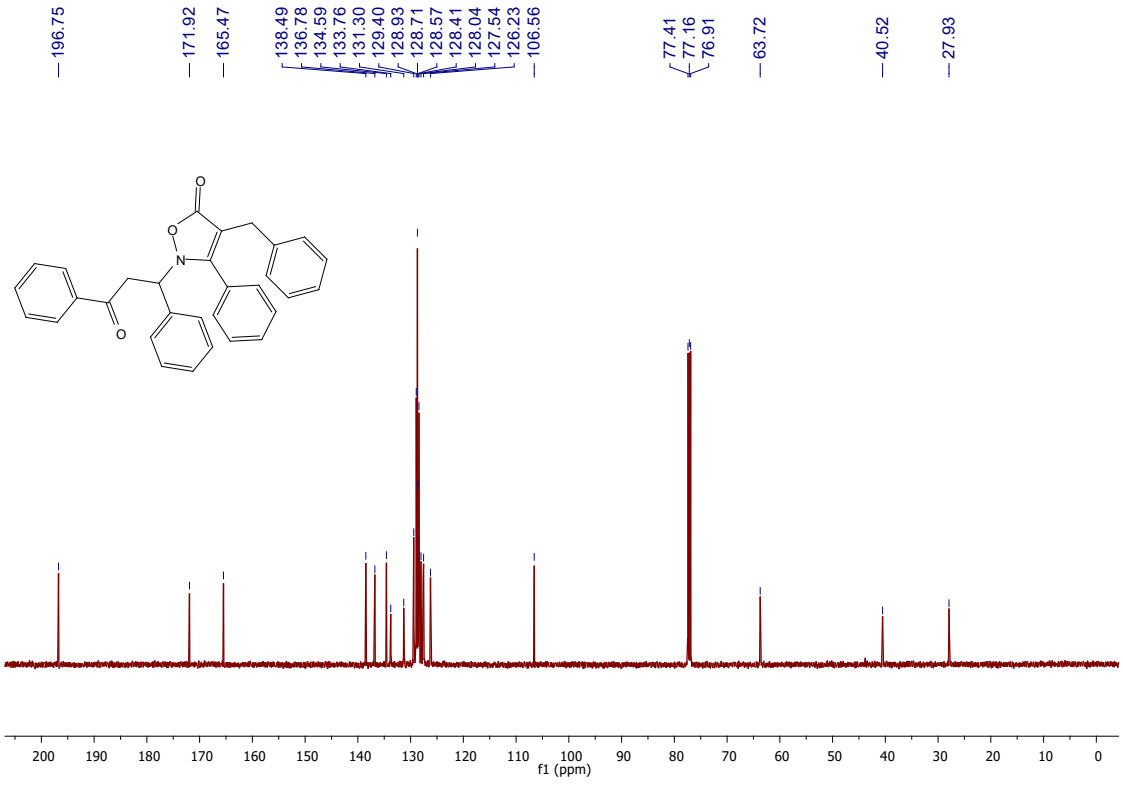


Figure S94. IR (ATR) of *4-benzyl-2-(1-(4-chlorophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3s).

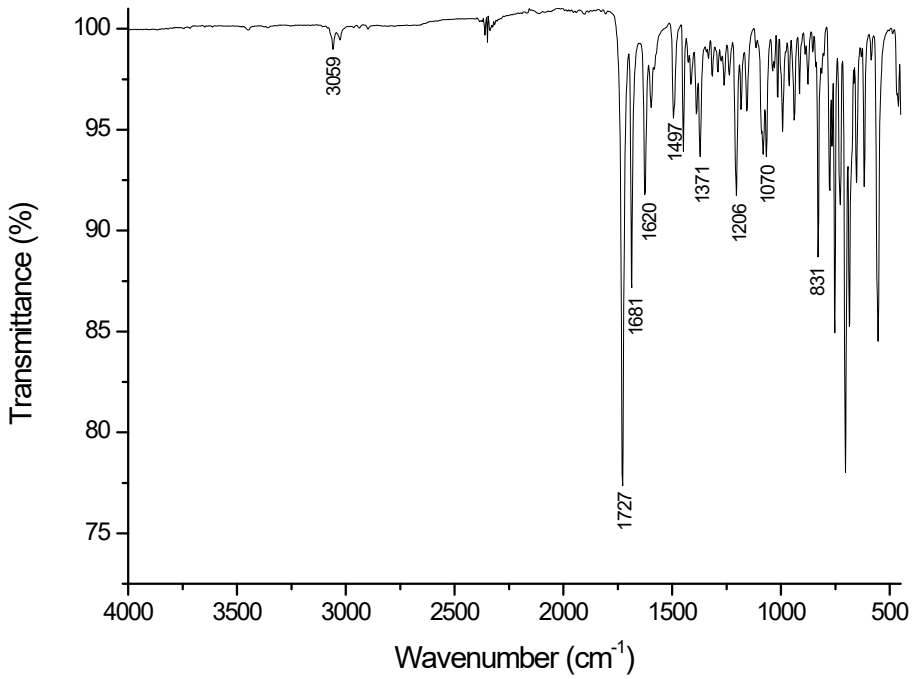


Figure S95. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(1-(4-chlorophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3s).

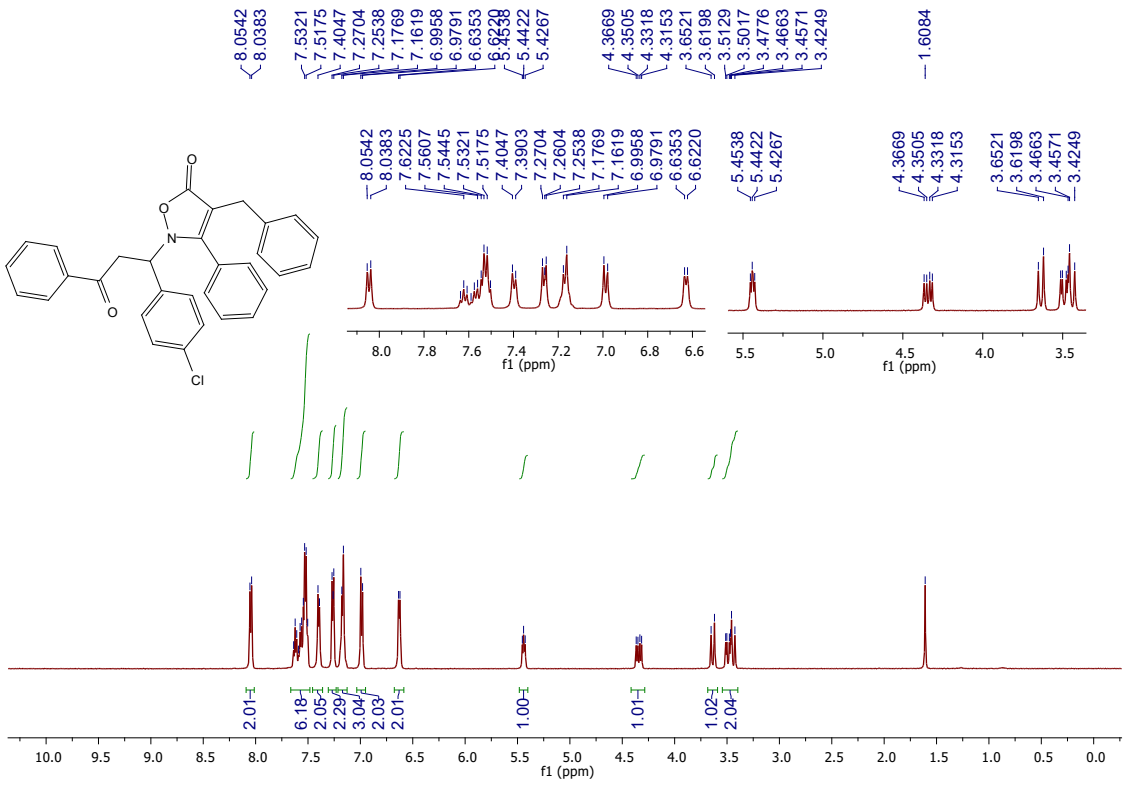


Figure S96. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(1-(4-chlorophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3s).

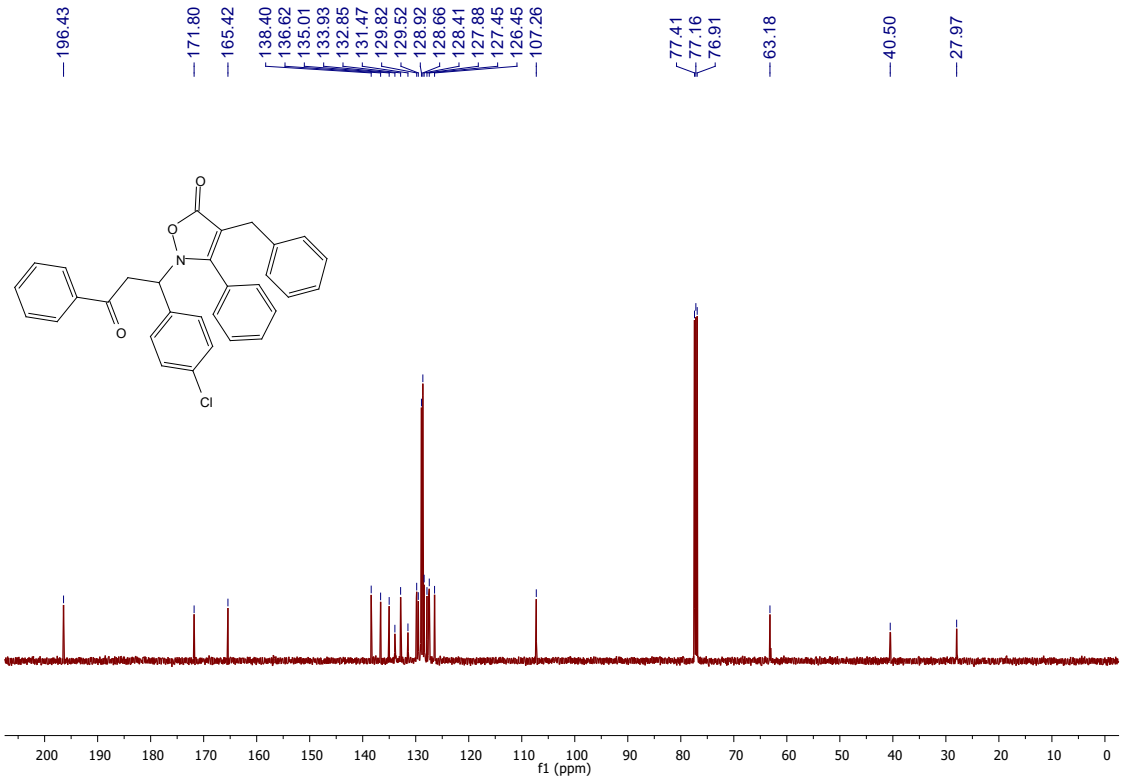


Figure S97. IR (ATR) of *4-benzyl-2-(3-oxo-3-phenyl-1-(p-tolyl)propyl)-3-phenylisoxazol-5(2H)-one* (3t).

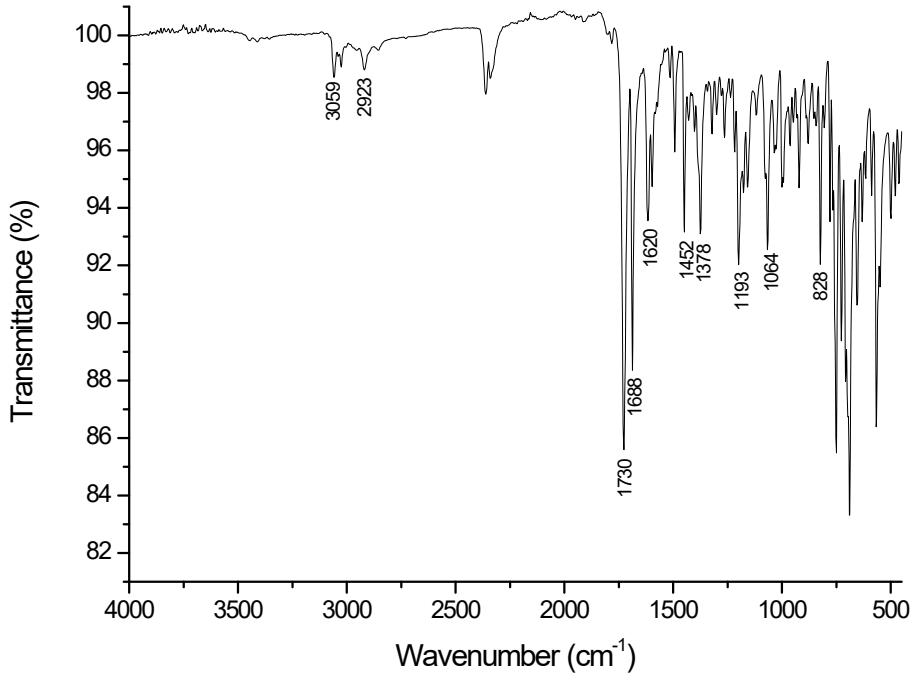


Figure S98. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxo-3-phenyl-1-(p-tolyl)propyl)-3-phenylisoxazol-5(2H)-one* (3t).

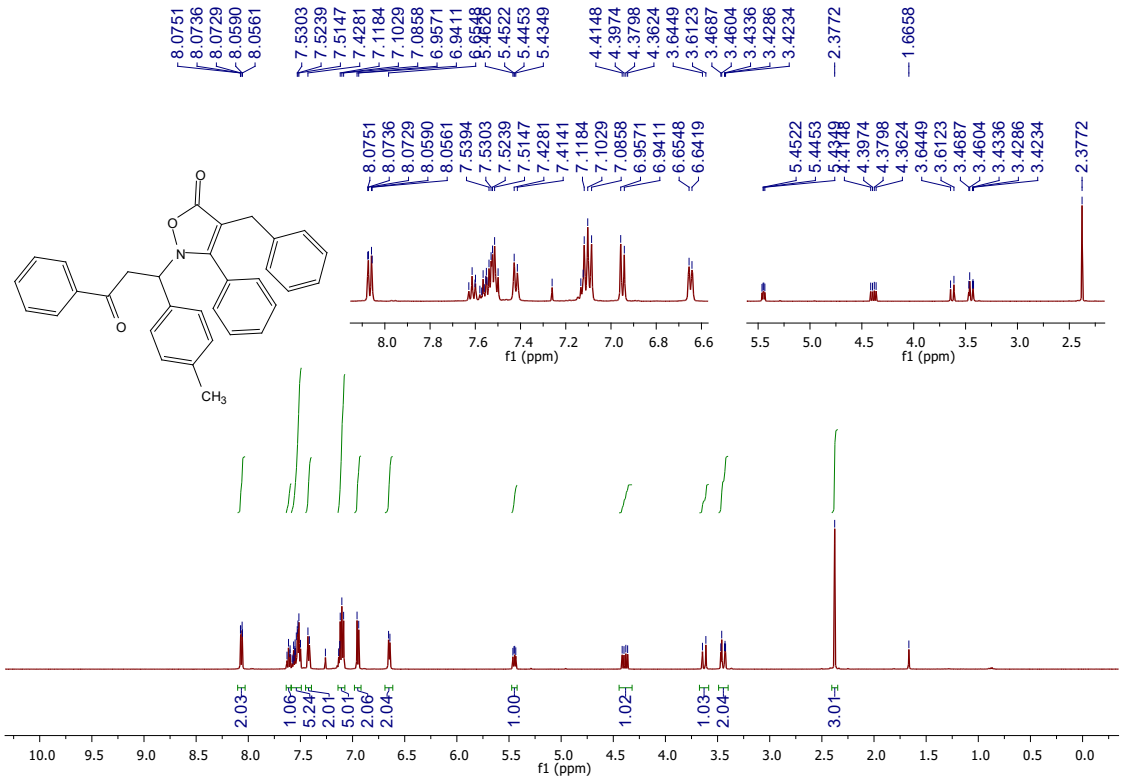


Figure S99. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(3-oxo-3-phenyl-1-(p-tolyl)propyl)-3-phenylisoxazol-5(2H)-one* (3t).

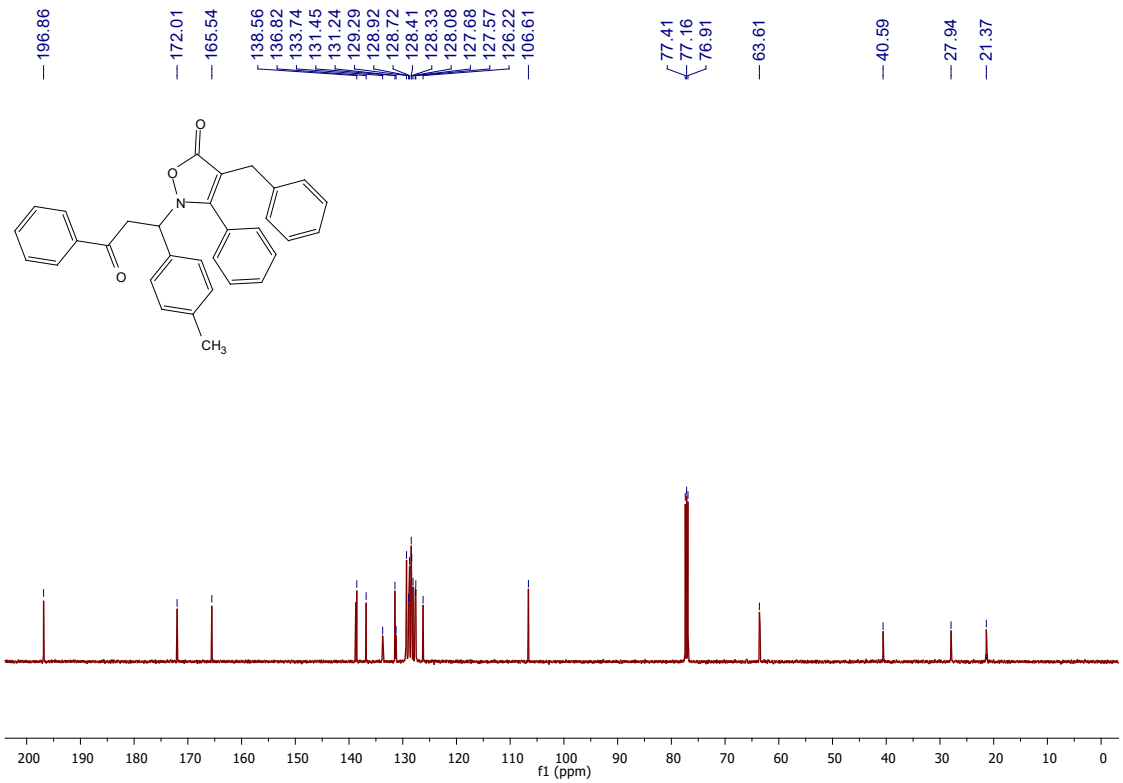


Figure S100. IR (ATR) of *4-benzyl-2-(1-(4-bromophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3u).

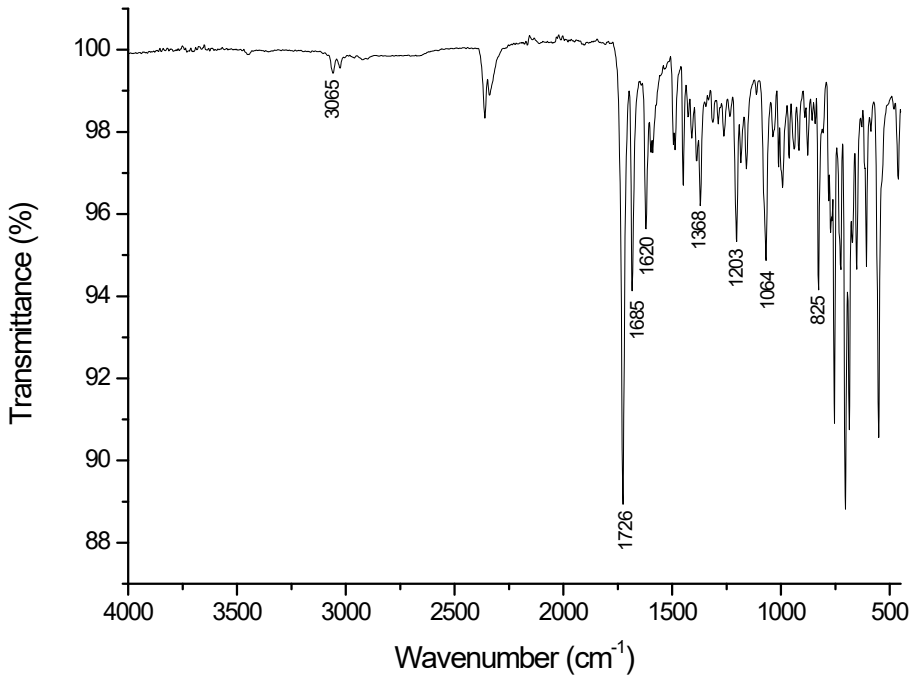


Figure S101. ^{1}H NMR (500 MHz, $CDCl_3$) of *4-benzyl-2-(1-(4-bromophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3u).

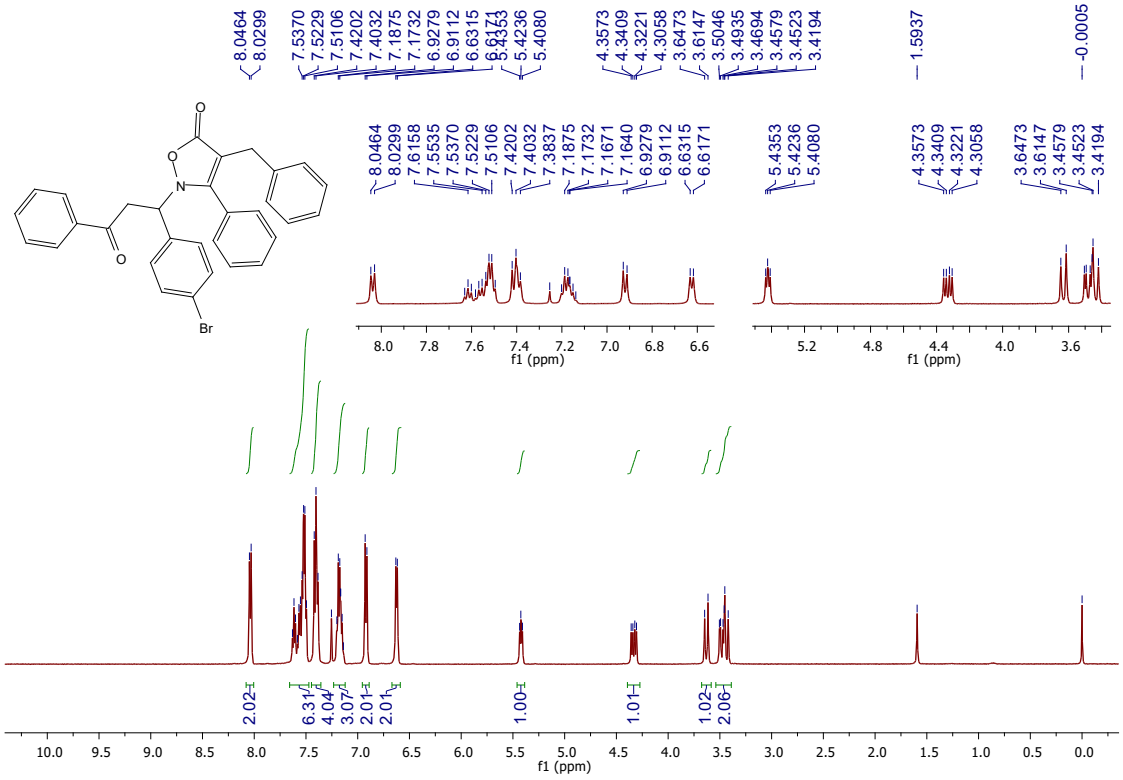


Figure S102. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *4-benzyl-2-(1-(4-bromophenyl)-3-oxo-3-phenylpropyl)-3-phenylisoxazol-5(2H)-one* (3u).

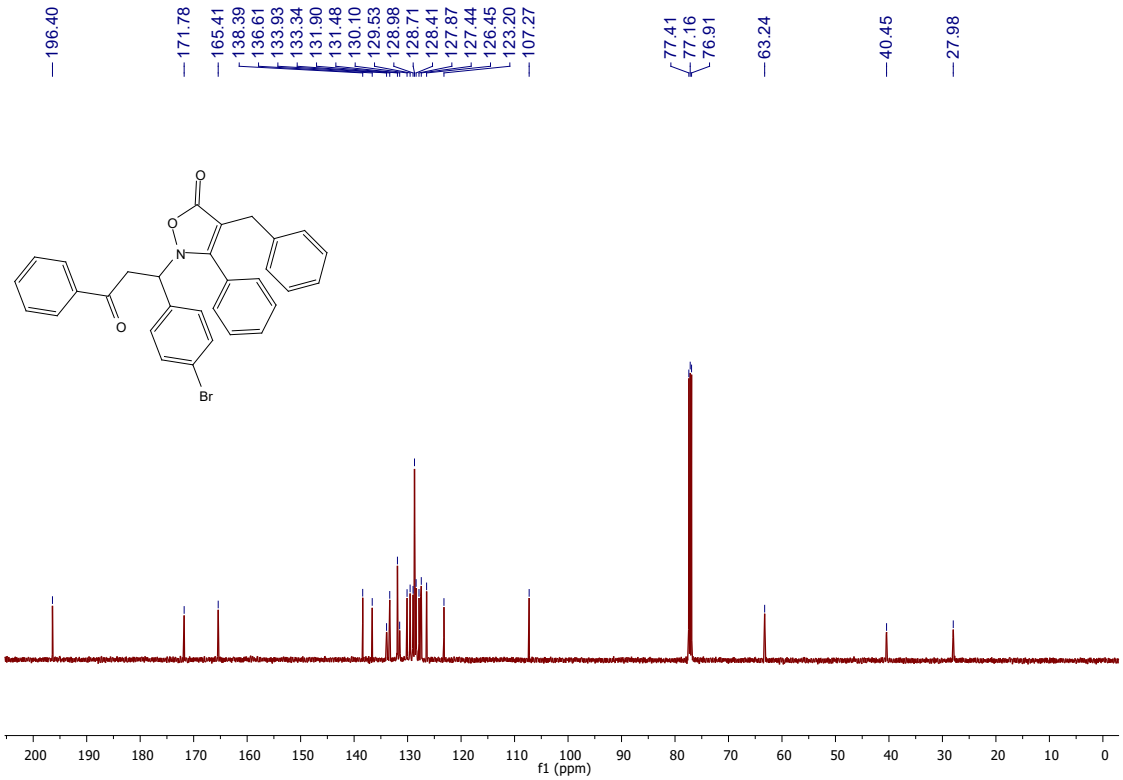


Figure S103. IR (ATR) of *(E)-4-benzyl-2-(3-hydroxy-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one (4a).*

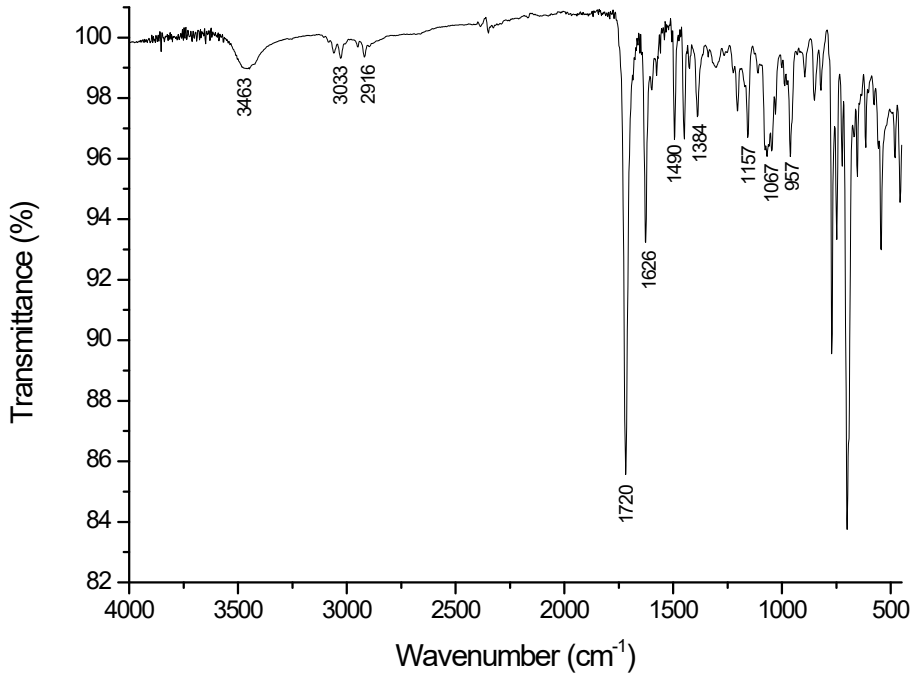


Figure S104. ^{1}H NMR (500 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-hydroxy-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one (4a).*

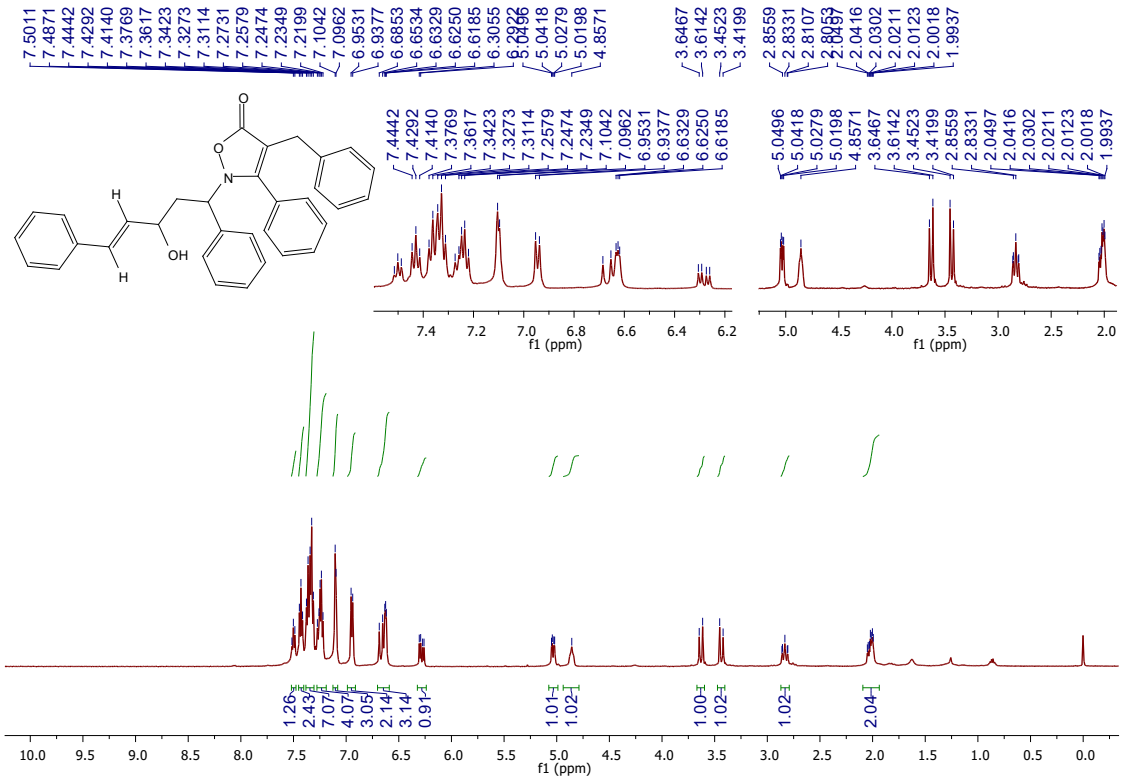
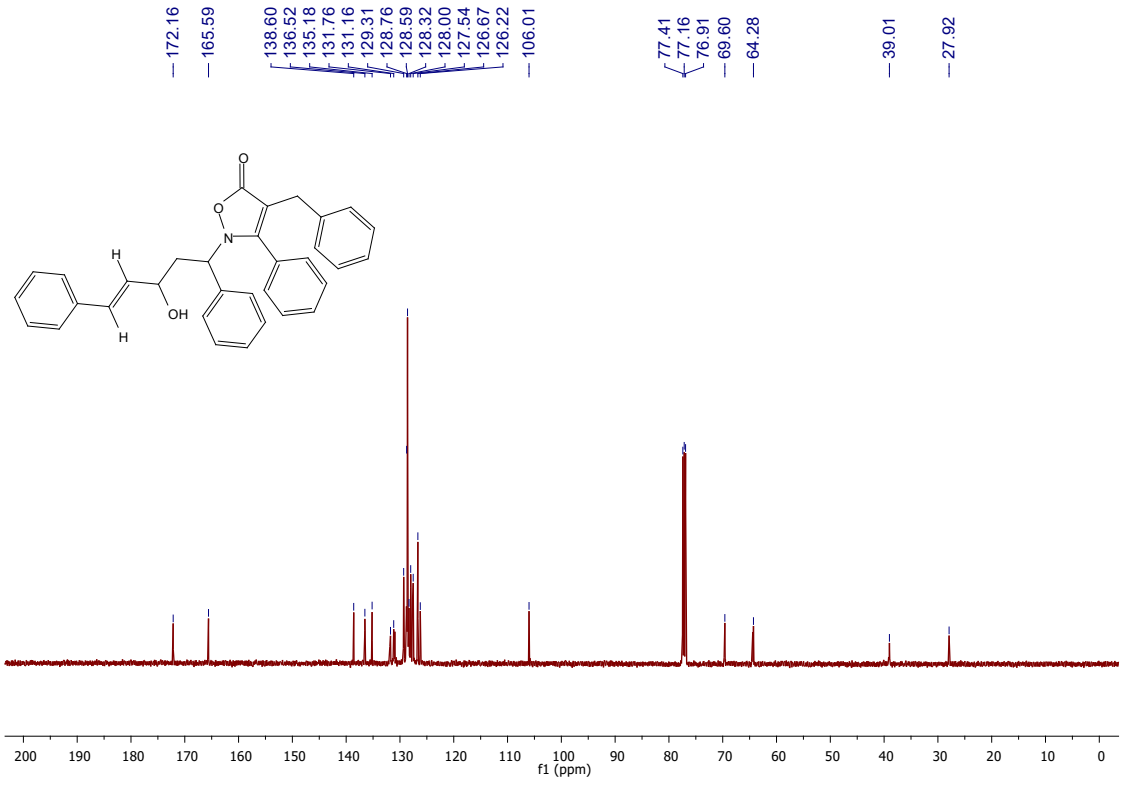


Figure S105. ^{13}C {1H} NMR (125 MHz, $CDCl_3$) of *(E)-4-benzyl-2-(3-hydroxy-1,5-diphenylpent-4-en-1-yl)-3-phenylisoxazol-5(2H)-one (4a).*



3. X-ray measurement

Single crystals of $C_{33}H_{27}NO_3$ (CCDC 2226174) were crystallized by multisolvent crystallization using a mixture of dichloromethane and hexanes as solvent. The compound (approximately 100 mg) was transferred to a 25 mL Erlenmeyer and added 5 mL of dichloromethane so that the whole sample was diluted then 15 mL of Hexane was added. The mixture was kept at room temperature for several days until small white crystals appeared. A suitable crystal was selected and mounted on a SuperNova, Dual, Cu at home/near, AtlasS2 diffractometer. The crystal was kept at 291.0(5) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimization.

[1] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
[2] Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
[3] Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination

Crystal Data for $C_{33}H_{27}NO_3$ (M = 485.55 g/mol): triclinic, space group P-1 (no. 2), a = 9.7053(4) Å, b = 9.7576(5) Å, c = 15.0112(6) Å, α = 86.996(4)°, β = 76.122(3)°, γ = 70.408(4)°, V = 1299.56(11)Å^3, Z = 2, T = 291.0(5) K, μ(Cu Kα) = 0.626 mm-1, D_{calc} = 1.241 g/cm^3, 8341 reflections measured (9.626° ≤ 2Θ ≤ 135.144°), 4686 unique (R_{int} = 0.0395, R_{sigma} = 0.0385) which were used in all calculations. The final R_1 was 0.0643 (I > 2σ(I)) and wR_2 was 0.2092 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1 Fixed Uiso

At 1.2 times of: All C(H) and C(H,H) groups

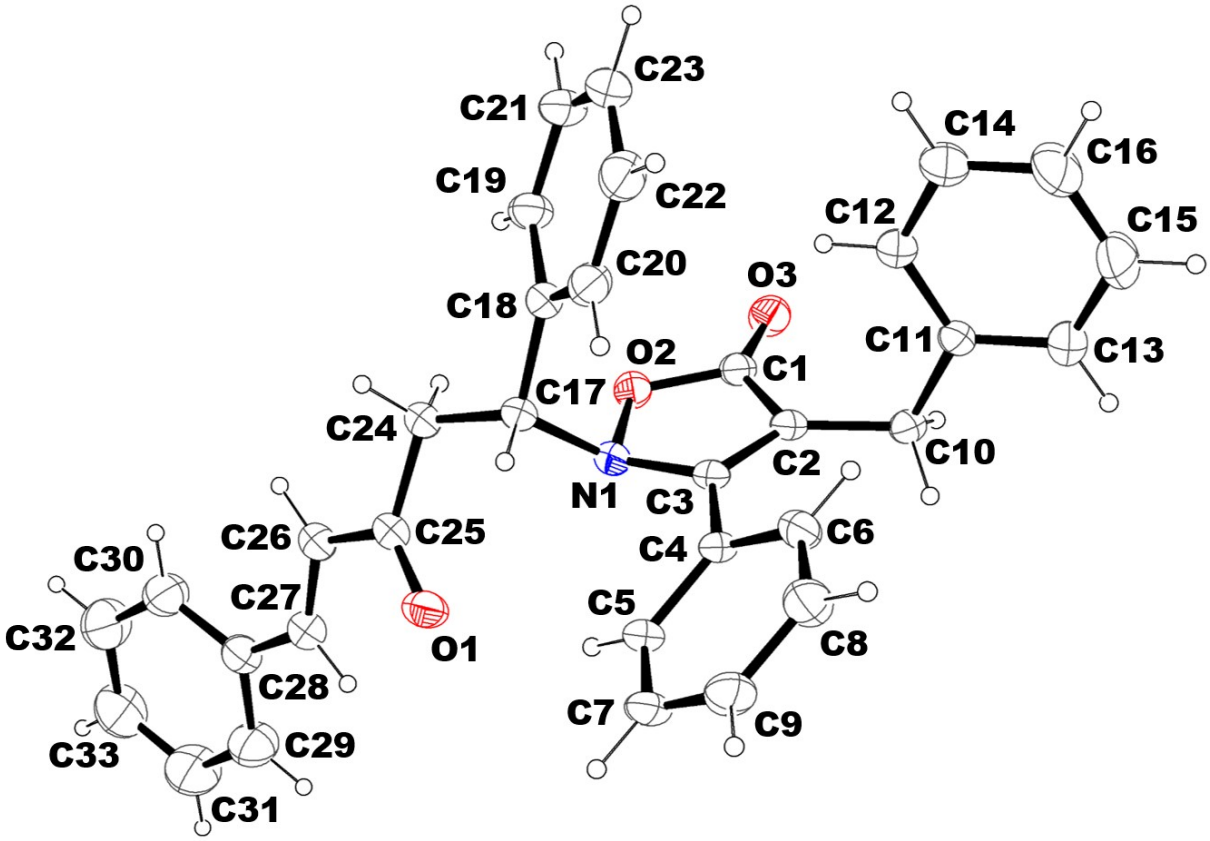
At 1.5 times of: All O(H) groups, All O(H,H) groups

2.a Ternary CH refined with riding coordinates: C17(H17)

2.b Secondary CH2 refined with riding coordinates: C10(H10A,H10B), C24(H24A,H24B)

2.c Aromatic/amide H refined with riding coordinates: C5(H5), C7(H7), C6(H6), C19(H19), C26(H26), C27(H27), C20(H20), C12(H12), C13(H13), C9(H9), C8(H8), C21(H21), C22(H22), C23(H23), C14(H14), C30(H30), C15(H15), C29(H29), C16(H16), C32(H32), C33(H33), C31(H31)

Figure S106. Crystal structure fragment of asymmetric unit for compound 3a. The water molecules crystallized from asymmetric unit were omitted to clarity. Ellipsoids are drawn with 25% with probability.



Diffractometer	SuperNova, Dual, Cu at home/near,
Radiation Source	AtlasS2Cu K_α(λ=1.54184Å)
Data Collection	
Collection Notes	CrysAlisPro 1.171.42.63a (Rigaku OD, 2022)

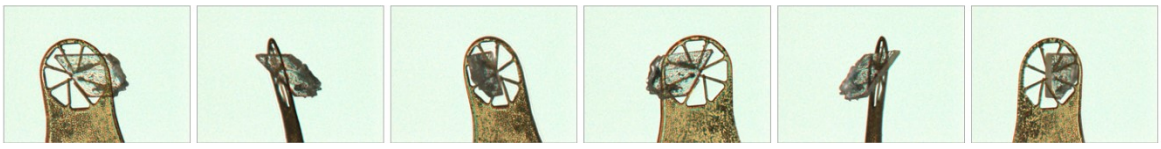


Table S1. Crystal data and structure refinement for compound **3a**.

Identification code	**3a**
Empirical formula	$C_{33}H_{27}NO_3$
Chemical_formula_moiety	$C_{33}H_{27}NO_3$, 2(H_2O)
Formula weight	485.55
Temperature/K	291.0(5)
Crystal system	triclinic
Space group	P-1
a/Å	9.7053(4)
b/Å	9.7576(5)
c/Å	15.0112(6)
α/°	86.996(4)
β/°	76.122(3)
γ/°	70.408(4)
Volume/Å^3	1299.56(11)
Z	2
ρ_{calc}mg/mm^3	1.241
μ/mm^{-1}	0.626
F(000)	512.0
Crystal size/mm^3	0.503×0.331×0.076
2Θ range for data collection	9.626 to 135.144°
Index ranges	-9 ≤ h ≤ 11, -11 ≤ k ≤ 11, -10 ≤ l ≤ 17
Reflections collected	8341
Independent reflections	4686[R(int) = 0.0395]
Data/restraints/parameters	4686/0/334
Goodness-of-fit on F^2	1.079
Final R indexes [I>=2σ (I)]	R1 = 0.0643, wR2 = 0.1991
Final R indexes [all data]	R1 = 0.0723, wR2 = 0.2092
Largest diff. peak/hole / e Å^{-3}	0.23/-0.33

Table S2. Bond Lengths for compound **3a**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O2	N1	1.427(2)	C25	C26	1.476(3)
O2	C1	1.382(2)	C7	C9	1.380(4)
O3	C1	1.206(2)	C6	C8	1.381(3)
O1	C25	1.216(3)	C19	C21	1.387(3)
N1	C3	1.402(2)	C26	C27	1.327(3)
N1	C17	1.494(2)	C27	C28	1.459(3)
C3	C2	1.358(3)	C20	C22	1.390(4)
C3	C4	1.467(3)	C12	C14	1.370(4)
C2	C10	1.495(3)	C28	C30	1.375(4)
C2	C1	1.438(3)	C28	C29	1.392(4)
C4	C5	1.402(3)	C13	C15	1.375(4)
C4	C6	1.391(3)	C9	C8	1.384(4)
C18	C17	1.517(3)	C21	C23	1.364(5)
C18	C19	1.391(3)	C22	C23	1.375(5)
C18	C20	1.383(3)	C14	C16	1.371(5)
C10	C11	1.513(3)	C30	C32	1.373(4)
C17	C24	1.525(3)	C15	C16	1.369(5)
C5	C7	1.380(3)	C29	C31	1.378(5)
C11	C12	1.384(3)	C32	C33	1.373(5)
C11	C13	1.383(3)	C33	C31	1.366(6)
C25	C24	1.509(3)			

Table S3. Bond Angles for compound **3a**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	O2	N1	108.22(13)	O1	C25	C26	121.25(19)
O2	N1	C17	107.89(13	C26	C25	C24	116.80(18)
C3	N1	O2	106.24(14)	C25	C24	C17	113.39(16)
C3	N1	C17	119.60(16)	C9	C7	C5	120.6(2)
N1	C3	C4	118.97(16)	C8	C6	C4	120.2(2)
C2	C3	N1	110.35(17)	C21	C19	C18	120.5(2)
C2	C3	C4	130.55(17)	C27	C26	C25	120.2(2)
C3	C2	C10	130.56(18)	C26	C27	C28	128.7(2)
C3	C2	C1	107.30(16)	C18	C20	C22	120.5(2)
C1	C2	C10	122.11(17)	C14	C12	C11	121.2(2)
C5	C4	C3	120.49(18)	C30	C28	C29	117.4(3)
C6	C4	C3	120.45(17)	C30	C28	C27	123.8(2)
C6	C4	C5	119.05(19)	C29	C28	C27	118.6(2)
C19	C18	C17	121.74(19)	C15	C13	C11	120.9(2)
C20	C18	C17	119.69(18)	C7	C9	C8	119.7(2)
C20	C18	C19	118.45(19)	C6	C8	C9	120.4(2)
C2	C10	C11	114.81(15)	C23	C21	C19	120.4(3)
N1	C17	C18	110.70(15)	C23	C22	C20	120.2(3)
N1	C17	C24	108.34(17)	C21	C23	C22	119.9(2)
C18	C17	C24	114.62(15)	C12	C14	C16	120.4(2)
O2	C1	C2	107.71(16)	C32	C30	C28	121.3(3)
O3	C1	O2	119.47(18)	C16	C15	C13	120.5(3)
O3	C1	C2	132.81(19)	C31	C29	C28	121.0(3)
C7	C5	C4	120.0(2)	C15	C16	C14	119.2(3)
C12	C11	C10	122.44(18)	C30	C32	C33	120.8(3)
C13	C11	C10	119.84(17)	C31	C33	C32	118.9(3)
C13	C11	C12	117.7(2)	C33	C31	C29	120.6(3)
O1	C25	C24	121.9(2)	C41	C43	Cl3	120.5(2)

Table S4. Hydrogen Bonds for compound **3a**.

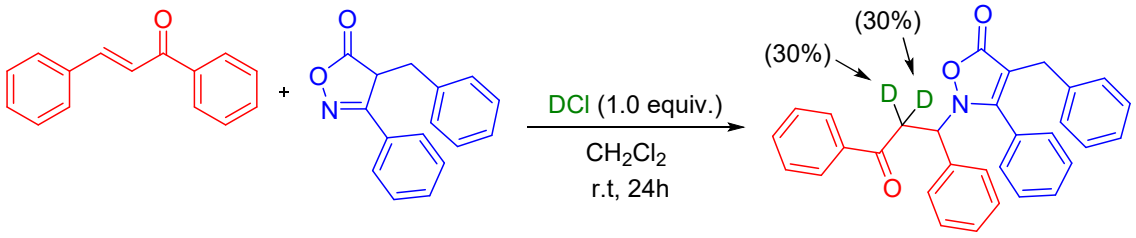
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
C10	H10A	O3[i]	0.97	2.565	3.442(3)	150.4
C10	H10B	O1[ii]	0.97	2.693	3.577(2)	151.7
C19	H19	O2[iii]	0.93	2.587	3.476(2)	160.2

(i) -X,-Y,1-Z; (ii) -X,1-Y,1-Z e (iii) 1-X,-Y,1-Z.

4. Control experiments

4.1. Reaction with DCl

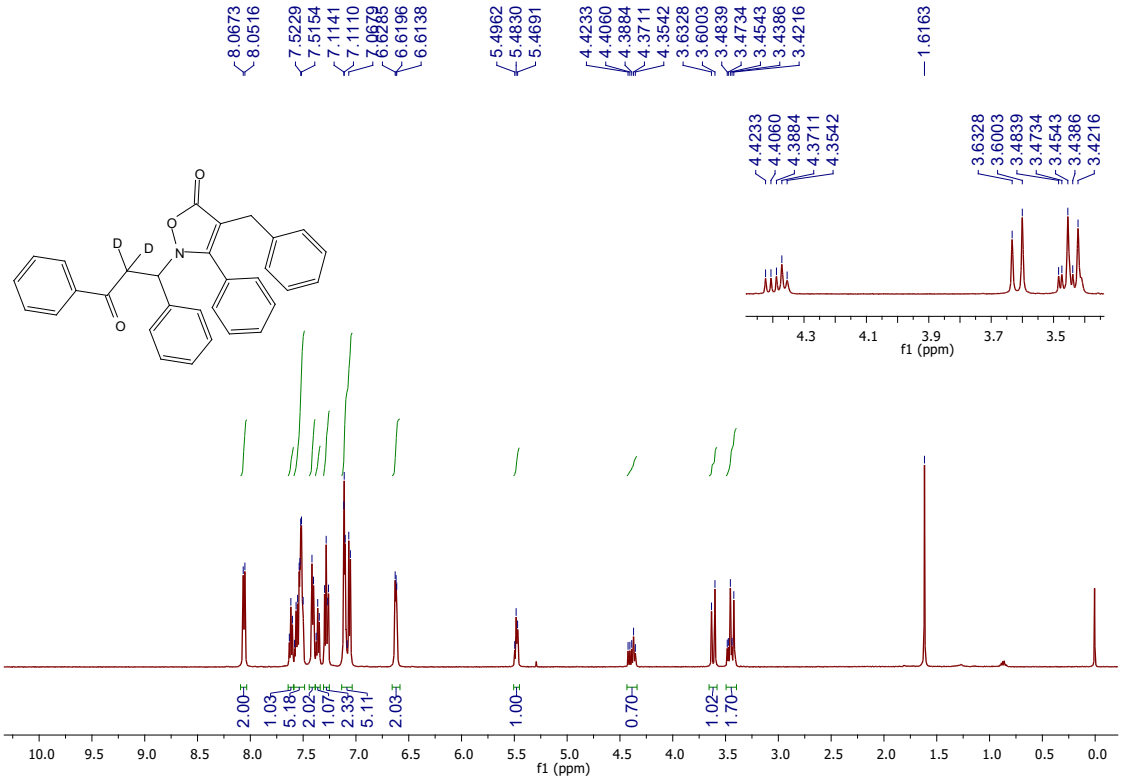
Scheme S1. Reaction using DCi.



84% yield

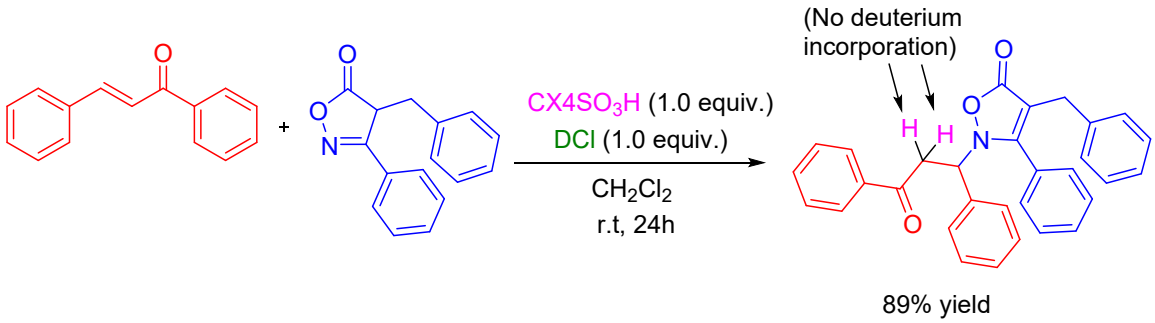
General procedure: In a 5.0 mL vial, 1.5 mL of dichloromethane was added. Then, 0.20 mmol (1.0 equiv.) of isoxazol-5-one **2a** and 0.20 mmol (1.0 equiv.) of chalcone were added. After 5 minutes under magnetic stirring, 0.20 mmol (1.0 equiv) of DCl was added. The reaction mixture was maintained under magnetic stirring at room temperature for 24 hours. Then, the crude reaction mixture was transferred to a round bottom flask, the solvent was removed under reduced pressure, and the product was purified by column chromatography.

Figure S107. ^{1}H NMR (500 MHz, $CDCl_3$) of product **3r** with 60% deuterium incorporation



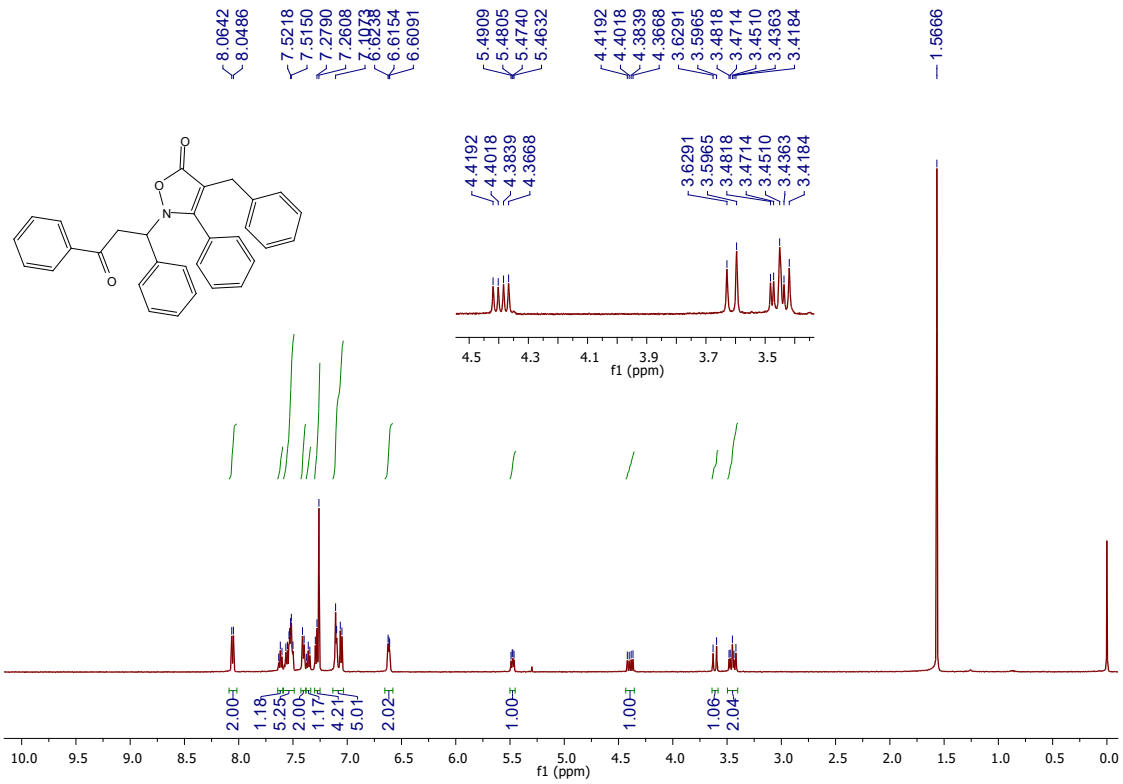
4.2. Competition experiment between DCl and $CX4SO_3H$

Scheme S2. Competition reaction between DCl and $CX4SO_3H$



In a 5.0 mL vial, 1.5 mL of dichloromethane was added. Then, 0.20 mmol (1.0 equiv.) of intermediate **2a** and 0.20 mmol (1.0 equiv.) of chalcone were added. After 5 minutes under magnetic stirring, 0.20 mmol (1.0 equiv) of DCl and 0.20 mmol (1.0 equiv) of calix[4]arene *p*-sulfonic acid ($CX4SO_3H$) were added. The reaction mixture was maintained under magnetic stirring at room temperature for 24 hours. Then, the crude reaction mixture was transferred to a round bottom flask, the solvent was removed under reduced pressure, and the product was purified by column chromatography.

Figure S107. ^1H NMR (500 MHz, $CDCl_3$) of product **3r** obtained in the competition experiment between DCl and $CX4SO_3H$



5. General procedure for the synthesis of *p*-sulfonic acid calix[4]arene ($CX4SO_3H$)

The *p*-sulfonic acid calix[4]arene was synthesized according to the methodologies described by Gustche et al. [1] and Shinkai et al. [2] First, the synthesis of *p*-tert-butylcalix[4]arene was performed using *p*-tert-butylphenol, formaldehyde solution (37%), sodium hydroxide, and heating at 110 °C for four hours. After this period, diphenyl ether was added, and a white precipitate of *p*-tert-butyl calix[4]arene was obtained in 55% yield. The *p*-sulfonic acid calix[4]arene was obtained by treating *p*-tert-butyl calix[4]arene with concentrated H_2SO_4 at 100 °C for 4 hours with 78% yield.

[1] Gutsche, C. D.; Iqbal, M. *Organic Syntheses* **1990**, 68, 234-235, doi: 10.15227/orgsyn.068.0234.

[2] Shinkai, S.; Mori, S.; Tsubaki, T.; Sone, T.; Manabe, O. *Tetrahedron Lett.* **1984**, 25, 5315–5318, doi: 10.1016/S0040-4039(01)81592-6.

5.1. NMR and IR spectra of $CX4SO_3H$

^{1}H NMR (300 MHz; D_2O; δ_{HDO} 4,67; 25 °C) δ 3.88 (s, 8H, H-4), 7.42 (s, 8H, H-2).

^{13}C NMR (75 MHz; D_2O; 25 °C) δ 32.0 (C-4), 126.1 (C-3), 130.7 (C-2), 133.7 (C-1), 155.9 (C-5).

Figure S108. IR (ATR) of *p*-sulfonic acid calix[4]arene ($CX4SO_3H$)

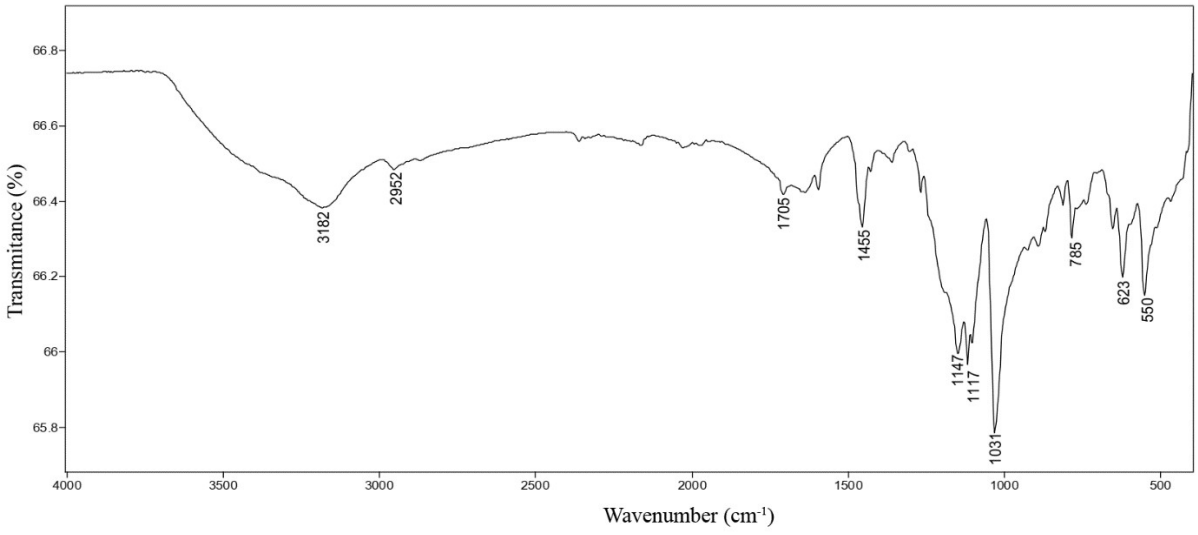


Figure S109. ^{1}H NMR (300 MHz, D_2O) of *p*-sulfonic acid calix[4]arene ($CX4SO_3H$).

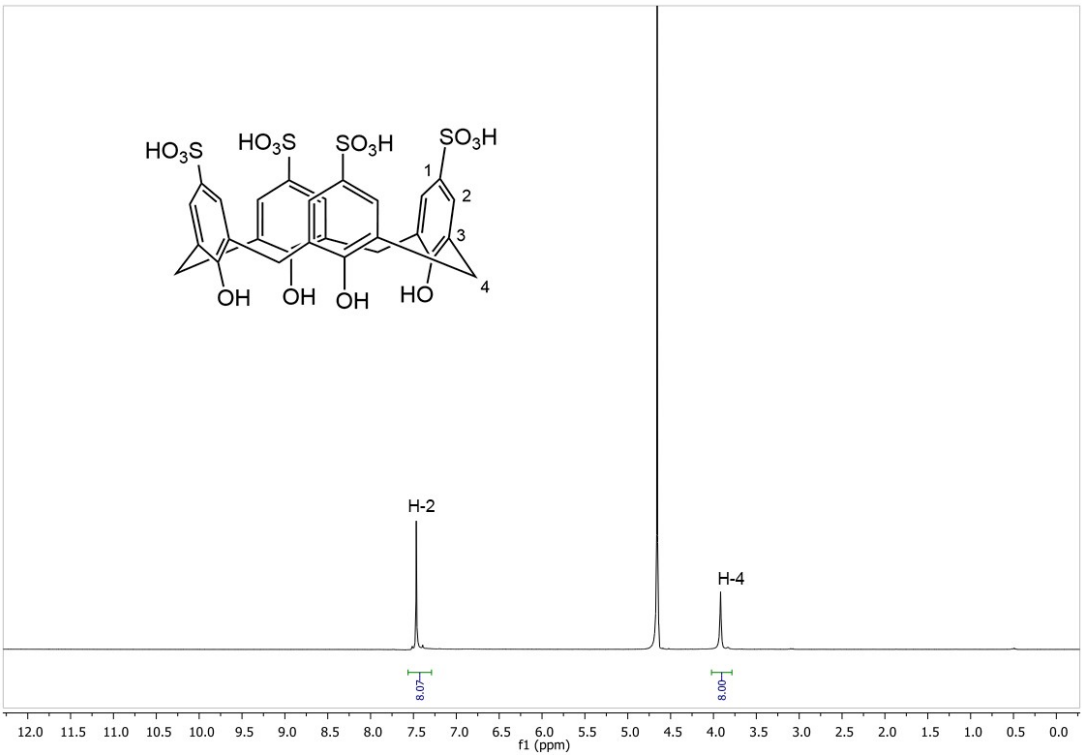
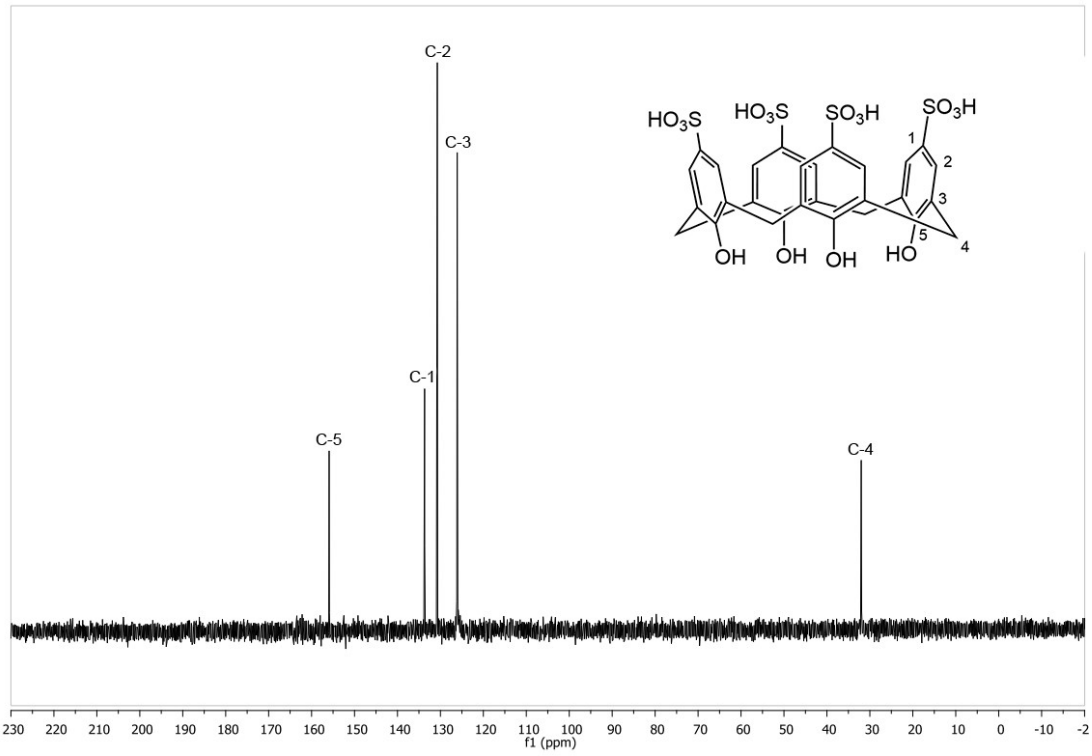


Figure S110. ^{13}C {1H} NMR (75,459 MHz, D_2O) of *p*-sulfonic acid calix[4]arene ($CX4SO_3H$).



6. Energy profile of the evaluated mechanisms

Figure S111. Energy profile (ΔG) for the first reaction pathway

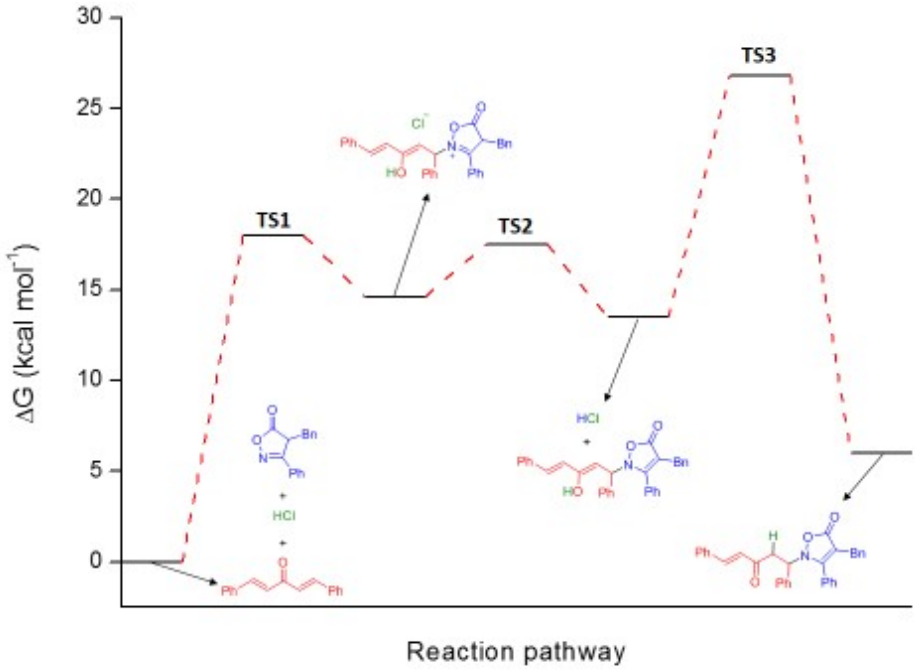
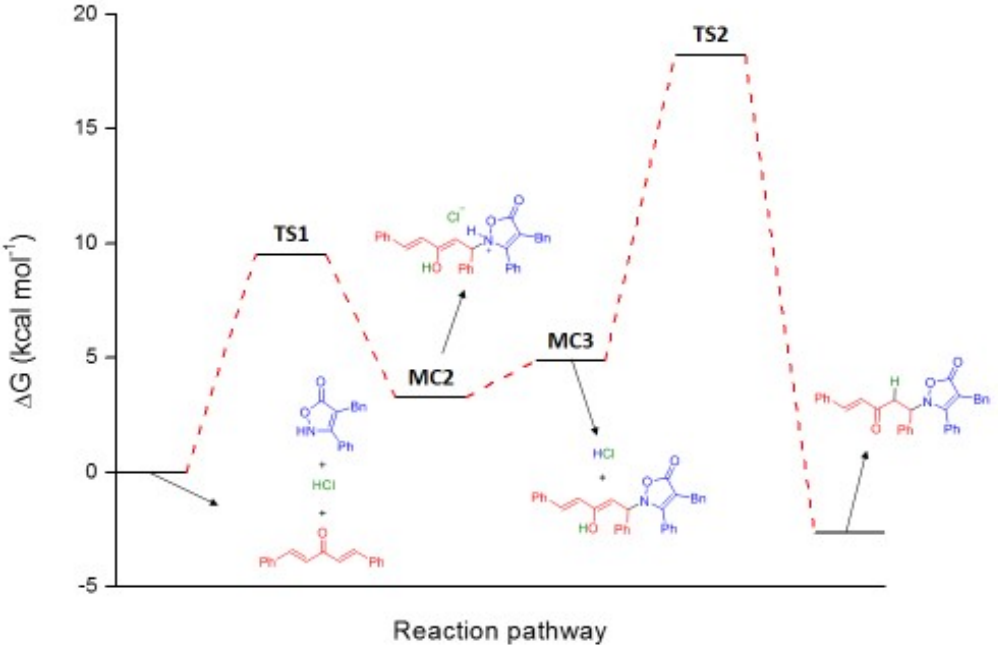
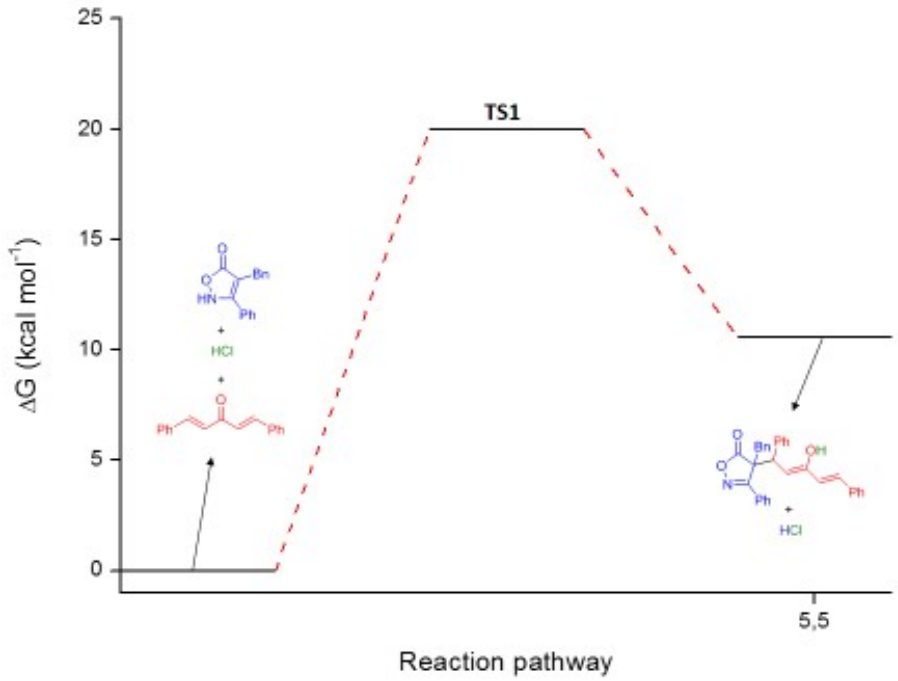


Figure S112. Energy profile (ΔG) for the second reaction pathway



Note: The conversion of the molecular complex 2 (MC2) into the molecular complex 3 (MC3) is barrierless (the barrier is lower than *k*T, in which *k* is the Boltzmann constant and T is the temperature). This observation was confirmed by the scan analysis of the acid-base reaction involved in this step.

Figure S113. Energy profile (ΔG) for the third reaction pathway



7. Imaginary frequencies for all transition states and intrinsic reaction coordinates

Table S5. Imaginary frequencies of TS structures

Reaction pathway		Frequency (cm^{-1})
1	**Transition state 1 (TS1)**	-327.67
	Transition state 2 (TS2)	-616.85
	Transition state 3 (TS3)	-768.49
2	**Transition state 1 (TS1)**	-226.36
	Transition state 3 (TS3)	-768.49
3	**Transition state 1 (TS1)**	-336.73

8. Electronic energies (E), Enthalpies (H) and Gibbs free energies (G) of all optimized structures

Note: All energies values presented below are expressed in Hartree. The energies were calculated using M06-2X/6-31++G(d,p)/SMD= diethyl ether//M06-2X/6-31G(d) level of theory.

Table S6. Electronic energies (E), Enthalpies (H) and Gibbs free energies (G) for reaction pathway 1.

		E	H	G
	Molecular complex 1	-2014.401357	-2013.836383	-2013.941961
Step 1	**Transition state 1**	-2014.376536	-2013.811247	-2013.913294
	Molecular complex 2	-2014.382997	-2013.815774	-2013.918675
	Molecular complex 3	-2014.387102	-2013.819632	-2013.921388
Step 2	**Transition state 2**	-2014.375621	-2013.813639	-2013.916768
	Molecular complex 4	-2014.380469	-2013.815713	-2013.923165
	Molecular complex 5	-2014.386734	-2013.82147	-2013.929386
Step 3	**Transition state 3**	-2014.369424	-2013.807392	-2013.908155
	Molecular complex 6	-2014.404071	-2013.838731	-2013.941344

Table S7. Electronic energies (E), Enthalpies (H) and Gibbs free energies (G) for reaction pathway 2.

		E	H	G
	Molecular complex 1	-2014.400151	-2013.834461	-2013.93719
Step 1	**Transition state 1**	-2014.38478	-2013.819741	-2013.922058
	Molecular complex 2	-2014.393422	-2013.82783	-2013.931945
	Molecular complex 3	-2014.386734	-2013.82147	-2013.929386
Step 3	**Transition state 2**	-2014.369424	-2013.807392	-2013.908155
	Molecular complex 4	-2014.404071	-2013.838731	-2013.941344

Table S8. Electronic energies (E), Enthalpies (H) and Gibbs free energies (G) for reaction pathway 3.

		E	H	G
	Molecular complex 1	-2014.397744	-2013.832224	-2013.934647
Step 1	**Transition state 1**	-2014.366695	-2013.802082	-2013.902815
	Molecular complex 2	-2014.377691	-2013.813078	-2013.917818

9. Electronic energies (ΔE), enthalpies (ΔH) and Gibbs free energies (ΔG) variation along each reaction step

Note: All energies values presented below are expressed in kcal mol^{-1}. The energies were calculated using M06-2X/6-31++G(d,p)/SMD= diethyl ether//M06-2X/6-31G(d) level of theory.

Table S9. Electronic energies (ΔE), Enthalpies (ΔH) and Gibbs free energies (ΔG) for reaction pathway 1.

		ΔE	ΔH	ΔG
	Molecular complex 1	0.00	0.00	0.00
Step 1	**Transition state 1**	15,58	15,77	17,99
	Molecular complex 2	11,52	12,93	14,61
	Molecular complex 3	0.00	0.00	0.00
Step 2	**Transition state 2**	7,20	3,76	2,90
	Molecular complex 4	4,16	2,46	-1,12
	Molecular complex 5	0.00	0.00	0.00
Step 3	**Transition state 3**	10,86	8,83	13,32
	Molecular complex 6	-10,88	-10,83	-7,50

Table S10. Electronic energies (ΔE), Enthalpies (ΔH) and Gibbs free energies (ΔG) for reaction pathway 2.

		ΔE	ΔH	ΔG
	Molecular complex 1	0.00	0.00	0.00
Step 1	**Transition state 1**	9.65	9.24	9.50
	Molecular complex 2	4.22	4.16	3.29
	Molecular complex 5	0.00	0.00	0.00
Step 3	**Transition state 3**	10,86	8,83	13,32
	Molecular complex 6	-10,88	-10,83	-7,50

Table S11. Electronic energies (ΔE), Enthalpies (ΔH) and Gibbs free energies (ΔG) for reaction pathway 3.

		ΔE	ΔH	ΔG
	Molecular complex 1	0.00	0.00	0.00
Step 1	**Transition state 1**	19.48	18.91	19.97
	Molecular complex 2	12.58	12.01	10.56

10. Images of all optimized structures and selected bond lengths

Figure S114. Molecular complex 1 (reaction pathway 1)

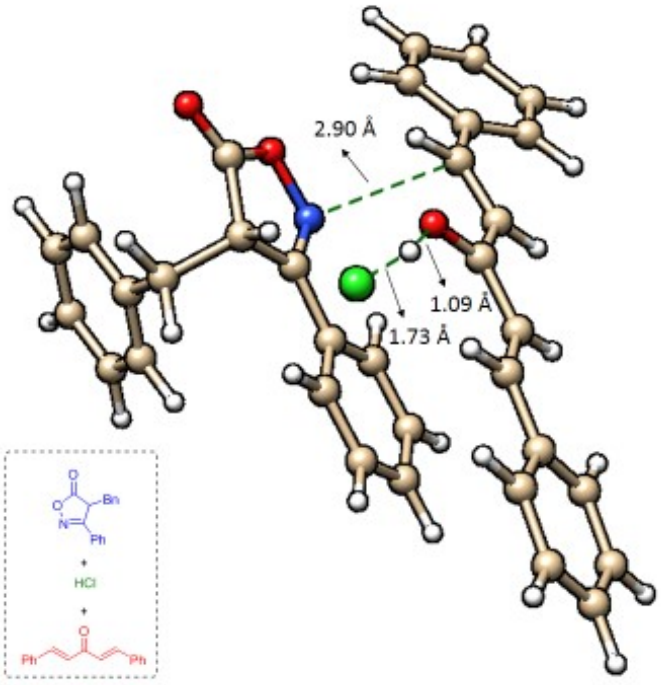


Figure S115. Transition State 1 (TS1) (reaction pathway 1)

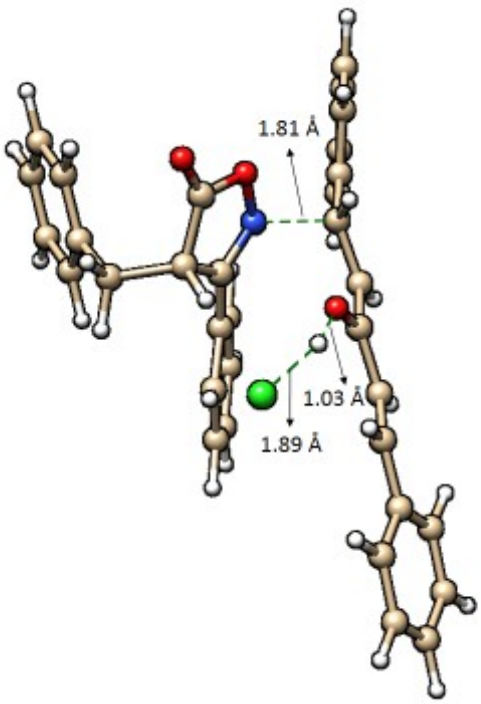


Figure S116. Molecular complex 2 (reaction pathway 1)

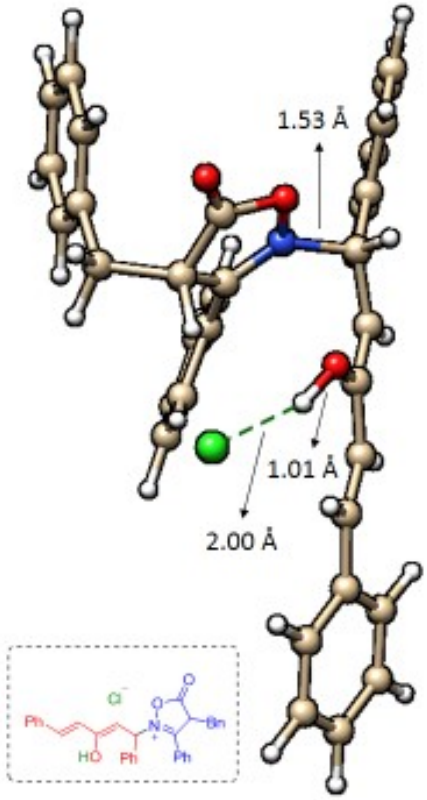


Figure S117. Molecular complex 3 (reaction pathway 1)

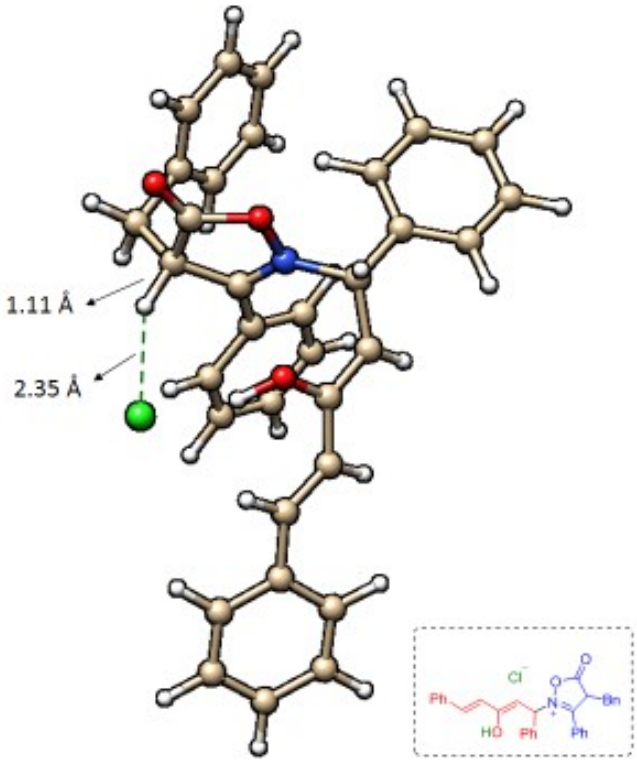


Figure S118. Transition State 2 (TS2) (reaction pathway 1)

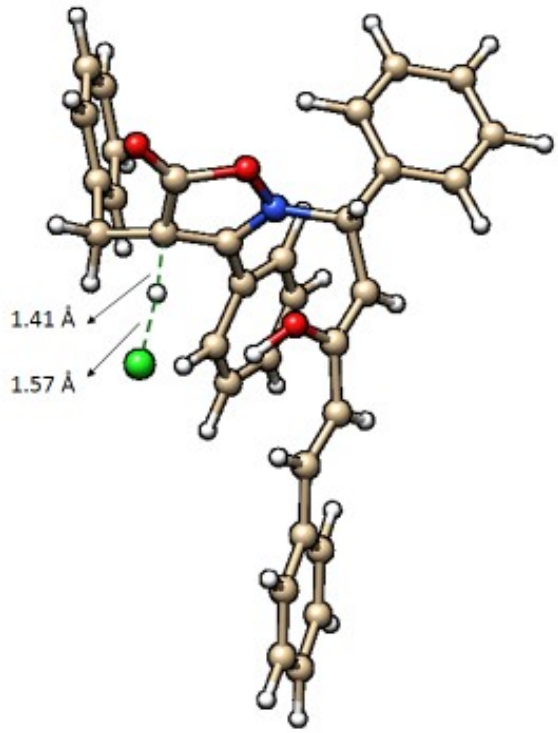


Figure S119. Molecular complex 4 (reaction pathway 1)

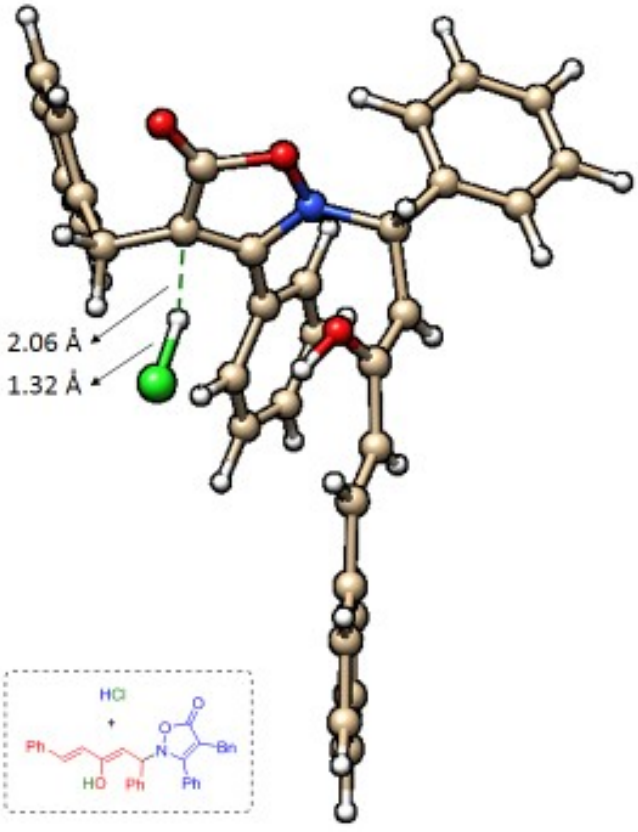


Figure S120. Molecular complex 5 (reaction pathway 1)

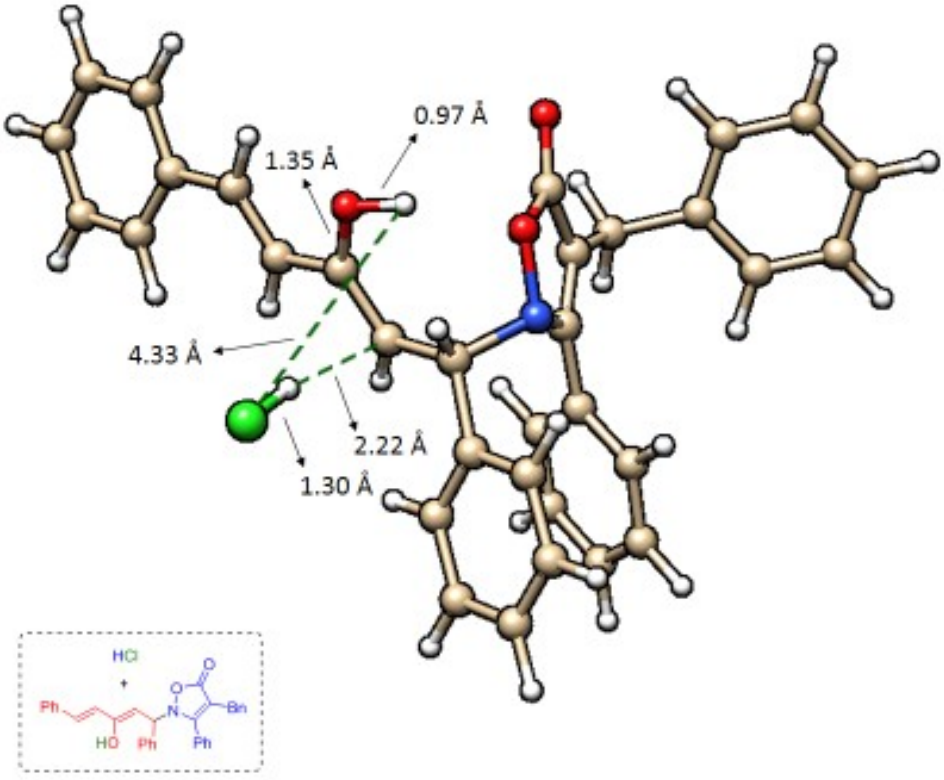


Figure S121. Transition State 3 (TS3) (reaction pathway 1)

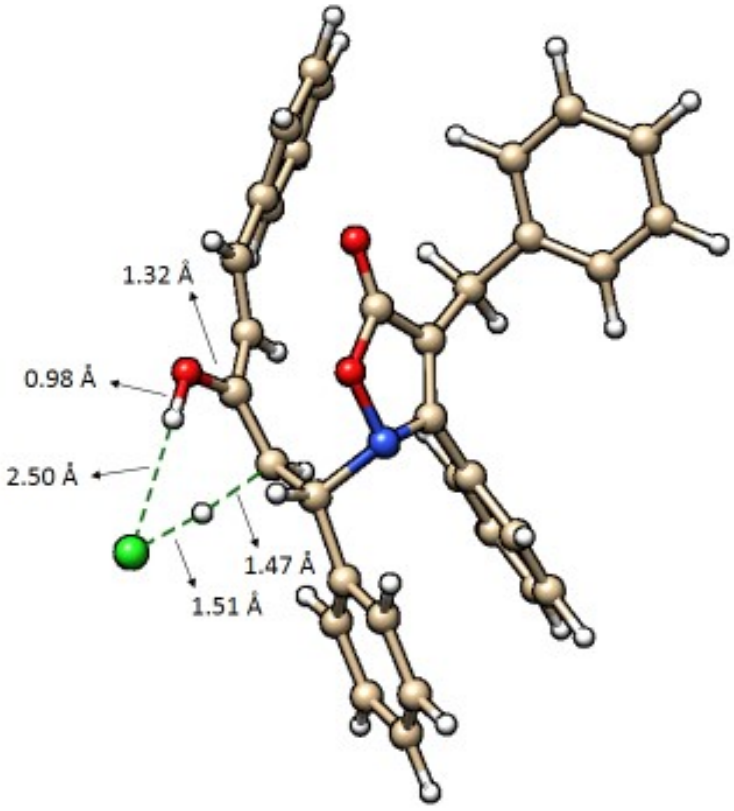


Figure S122. Molecular complex 6 (reaction pathway 1)

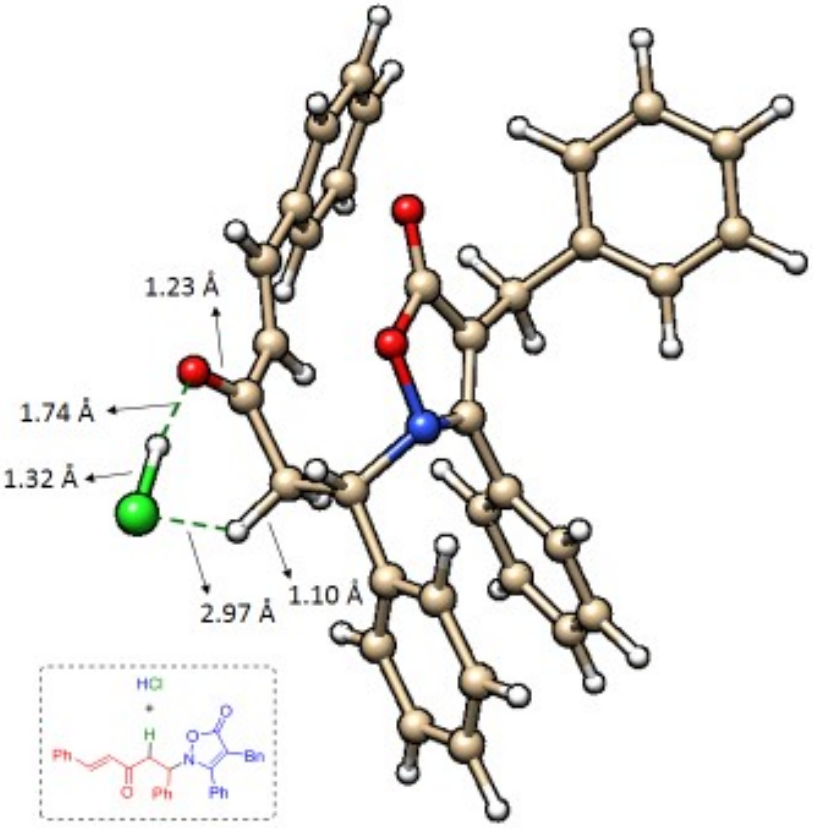


Figure S123. Molecular complex 1 (reaction pathway 2)

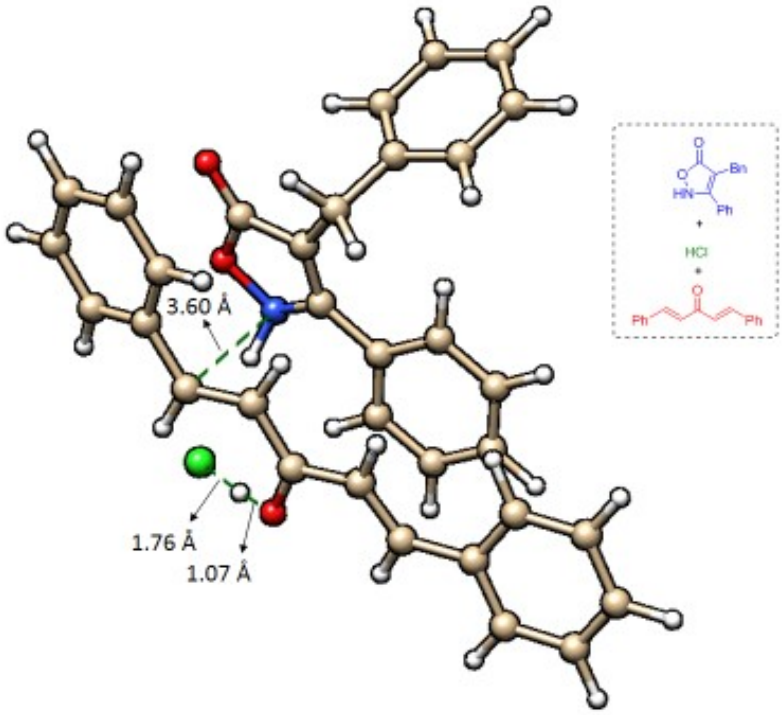


Figure S124. Transition State 1 (TS1) (reaction pathway 2)

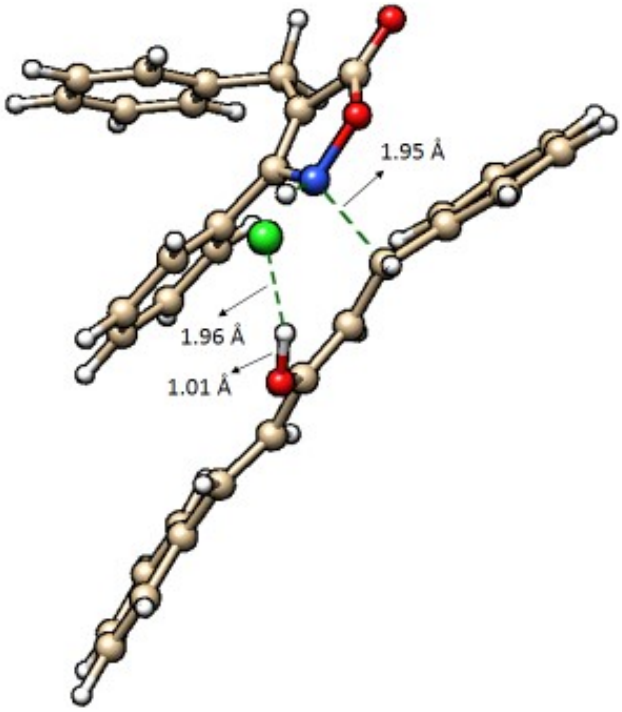


Figure S125. Molecular complex 2 (reaction pathway 2)

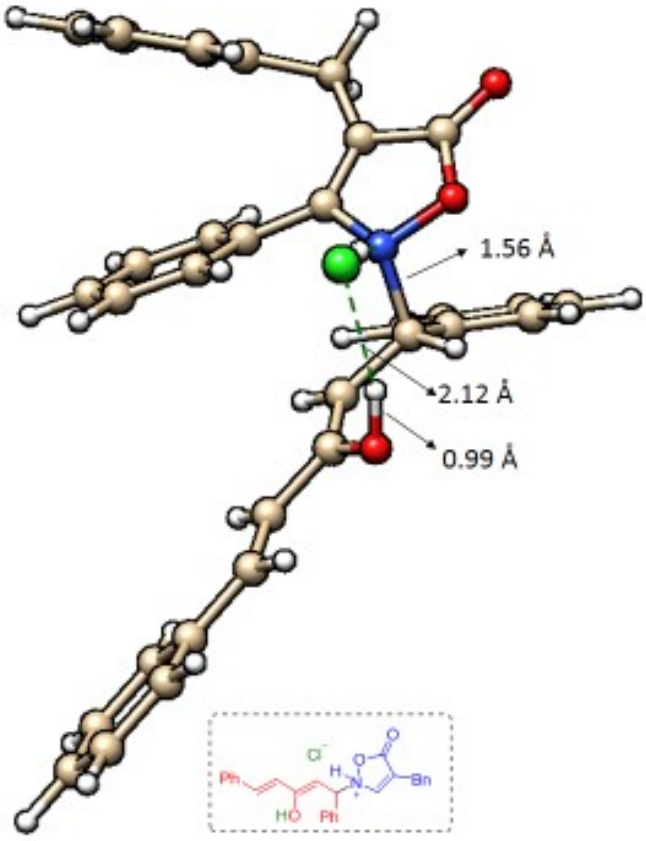


Figure S126. Molecular complex 3 (reaction pathway 2)

Figure S127. Transition State 2 (TS2) (reaction pathway 2)

Figure S128. Molecular complex 4 (reaction pathway 2)

Figure S129. Molecular complex 1 (reaction pathway 3)

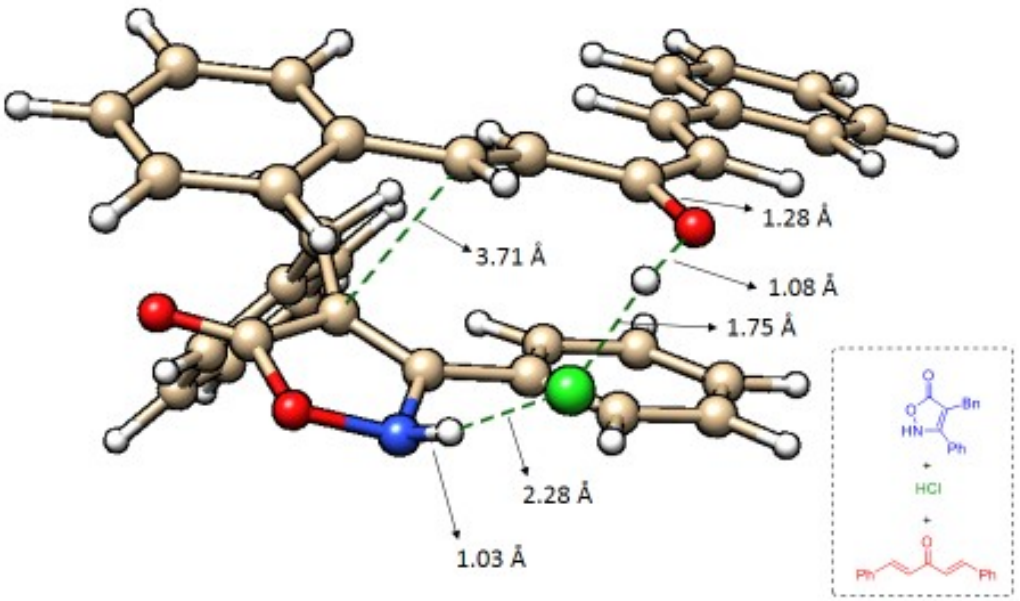


Figure S130. Transition State 1 (TS1) (reaction pathway 3)

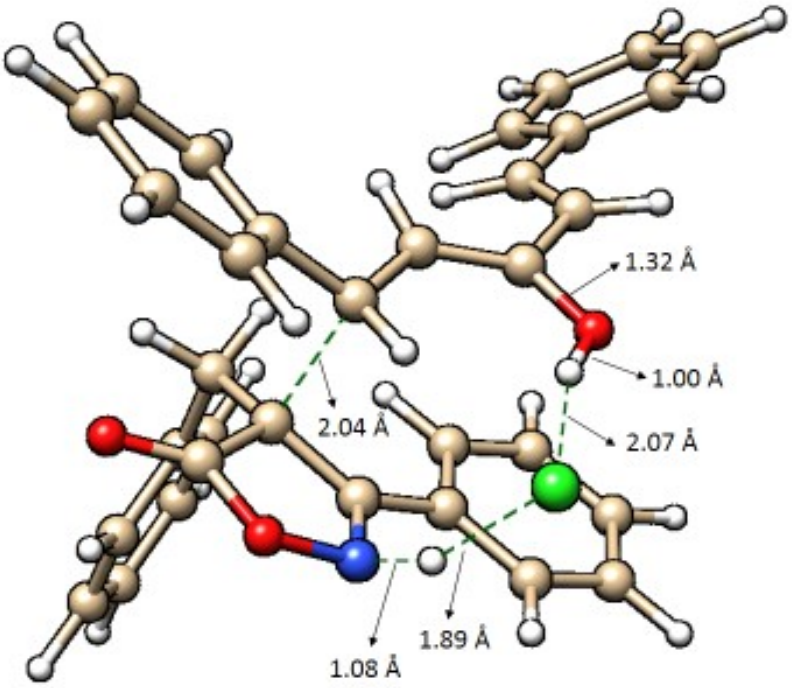
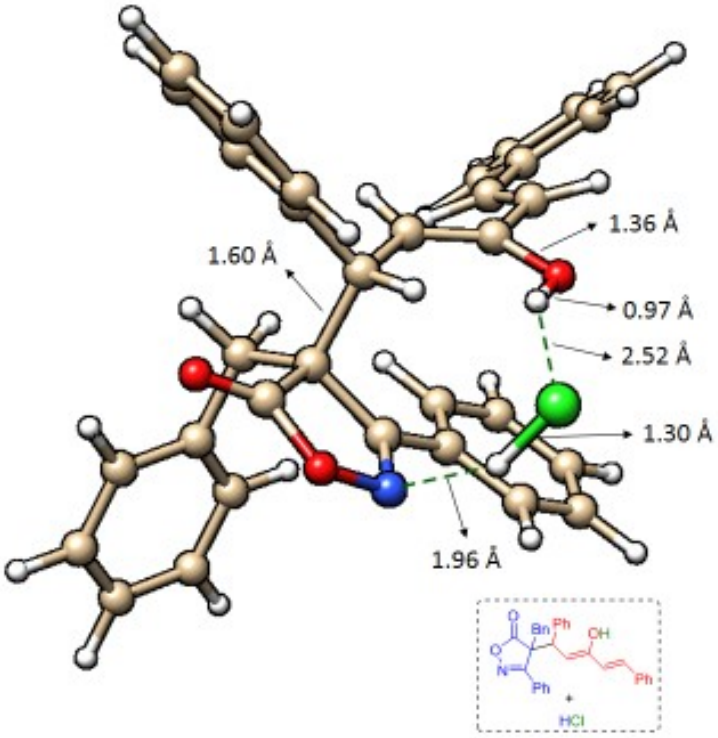


Figure S131. Molecular complex 2 (reaction pathway 3)



11. Coordinates of Optimized Stationary Points

- Molecular complex 1 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.12202	1.71748	-0.88895
C	-0.2291	2.70473	-0.32584
H	-0.62073	3.32452	0.47403
C	-2.43235	1.58281	-0.29914
H	-2.61733	2.21599	0.56252
C	1.06565	2.77058	-0.7099
H	1.39825	2.07468	-1.47647
C	-3.357	0.70159	-0.7425
H	-3.12147	0.08886	-1.61155
O	-0.6766	1.01345	-1.85807
C	-4.66645	0.44689	-0.15737
C	-5.46719	-0.52978	-0.76751
C	-5.14191	1.10033	0.99066
C	-6.71804	-0.84349	-0.24756
H	-5.08876	-1.04261	-1.64866
C	-6.39012	0.78715	1.50676
H	-4.5303	1.84998	1.48375
C	-7.18074	-0.18438	0.88811
H	-7.32952	-1.60081	-0.72699
H	-6.75266	1.29712	2.39356
H	-8.15699	-0.42653	1.29648
C	2.0821	3.65757	-0.16132
C	3.42944	3.31738	-0.35046
C	1.76111	4.82216	0.55311
C	4.43461	4.11602	0.18179
H	3.67409	2.40679	-0.89101
C	2.76748	5.62351	1.07169
H	0.72177	5.11209	0.67697
C	4.10545	5.26912	0.89026
H	5.47449	3.83984	0.04179
H	2.51352	6.52909	1.6132
H	4.89086	5.89778	1.29831
C	1.0957	-0.7726	-0.15389
C	1.38086	-1.65842	-1.32838
C	2.6871	-1.05495	-1.79513
N	1.99664	0.12416	0.03179
C	-0.09288	-0.81577	0.71236
C	-1.16939	-1.64773	0.38785
C	-0.17728	0.02057	1.83431
C	-2.31276	-1.64926	1.18308
H	-1.14229	-2.25307	-0.51257
C	-1.32418	0.01717	2.62013
H	0.66339	0.66397	2.07584
C	-2.39339	-0.81918	2.29815
H	-1.38101	0.66357	3.49093
H	-3.29146	-0.81743	2.90895
C	1.56687	-3.1629	-1.02712
H	0.58777	-3.61215	-0.84093
H	1.96569	-3.61308	-1.94203
C	2.49416	-3.40931	0.139
C	3.87873	-3.44888	-0.0488
C	1.98353	-3.55486	1.43154
C	4.73388	-3.63007	1.03479
H	4.28469	-3.33715	-1.05111
C	2.83742	-3.7376	2.51525
H	0.90716	-3.52601	1.58667
C	4.21557	-3.77503	2.31891
H	5.80706	-3.66195	0.87365
H	2.42549	-3.8534	3.51315
H	4.88276	-3.91981	3.16305
O	2.98584	-0.00505	-0.95992
O	3.41366	-1.38106	-2.68605
Cl	-1.77911	-1.31055	-2.98927
H	-1.21285	0.14947	-2.25101
H	0.61515	-1.53858	-2.11026
H	-3.15084	-2.28492	0.91379

- Transition state 1 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.36905	1.25477	-0.94573
C	-0.39472	2.1114	-0.47941
H	-0.62892	2.78117	0.33703
C	-2.71202	1.26465	-0.38091
H	-2.85048	1.92369	0.47238
C	0.93006	2.03301	-1.01269
H	0.96707	1.82265	-2.08207
C	-3.71092	0.48882	-0.83516
H	-3.52136	-0.18712	-1.66569
O	-1.01043	0.38939	-1.87548
C	-5.05771	0.39979	-0.2681
C	-5.82859	-0.72686	-0.58582
C	-5.59921	1.37595	0.57993
C	-7.10343	-0.88349	-0.05308
H	-5.40456	-1.4841	-1.24096

C	-6.8753	1.22164	1.10455
H	-5.027	2.27042	0.80904
C	-7.62944	0.09001	0.79238
H	-7.68765	-1.76395	-0.30119
H	-7.28908	1.9882	1.75247
H	-8.62784	-0.02666	1.20252
C	1.98524	2.97637	-0.55768
C	3.04504	3.26841	-1.42051
C	1.9565	3.56037	0.71257
C	4.05331	4.14185	-1.02754
H	3.07645	2.80109	-2.401
C	2.966	4.43133	1.10642
H	1.14559	3.33198	1.3984
C	4.01393	4.7255	0.23619
H	4.86919	4.36579	-1.70704
H	2.93512	4.88279	2.09294
H	4.79957	5.40817	0.54438
C	0.97871	-0.64645	-0.25543
C	1.17968	-1.84736	-1.11547
C	2.15125	-1.30337	-2.13382
N	1.62095	0.38136	-0.71788
C	0.18862	-0.55163	0.96156
C	-0.96257	-1.33555	1.10811
C	0.58192	0.33944	1.97028
C	-1.73378	-1.19555	2.25778
H	-1.28549	-1.99335	0.30157
C	-0.18768	0.45817	3.11859
H	1.50308	0.90399	1.84929
C	-1.34831	-0.30586	3.25839
H	0.11669	1.13777	3.90823
H	-1.9515	-0.20916	4.15599
C	1.70281	-3.11217	-0.40866
H	0.88537	-3.53002	0.18651
H	1.94063	-3.83515	-1.1953
C	2.90809	-2.82962	0.45673
C	4.18431	-2.74062	-0.10765
C	2.75774	-2.59924	1.82705
C	5.28537	-2.42233	0.68244
H	4.31301	-2.92676	-1.17101
C	3.8587	-2.28136	2.61779
H	1.77005	-2.67433	2.27651
C	5.12505	-2.19007	2.04626
H	6.27096	-2.36094	0.23153
H	3.72661	-2.1104	3.68187
H	5.98486	-1.94531	2.66212
O	2.34233	0.04513	-1.86238
O	2.73169	-1.83998	-3.0234
Cl	-2.11324	-2.27579	-2.07388
H	-1.57212	-0.46942	-1.9662
H	0.21811	-2.08189	-1.6201
H	-2.6441	-1.77641	2.36289

- Molecular complex 2 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.46142	1.17225	-1.11965
C	-0.47243	2.0142	-0.73433
H	-0.683	2.8141	-0.03907
C	-2.80555	1.24617	-0.55175
H	-2.94795	2.01342	0.20569
C	0.91166	1.82383	-1.2534
H	0.9069	1.8416	-2.34922
C	-3.79186	0.39388	-0.86927
H	-3.60129	-0.3968	-1.5917
O	-1.14643	0.21327	-2.00539
C	-5.13062	0.36838	-0.2703
C	-5.87198	-0.81726	-0.35948
C	-5.69328	1.46879	0.39029
C	-7.13493	-0.90777	0.21558
H	-5.43499	-1.67133	-0.87137
C	-6.95698	1.37894	0.95958
H	-5.14677	2.40658	0.4365
C	-7.6806	0.18944	0.87718
H	-7.69478	-1.83508	0.14395
H	-7.38518	2.24147	1.46124
H	-8.66951	0.123	1.32021
C	1.99171	2.76125	-0.75247
C	3.14142	2.92345	-1.52949
C	1.88357	3.45197	0.45536
C	4.16824	3.76038	-1.10635
H	3.22897	2.38754	-2.47125
C	2.90972	4.2938	0.87724
H	1.00113	3.33292	1.0766
C	4.0528	4.44934	0.09868
H	5.05496	3.87902	-1.72063
H	2.81239	4.83094	1.81543
H	4.85006	5.10807	0.42808
C	0.89962	-0.58481	-0.30623
C	1.1112	-1.89222	-0.9747
C	1.95452	-1.49897	-2.15315
N	1.35659	0.37034	-1.05549
C	0.25917	-0.36542	0.98313
C	-0.89235	-1.09099	1.30987
C	0.83581	0.52876	1.89442
C	-1.48961	-0.8747	2.54819

H	-1.33914	-1.77056	0.58273
C	0.24188	0.71338	3.13466
H	1.76017	1.03788	1.63712
C	-0.92597	0.01893	3.45629
H	0.68985	1.39269	3.85278
H	-1.39335	0.17123	4.42429
C	1.68357	-3.04428	-0.13598
H	0.90184	-3.38094	0.55115
H	1.88281	-3.8658	-0.83132
C	2.93158	-2.64419	0.61514
C	4.16709	-2.58717	-0.03796
C	2.86046	-2.27452	1.96092
C	5.30527	-2.16082	0.64047
H	4.23559	-2.88686	-1.0808
C	3.999	-1.84784	2.63993
H	1.90542	-2.32406	2.47938
C	5.22344	-1.78742	1.97996
H	6.25885	-2.12644	0.12281
H	3.92848	-1.56786	3.68664
H	6.11231	-1.45819	2.50903
O	2.00482	-0.10207	-2.18725
O	2.53131	-2.1444	-2.96624
Cl	-2.07142	-2.57954	-1.64307
H	-1.67317	-0.6402	-1.92004
H	0.09557	-2.19579	-1.35959
H	-2.40071	-1.40764	2.79873

- Molecular complex 3 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.43593	0.93655	-1.39318
C	-0.38393	1.73701	-1.09888
H	-0.49837	2.60332	-0.46023
C	-2.762	1.16188	-0.82294
H	-2.84811	2.02362	-0.16469
C	0.98912	1.31199	-1.51259
H	1.03236	1.17058	-2.59968
C	-3.79042	0.31929	-1.00131
H	-3.64829	-0.5691	-1.61263
O	-1.20031	-0.12922	-2.17474
C	-5.10699	0.43308	-0.36447
C	-5.88147	-0.72676	-0.2296
C	-5.61424	1.6449	0.1232
C	-7.12235	-0.68005	0.39663
H	-5.48598	-1.66714	-0.606
C	-6.8564	1.6913	0.74327
H	-5.04135	2.55875	-0.00745
C	-7.61304	0.52841	0.88526
H	-7.7084	-1.588	0.50038
H	-7.24192	2.63833	1.10883
H	-8.58508	0.56757	1.3673
C	2.12393	2.21768	-1.07089
C	3.2979	1.72037	-0.50169
C	1.99023	3.59249	-1.27722
C	4.31835	2.59356	-0.13229
H	3.4309	0.65268	-0.3383
C	3.01525	4.45978	-0.91445
H	1.08079	3.98051	-1.7278
C	4.18175	3.96279	-0.3372
H	5.22169	2.19081	0.31521
H	2.90061	5.52612	-1.08148
H	4.9796	4.64041	-0.05049
C	0.76381	-0.83003	-0.10477
C	1.06838	-2.26291	-0.38373
C	1.82663	-2.17247	-1.68231
N	1.24681	-0.09823	-1.05627
C	0.05958	-0.33026	1.07028
C	-1.04098	-1.05606	1.54224
C	0.49296	0.83021	1.72938
C	-1.72925	-0.58832	2.65841
H	-1.39921	-1.92568	0.99298
C	-0.18627	1.26605	2.85634
H	1.36925	1.36374	1.37019
C	-1.30293	0.56196	3.31475
H	0.14972	2.15669	3.37701
H	-1.83999	0.91599	4.18933
C	1.92108	-2.94254	0.7117
H	1.29429	-3.07797	1.5976
H	2.19137	-3.93355	0.33459
C	3.15027	-2.12337	1.04172
C	4.2814	-2.1683	0.21837
C	3.14931	-1.25474	2.13787
C	5.38305	-1.35776	0.48378
H	4.30261	-2.84825	-0.62944
C	4.24881	-0.4416	2.40216
H	2.28111	-1.21959	2.79129
C	5.36907	-0.49238	1.57573
H	6.2555	-1.41009	-0.1599
H	4.23226	0.22469	3.2592
H	6.23256	0.13082	1.7886
O	1.91958	-0.8227	-2.02493
O	2.3463	-3.00452	-2.34994
Cl	-2.14933	-2.77286	-1.21668
H	-1.69979	-0.96311	-1.90415
H	0.10579	-2.78986	-0.56287

H	-2.60565	-1.12489	3.0055

- Transition state 2 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.52234	1.3477	-1.09439
C	-0.53501	2.12343	-0.60774
H	-0.6919	2.72046	0.28195
C	-2.80757	1.19961	-0.41994
H	-2.89957	1.74309	0.51715
C	0.84475	2.02134	-1.19503
H	0.79557	2.18032	-2.27912
C	-3.80441	0.41772	-0.86155
H	-3.70348	-0.08195	-1.82435
O	-1.25717	0.62953	-2.2116
C	-5.0688	0.16785	-0.16019
C	-6.1435	-0.38126	-0.87055
C	-5.24086	0.44629	1.20353
C	-7.36371	-0.61959	-0.24809
H	-6.01587	-0.61701	-1.92375
C	-6.45896	0.20753	1.82595
H	-4.40743	0.83054	1.78478
C	-7.52675	-0.32214	1.10202
H	-8.18624	-1.04124	-0.81716
H	-6.57525	0.42602	2.88308
H	-8.47673	-0.51107	1.59192
C	1.86661	2.9743	-0.59932
C	3.18738	2.58277	-0.37446
C	1.48889	4.28965	-0.32244
C	4.11037	3.48935	0.14082
H	3.49905	1.5676	-0.60401
C	2.41455	5.1961	0.18559
H	0.46756	4.60782	-0.51246
C	3.72693	4.79699	0.42428
H	5.1328	3.17009	0.31635
H	2.10745	6.21561	0.39679
H	4.44766	5.50242	0.82533
C	0.94507	-0.41426	-0.3759
C	1.18556	-1.62949	-1.06946
C	1.94105	-1.22399	-2.25895
N	1.3171	0.60971	-1.12349
C	0.34668	-0.25732	0.95353
C	-0.7772	-1.02028	1.28714
C	0.90961	0.62527	1.88129
C	-1.34991	-0.87652	2.54715
H	-1.2194	-1.68893	0.55221
C	0.33965	0.74713	3.14247
H	1.79221	1.20031	1.61492
C	-0.79187	0.00185	3.47396
H	0.77918	1.42392	3.8679
H	-1.23633	0.10373	4.45916
C	1.52815	-2.94747	-0.39427
H	0.6867	-3.27221	0.2255
H	1.64397	-3.6886	-1.19194
C	2.79065	-2.83562	0.42981
C	4.04225	-2.87017	-0.19269
C	2.72463	-2.63093	1.80966
C	5.20509	-2.70558	0.55372
H	4.09679	-3.025	-1.26763
C	3.88875	-2.46644	2.55696
H	1.75416	-2.60097	2.30077
C	5.13138	-2.50313	1.93058
H	6.17137	-2.74056	0.0597
H	3.82327	-2.31345	3.63002
H	6.03937	-2.37923	2.51275
O	1.90986	0.18001	-2.29667
O	2.51285	-1.84125	-3.10835
Cl	-1.51109	-2.45348	-2.00243
H	-1.70968	-0.23947	-2.20801
H	-0.0993	-1.92939	-1.57518
H	-2.23422	-1.45219	2.80101

- Molecular complex 4 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.65065	1.19363	-0.96749
C	-0.72383	1.9953	-0.41825
H	-0.9197	2.4679	0.537
C	-2.91485	0.89063	-0.30416
H	-2.99514	1.26761	0.71217
C	0.63131	2.14778	-1.05291
H	0.49845	2.30411	-2.13043
C	-3.92246	0.19454	-0.85214
H	-3.8572	-0.11977	-1.89433
O	-1.36007	0.61658	-2.16514
C	-5.17279	-0.17343	-0.17706
C	-6.27849	-0.55503	-0.94693
C	-5.30061	-0.16581	1.21928
C	-7.48565	-0.89252	-0.34513
H	-6.18779	-0.57739	-2.02992
C	-6.50593	-0.50278	1.8208
H	-4.44251	0.08223	1.83746
C	-7.60454	-0.86374	1.04152
H	-8.33286	-1.18041	-0.95957

H	-6.58752	-0.49487	2.90335
H	-8.54415	-1.13069	1.51472
C	1.44764	3.30126	-0.48923
C	2.83134	3.20308	-0.33571
C	0.81301	4.50427	-0.17305
C	3.56441	4.28466	0.14599
H	3.33435	2.27705	-0.59774
C	1.54715	5.58642	0.3037
H	-0.26145	4.59701	-0.30718
C	2.92524	5.47809	0.46997
H	4.63967	4.19285	0.26418
H	1.03974	6.5149	0.54683
H	3.49795	6.3202	0.84559
C	1.13144	-0.2566	-0.29794
C	1.53136	-1.35777	-1.01221
C	2.09262	-0.85533	-2.25302
N	1.39564	0.87809	-0.99778
C	0.59323	-0.19221	1.07079
C	-0.45436	-1.03693	1.44979
C	1.13186	0.7115	1.99099
C	-0.96212	-0.97251	2.74306
H	-0.89299	-1.71629	0.72335
C	0.62157	0.76773	3.28384
H	1.94601	1.36429	1.68836
C	-0.42464	-0.07167	3.66124
H	1.04362	1.46772	3.99776
H	-0.82093	-0.0246	4.67076
C	1.77098	-2.76851	-0.5463
H	0.95029	-3.11464	0.08996
H	1.78989	-3.41214	-1.43288
C	3.08411	-2.8741	0.20173
C	4.28937	-2.91972	-0.50388
C	3.11055	-2.86505	1.59674
C	5.50086	-2.96707	0.17864
H	4.26736	-2.90799	-1.59109
C	4.32357	-2.91294	2.27995
H	2.17458	-2.81906	2.14966
C	5.52106	-2.9659	1.57226
H	6.43181	-3.00705	-0.37882
H	4.33173	-2.91105	3.36585
H	6.46692	-3.0068	2.10369
O	1.93509	0.52919	-2.22976
O	2.63324	-1.40349	-3.17876
Cl	-1.43266	-2.55055	-2.01021
H	-1.92016	-0.16253	-2.31058
H	-0.31945	-1.90801	-1.73114
H	-1.78137	-1.62386	3.03113

- Molecular complex 5 (pathway 1)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	2.07246	-0.26935	-0.82806
C	1.04484	-1.00238	-0.3305
H	1.0499	-1.19539	0.73693
C	3.22879	0.0845	-0.00781
H	3.23144	-0.31918	1.00116
C	-0.13769	-1.44227	-1.14097
H	0.17052	-1.58257	-2.18489
C	4.226	0.86089	-0.45614
H	4.14163	1.25971	-1.46471
O	2.15892	0.148	-2.10894
C	5.4227	1.2498	0.2982
C	6.21534	2.29756	-0.18729
C	5.80992	0.615	1.4872
C	7.34765	2.71658	0.50267
H	5.9301	2.78976	-1.11334
C	6.94141	1.03075	2.17569
H	5.23275	-0.22375	1.86473
C	7.71295	2.08563	1.68839
H	7.94604	3.53393	0.11258
H	7.22983	0.52532	3.09218
H	8.59877	2.40673	2.22733
C	-0.81789	-2.72952	-0.7024
C	-1.8209	-3.24307	-1.5299
C	-0.50847	-3.39921	0.47898
C	-2.52129	-4.38725	-1.17038
H	-2.06376	-2.71995	-2.45152
C	-1.21173	-4.54584	0.84308
H	0.27581	-3.03587	1.13399
C	-2.22223	-5.03904	0.02527
H	-3.29824	-4.77277	-1.82332
H	-0.96543	-5.05143	1.7715
H	-2.76825	-5.93279	0.31103
C	-1.58859	0.27565	-0.06703
C	-1.38199	1.60684	-0.12751
C	-0.7498	1.87756	-1.40988
N	-1.18688	-0.36369	-1.25117
C	-2.16133	-0.53188	1.02426
C	-1.58787	-0.4722	2.29683
C	-3.24612	-1.38135	0.78655
C	-2.08581	-1.2719	3.32205
H	-0.7373	0.18269	2.46771
C	-3.73723	-2.17951	1.8117
H	-3.68134	-1.4232	-0.20668
C	-3.15556	-2.12885	3.07831

H	-4.56938	-2.84926	1.61988
H	-3.53771	-2.75868	3.87566
C	-1.81093	2.70499	0.79768
H	-1.88825	2.32282	1.81961
H	-1.03984	3.48268	0.78811
C	-3.1418	3.28842	0.36381
C	-3.1983	4.23258	-0.6639
C	-4.32824	2.84706	0.95076
C	-4.42532	4.73396	-1.08864
H	-2.27552	4.56051	-1.13558
C	-5.55554	3.35003	0.52724
H	-4.2875	2.10378	1.74416
C	-5.60614	4.29621	-0.49302
H	-4.45891	5.46922	-1.88687
H	-6.47202	3.00381	0.99556
H	-6.56212	4.6908	-0.82327
O	-0.62696	0.65143	-2.05796
O	-0.37685	2.89138	-1.93481
Cl	2.58136	-3.79561	-1.71692
H	1.26602	0.25305	-2.48165
H	2.22194	-2.72715	-1.06975
H	-1.63305	-1.23055	4.30765

- Transition state 3 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.36616	-2.48735	-0.33703
C	-1.51715	-1.78844	0.03655
H	-1.46612	-1.38117	1.04412
C	0.82126	-2.51804	0.49257
H	0.71228	-2.13457	1.50335
C	-2.16434	-0.84508	-0.96719
H	-2.29249	-1.34321	-1.93368
C	2.03352	-2.72854	-0.05396
H	2.0842	-2.98284	-1.11027
O	-0.27571	-3.13813	-1.48309
C	3.30589	-2.48973	0.62982
C	4.40282	-2.06385	-0.13164
C	3.44707	-2.62233	2.01764
C	5.60971	-1.75608	0.48679
H	4.28402	-1.94417	-1.20511
C	4.65771	-2.32509	2.63094
H	2.61098	-2.98403	2.60997
C	5.73947	-1.88638	1.86805
H	6.45031	-1.41538	-0.10957
H	4.76165	-2.44091	3.70517
H	6.68359	-1.65248	2.34984
C	-3.50859	-0.27827	-0.5544
C	-4.1741	0.55037	-1.46196
C	-4.08688	-0.53078	0.68668
C	-5.38337	1.14305	-1.12226
H	-3.72087	0.74518	-2.43078
C	-5.29886	0.06499	1.02992
H	-3.60126	-1.19454	1.39461
C	-5.94509	0.90795	0.13223
H	-5.88986	1.78572	-1.83579
H	-5.73684	-0.13473	2.00275
H	-6.88936	1.37079	0.40207
C	-0.57631	0.91071	-0.20427
C	0.76371	0.78312	-0.29701
C	1.02673	0.00136	-1.49869
N	-1.22334	0.29003	-1.29231
C	-1.39109	1.55992	0.83683
C	-1.18331	1.23963	2.18144
C	-2.39589	2.46775	0.48709
C	-1.98582	1.80798	3.16651
H	-0.40707	0.52579	2.44664
C	-3.19728	3.02947	1.47254
H	-2.55397	2.70769	-0.55923
C	-2.99604	2.6977	2.81197
H	-3.98644	3.72039	1.194
H	-3.62848	3.13296	3.57932
C	1.87873	1.3178	0.54655
H	1.46828	1.75173	1.46378
H	2.5272	0.47985	0.83393
C	2.69134	2.3576	-0.19997
C	3.90529	2.02397	-0.79888
C	2.20586	3.661	-0.32266
C	4.62957	2.98373	-1.50187
H	4.27316	1.00441	-0.71864
C	2.92823	4.62129	-1.02312
H	1.25305	3.91963	0.13539
C	4.14431	4.28354	-1.61392
H	5.57368	2.71407	-1.96534
H	2.54356	5.63313	-1.10787
H	4.7099	5.03137	-2.1612
O	-0.19789	-0.27101	-2.07548
O	2.05408	-0.39672	-1.98514
Cl	-3.32429	-3.9121	-0.87244
H	-1.15466	-3.21109	-1.90694
H	-2.47444	-2.888	-0.15327
H	-1.8271	1.54883	4.20839

- Molecular complex 6 (pathway 1)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.66413	-2.73741	0.23571
C	-1.84013	-1.83402	0.56997
H	-1.62592	-1.23514	1.4607
C	0.61278	-2.46432	0.9157
H	0.58907	-1.81972	1.79085
C	-2.22098	-0.91427	-0.60622
H	-2.37962	-1.54175	-1.48891
C	1.77768	-2.84374	0.36482
H	1.73863	-3.38802	-0.57768
O	-0.77859	-3.62623	-0.59955
C	3.0986	-2.46514	0.87558
C	4.15717	-2.3121	-0.02921
C	3.3171	-2.19338	2.23312
C	5.39893	-1.86707	0.4114
H	3.98122	-2.50289	-1.08334
C	4.56094	-1.75677	2.67223
H	2.51202	-2.34564	2.94667
C	5.60234	-1.58538	1.76084
H	6.20873	-1.73798	-0.29989
H	4.72202	-1.55506	3.72657
H	6.57263	-1.24043	2.10419
C	-3.48301	-0.10246	-0.36979
C	-4.02379	0.59095	-1.45628
C	-4.09588	0.00642	0.87636
C	-5.14308	1.3976	-1.29477
H	-3.54374	0.50637	-2.42798
C	-5.21924	0.81459	1.0406
H	-3.69386	-0.51697	1.738
C	-5.74136	1.51606	-0.0405
H	-5.55218	1.93113	-2.14714
H	-5.68028	0.89864	2.01977
H	-6.61568	2.14646	0.08907
C	-0.41288	0.74668	-0.07989
C	0.91879	0.57855	-0.23812
C	1.09017	-0.38072	-1.31925
N	-1.12725	0.0000	-1.02401
C	-1.14217	1.61547	0.86338
C	-0.94818	1.47071	2.23916
C	-2.03709	2.57811	0.38486
C	-1.66336	2.26516	3.1318
H	-0.24691	0.72387	2.60419
C	-2.7488	3.36789	1.27837
H	-2.18393	2.68194	-0.68545
C	-2.56728	3.20871	2.65205
H	-3.45386	4.10225	0.90233
H	-3.12961	3.82302	3.34828
C	2.08472	1.2305	0.43848
H	1.73459	1.77225	1.32325
H	2.77444	0.44729	0.77816
C	2.80987	2.17804	-0.4968
C	3.93479	1.75798	-1.20606
C	2.32902	3.47506	-0.68615
C	4.57613	2.62752	-2.08481
H	4.29415	0.74089	-1.07343
C	2.96972	4.34555	-1.56192
H	1.44444	3.79994	-0.14153
C	4.09728	3.92257	-2.26286
H	5.45073	2.29123	-2.63333
H	2.5905	5.354	-1.69723
H	4.59906	4.60019	-2.94679
O	-0.17356	-0.74809	-1.73651
O	2.07644	-0.84938	-1.82913
Cl	-3.64276	-4.07525	-1.53949
H	-2.36684	-3.96479	-1.21851
H	-2.70837	-2.46994	0.77923
H	-1.51617	2.14377	4.20026

- Molecular complex 1 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.30448	-1.99123	-0.68247
C	0.00533	-1.72277	-1.19838
H	0.11913	-0.79106	-1.74457
C	-2.39484	-1.13221	-1.09206
H	-2.16241	-0.35687	-1.81416
C	1.06599	-2.54527	-0.99023
H	0.91469	-3.46224	-0.4267
C	-3.6247	-1.2734	-0.55529
H	-3.76306	-2.08853	0.15334
O	-1.57506	-2.9422	0.13479
C	-4.79164	-0.43832	-0.81533
C	-4.71431	0.76773	-1.5299
C	-6.03153	-0.84197	-0.30144
C	-5.85041	1.53664	-1.73338
H	-3.75639	1.11358	-1.90626
C	-7.17112	-0.07355	-0.50982
H	-6.09468	-1.76929	0.26177
C	-7.08195	1.11647	-1.22694
H	-5.77978	2.46979	-2.28292
H	-8.1256	-0.40047	-0.11053
H	-7.96836	1.722	-1.38722
C	2.43001	-2.2879	-1.40392
C	3.45033	-3.00774	-0.76209

C	2.76741	-1.32235	-2.36877
C	4.78159	-2.7467	-1.05808
H	3.18178	-3.73581	-0.00065
C	4.09571	-1.08366	-2.67754
H	1.98434	-0.7777	-2.88917
C	5.10317	-1.78844	-2.01501
H	5.56724	-3.28187	-0.53601
H	4.35451	-0.33967	-3.42383
H	6.14357	-1.57957	-2.24213
C	1.06078	0.12536	1.22512
C	1.95221	0.68244	0.35967
C	3.23971	0.07169	0.65247
N	1.71275	-0.75777	2.07232
C	-0.38129	0.35294	1.42379
C	-1.14288	-0.52933	2.20299
C	-1.00704	1.47658	0.86319
C	-2.50112	-0.29963	2.39669
H	-0.68643	-1.40423	2.65722
C	-2.36499	1.69989	1.06116
H	-0.41841	2.20958	0.32347
C	-3.11786	0.81206	1.82661
H	-2.83298	2.58093	0.63211
H	-4.17881	0.98871	1.9786
C	1.83959	1.68311	-0.75073
H	2.65533	1.45039	-1.44832
H	0.89907	1.55021	-1.30053
C	1.97563	3.13215	-0.32006
C	1.0689	4.10063	-0.74956
C	3.04225	3.51863	0.49712
C	1.21219	5.43286	-0.36435
H	0.24263	3.81066	-1.39667
C	3.18768	4.84673	0.88089
H	3.76436	2.77052	0.81492
C	2.27135	5.80798	0.45457
H	0.49534	6.1742	-0.70452
H	4.02087	5.13451	1.51478
H	2.38589	6.84376	0.75869
O	3.03811	-0.85443	1.64819
O	4.33826	0.2802	0.19195
Cl	0.39595	-3.75639	1.99177
H	-0.77879	-3.30242	0.75834
H	-3.07484	-0.99378	3.00316
H	1.34266	-1.71735	2.15864

- Transition state 1 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.5216	-2.01619	0.17912
C	-0.32717	-1.94262	-0.50466
H	-0.38163	-1.48136	-1.48332
C	-2.7234	-1.49395	-0.46768
H	-2.60448	-1.1378	-1.48682
C	0.94637	-2.38253	-0.04382
H	0.95439	-3.0932	0.78456
C	-3.89656	-1.39306	0.17667
H	-3.95811	-1.79994	1.18422
O	-1.71698	-2.48527	1.39139
C	-5.10714	-0.76278	-0.35601
C	-5.06787	0.14239	-1.42734
C	-6.34446	-1.04768	0.23606
C	-6.23594	0.72097	-1.90638
H	-4.11136	0.41261	-1.86621
C	-7.51447	-0.4724	-0.24659
H	-6.38223	-1.73593	1.07628
C	-7.46363	0.41158	-1.32138
H	-6.19049	1.42277	-2.73344
H	-8.46568	-0.71089	0.21863
H	-8.37496	0.86658	-1.6964
C	2.05491	-2.53342	-1.00711
C	3.03194	-3.50962	-0.78063
C	2.20229	-1.6614	-2.09497
C	4.12236	-3.62761	-1.63257
H	2.93787	-4.16311	0.082
C	3.30039	-1.77244	-2.94029
H	1.46857	-0.87893	-2.26915
C	4.26008	-2.75584	-2.71067
H	4.87414	-4.38699	-1.44565
H	3.41078	-1.08834	-3.77563
H	5.12021	-2.83717	-3.36751
C	1.61296	0.29164	0.56313
C	2.82033	0.70057	0.11679
C	3.78781	-0.33727	0.49539
N	1.73895	-1.01429	1.10241
C	0.27197	0.88629	0.51352
C	-0.61595	0.71017	1.583
C	-0.13441	1.5997	-0.61903
C	-1.89556	1.24868	1.51135
H	-0.31902	0.14204	2.46247
C	-1.41602	2.13431	-0.68251
H	0.55218	1.72371	-1.45138
C	-2.29853	1.95906	0.38209
H	-1.72486	2.68807	-1.5637
H	-3.30451	2.36421	0.32657
C	3.28901	1.93827	-0.58541
H	4.36046	2.03259	-0.36657

H	3.22616	1.78078	-1.67091
C	2.56136	3.21418	-0.21601
C	2.17217	4.11189	-1.20998
C	2.27075	3.51735	1.11598
C	1.49597	5.28557	-0.88575
H	2.39483	3.8859	-2.25063
C	1.59301	4.68665	1.44344
H	2.56329	2.82351	1.90027
C	1.20058	5.57362	0.44298
H	1.1972	5.97137	-1.67271
H	1.36756	4.90409	2.4828
H	0.66772	6.48382	0.69938
O	3.08767	-1.31258	1.19852
O	4.96858	-0.41821	0.32181
Cl	0.43838	-2.30457	3.39907
H	-0.90612	-2.54119	1.98834
H	-2.58368	1.09899	2.33702
H	1.2832	-1.28442	2.03827

- Molecular complex 2 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-2.31395	-1.20733	0.40234
C	-1.11107	-1.19079	-0.21637
H	-1.02235	-0.60893	-1.12599
C	-3.46203	-0.51496	-0.18176
H	-3.29499	-0.04774	-1.14905
C	0.04663	-2.01648	0.21983
H	-0.29695	-2.76421	0.9425
C	-4.6488	-0.44506	0.43907
H	-4.7275	-0.91393	1.41752
O	-2.56991	-1.876	1.54805
C	-5.85581	0.22108	-0.06236
C	-5.98239	0.67936	-1.38203
C	-6.93393	0.40847	0.81229
C	-7.14149	1.3168	-1.80324
H	-5.17318	0.52087	-2.08859
C	-8.09508	1.04823	0.39237
H	-6.85065	0.0502	1.835
C	-8.20208	1.5068	-0.91736
H	-7.22335	1.66162	-2.82954
H	-8.91704	1.18643	1.08789
H	-9.10817	2.00331	-1.25025
C	0.83079	-2.68028	-0.88862
C	1.32338	-3.97276	-0.6974
C	1.11148	-2.01699	-2.08701
C	2.07886	-4.5965	-1.68621
H	1.11937	-4.48768	0.2372
C	1.8702	-2.6379	-3.07397
H	0.7384	-1.01063	-2.25538
C	2.35382	-3.92942	-2.87617
H	2.45345	-5.60186	-1.5238
H	2.07873	-2.11422	-4.00176
H	2.94264	-4.41403	-3.6486
C	1.81706	-0.1564	0.44749
C	3.12234	-0.45867	0.52039
C	3.24382	-1.73553	1.24338
N	1.04392	-1.20672	1.09907
C	1.1134	1.00059	-0.11425
C	0.06869	1.61433	0.58843
C	1.53567	1.52315	-1.34165
C	-0.53566	2.7497	0.06134
H	-0.26415	1.2108	1.54195
C	0.9283	2.66037	-1.85902
H	2.33949	1.0332	-1.88378
C	-0.10676	3.27437	-1.15646
H	1.26474	3.06718	-2.80699
H	-0.58138	4.16334	-1.56007
C	4.36602	0.25833	0.08589
H	5.16522	-0.07436	0.76082
H	4.65298	-0.1069	-0.9086
C	4.27664	1.76938	0.07052
C	4.75493	2.48769	-1.02466
C	3.7064	2.46616	1.13832
C	4.6524	3.87626	-1.06469
H	5.20235	1.95389	-1.8602
C	3.59488	3.85133	1.0982
H	3.3241	1.91847	1.99667
C	4.06417	4.56072	-0.00595
H	5.02625	4.42038	-1.92665
H	3.1366	4.3775	1.92966
H	3.97303	5.64184	-0.03784
O	1.96675	-2.13014	1.61531
O	4.20411	-2.37557	1.54411
Cl	-0.47602	-0.62202	3.43426
H	-1.90769	-1.63547	2.23917
H	-1.34357	3.22521	0.6074
H	0.44612	-0.86362	2.04171

- Molecular complex 3 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	2.07246	-0.26935	-0.82806
C	1.04484	-1.00238	-0.3305

H	1.0499	-1.19539	0.73693
C	3.22879	0.0845	-0.00781
H	3.23144	-0.31918	1.00116
C	-0.13769	-1.44227	-1.14097
H	0.17052	-1.58257	-2.18489
C	4.226	0.86089	-0.45614
H	4.14163	1.25971	-1.46471
O	2.15892	0.148	-2.10894
C	5.4227	1.2498	0.2982
C	6.21534	2.29756	-0.18729
C	5.80992	0.615	1.4872
C	7.34765	2.71658	0.50267
H	5.9301	2.78976	-1.11334
C	6.94141	1.03075	2.17569
H	5.23275	-0.22375	1.86473
C	7.71295	2.08563	1.68839
H	7.94604	3.53393	0.11258
H	7.22983	0.52532	3.09218
H	8.59877	2.40673	2.22733
C	-0.81789	-2.72952	-0.7024
C	-1.8209	-3.24307	-1.5299
C	-0.50847	-3.39921	0.47898
C	-2.52129	-4.38725	-1.17038
H	-2.06376	-2.71995	-2.45152
C	-1.21173	-4.54584	0.84308
H	0.27581	-3.03587	1.13399
C	-2.22223	-5.03904	0.02527
H	-3.29824	-4.77277	-1.82332
H	-0.96543	-5.05143	1.7715
H	-2.76825	-5.93279	0.31103
C	-1.58859	0.27565	-0.06703
C	-1.38199	1.60684	-0.12751
C	-0.7498	1.87756	-1.40988
N	-1.18688	-0.36369	-1.25117
C	-2.16133	-0.53188	1.02426
C	-1.58787	-0.4722	2.29683
C	-3.24612	-1.38135	0.78655
C	-2.08581	-1.2719	3.32205
H	-0.7373	0.18269	2.46771
C	-3.73723	-2.17951	1.8117
H	-3.68134	-1.4232	-0.20668
C	-3.15556	-2.12885	3.07831
H	-4.56938	-2.84926	1.61988
H	-3.53771	-2.75868	3.87566
C	-1.81093	2.70499	0.79768
H	-1.88825	2.32282	1.81961
H	-1.03984	3.48268	0.78811
C	-3.1418	3.28842	0.36381
C	-3.1983	4.23258	-0.6639
C	-4.32824	2.84706	0.95076
C	-4.42532	4.73396	-1.08864
H	-2.27552	4.56051	-1.13558
C	-5.55554	3.35003	0.52724
H	-4.2875	2.10378	1.74416
C	-5.60614	4.29621	-0.49302
H	-4.45891	5.46922	-1.88687
H	-6.47202	3.00381	0.99556
H	-6.56212	4.6908	-0.82327
O	-0.62696	0.65143	-2.05796
O	-0.37685	2.89138	-1.93481
Cl	2.58136	-3.79561	-1.71692
H	1.26602	0.25305	-2.48165
H	2.22194	-2.72715	-1.06975
H	-1.63305	-1.23055	4.30765

- Transition state 2 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.36616	-2.48735	-0.33703
C	-1.51715	-1.78844	0.03655
H	-1.46612	-1.38117	1.04412
C	0.82126	-2.51804	0.49257
H	0.71228	-2.13457	1.50335
C	-2.16434	-0.84508	-0.96719
H	-2.29249	-1.34321	-1.93368
C	2.03352	-2.72854	-0.05396
H	2.0842	-2.98284	-1.11027
O	-0.27571	-3.13813	-1.48309
C	3.30589	-2.48973	0.62982
C	4.40282	-2.06385	-0.13164
C	3.44707	-2.62233	2.01764
C	5.60971	-1.75608	0.48679
H	4.28402	-1.94417	-1.20511
C	4.65771	-2.32509	2.63094
H	2.61098	-2.98403	2.60997
C	5.73947	-1.88638	1.86805
H	6.45031	-1.41538	-0.10957
H	4.76165	-2.44091	3.70517
H	6.68359	-1.65248	2.34984
C	-3.50859	-0.27827	-0.5544
C	-4.1741	0.55037	-1.46196
C	-4.08688	-0.53078	0.68668
C	-5.38337	1.14305	-1.12226
H	-3.72087	0.74518	-2.43078
C	-5.29886	0.06499	1.02992

H	-3.60126	-1.19454	1.39461
C	-5.94509	0.90795	0.13223
H	-5.88986	1.78572	-1.83579
H	-5.73684	-0.13473	2.00275
H	-6.88936	1.37079	0.40207
C	-0.57631	0.91071	-0.20427
C	0.76371	0.78312	-0.29701
C	1.02673	0.00136	-1.49869
N	-1.22334	0.29003	-1.29231
C	-1.39109	1.55992	0.83683
C	-1.18331	1.23963	2.18144
C	-2.39589	2.46775	0.48709
C	-1.98582	1.80798	3.16651
H	-0.40707	0.52579	2.44664
C	-3.19728	3.02947	1.47254
H	-2.55397	2.70769	-0.55923
C	-2.99604	2.6977	2.81197
H	-3.98644	3.72039	1.194
H	-3.62848	3.13296	3.57932
C	1.87873	1.3178	0.54655
H	1.46828	1.75173	1.46378
H	2.5272	0.47985	0.83393
C	2.69134	2.3576	-0.19997
C	3.90529	2.02397	-0.79888
C	2.20586	3.661	-0.32266
C	4.62957	2.98373	-1.50187
H	4.27316	1.00441	-0.71864
C	2.92823	4.62129	-1.02312
H	1.25305	3.91963	0.13539
C	4.14431	4.28354	-1.61392
H	5.57368	2.71407	-1.96534
H	2.54356	5.63313	-1.10787
H	4.7099	5.03137	-2.1612
O	-0.19789	-0.27101	-2.07548
O	2.05408	-0.39672	-1.98514
Cl	-3.32429	-3.9121	-0.87244
H	-1.15466	-3.21109	-1.90694
H	-2.47444	-2.888	-0.15327
H	-1.8271	1.54883	4.20839

- Molecular complex 4 (pathway 2)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.66413	-2.73741	0.23571
C	-1.84013	-1.83402	0.56997
H	-1.62592	-1.23514	1.4607
C	0.61278	-2.46432	0.9157
H	0.58907	-1.81972	1.79085
C	-2.22098	-0.91427	-0.60622
H	-2.37962	-1.54175	-1.48891
C	1.77768	-2.84374	0.36482
H	1.73863	-3.38802	-0.57768
O	-0.77859	-3.62623	-0.59955
C	3.0986	-2.46514	0.87558
C	4.15717	-2.3121	-0.02921
C	3.3171	-2.19338	2.23312
C	5.39893	-1.86707	0.4114
H	3.98122	-2.50289	-1.08334
C	4.56094	-1.75677	2.67223
H	2.51202	-2.34564	2.94667
C	5.60234	-1.58538	1.76084
H	6.20873	-1.73798	-0.29989
H	4.72202	-1.55506	3.72657
H	6.57263	-1.24043	2.10419
C	-3.48301	-0.10246	-0.36979
C	-4.02379	0.59095	-1.45628
C	-4.09588	0.00642	0.87636
C	-5.14308	1.3976	-1.29477
H	-3.54374	0.50637	-2.42798
C	-5.21924	0.81459	1.0406
H	-3.69386	-0.51697	1.738
C	-5.74136	1.51606	-0.0405
H	-5.55218	1.93113	-2.14714
H	-5.68028	0.89864	2.01977
H	-6.61568	2.14646	0.08907
C	-0.41288	0.74668	-0.07989
C	0.91879	0.57855	-0.23812
C	1.09017	-0.38072	-1.31925
N	-1.12725	0.0000	-1.02401
C	-1.14217	1.61547	0.86338
C	-0.94818	1.47071	2.23916
C	-2.03709	2.57811	0.38486
C	-1.66336	2.26516	3.1318
H	-0.24691	0.72387	2.60419
C	-2.7488	3.36789	1.27837
H	-2.18393	2.68194	-0.68545
C	-2.56728	3.20871	2.65205
H	-3.45386	4.10225	0.90233
H	-3.12961	3.82302	3.34828
C	2.08472	1.2305	0.43848
H	1.73459	1.77225	1.32325
H	2.77444	0.44729	0.77816
C	2.80987	2.17804	-0.4968
C	3.93479	1.75798	-1.20606
C	2.32902	3.47506	-0.68615

C	4.57613	2.62752	-2.08481
H	4.29415	0.74089	-1.07343
C	2.96972	4.34555	-1.56192
H	1.44444	3.79994	-0.14153
C	4.09728	3.92257	-2.26286
H	5.45073	2.29123	-2.63333
H	2.5905	5.354	-1.69723
H	4.59906	4.60019	-2.94679
O	-0.17356	-0.74809	-1.73651
O	2.07644	-0.84938	-1.82913
Cl	-3.64276	-4.07525	-1.53949
H	-2.36684	-3.96479	-1.21851
H	-2.70837	-2.46994	0.77923
H	-1.51617	2.14377	4.20026

- Molecular complex 1 (pathway 3)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.78124	-2.66766	-0.51633
C	0.29516	-1.89847	-1.07348
H	0.07216	-0.9001	-1.43061
C	-2.17313	-2.28301	-0.65508
H	-2.86485	-2.95688	-0.16026
C	1.56831	-2.36421	-1.11936
H	1.78343	-3.35717	-0.73569
C	-2.58814	-1.14428	-1.24431
H	-1.8547	-0.49208	-1.71362
O	-0.59311	-3.7368	0.16395
C	-3.9588	-0.64358	-1.29465
C	-4.19187	0.59309	-1.91107
C	-5.04054	-1.32595	-0.71673
C	-5.46986	1.13823	-1.95387
H	-3.35715	1.13035	-2.35496
C	-6.31599	-0.78277	-0.76084
H	-4.88252	-2.28103	-0.22583
C	-6.53439	0.45028	-1.37824
H	-5.63438	2.09729	-2.43398
H	-7.14559	-1.31873	-0.31124
H	-7.53401	0.87205	-1.40775
C	2.71465	-1.61744	-1.60259
C	3.98452	-1.99697	-1.14196
C	2.59354	-0.51881	-2.47024
C	5.1072	-1.26993	-1.5159
H	4.06649	-2.8343	-0.45349
C	3.72027	0.18494	-2.86245
H	1.61708	-0.23903	-2.85681
C	4.97591	-0.18385	-2.37665
H	6.08273	-1.54493	-1.12989
H	3.62537	1.03031	-3.53619
H	5.85289	0.38649	-2.66489
C	0.98038	0.11847	1.33759
C	1.53885	0.99191	0.45549
C	2.9787	0.82191	0.57101
N	1.97257	-0.55169	2.03458
C	-0.43021	-0.15162	1.66458
C	-0.80262	-1.34397	2.2993
C	-1.41961	0.79085	1.35098
C	-2.14243	-1.5989	2.5796
H	-0.05659	-2.08854	2.56567
C	-2.7559	0.53136	1.63781
H	-1.13716	1.75102	0.9333
C	-3.1227	-0.66758	2.24514
H	-3.51204	1.27043	1.38954
H	-4.16719	-0.86722	2.46606
C	0.96635	1.94873	-0.5462
H	1.69923	2.01019	-1.36182
H	0.03876	1.54555	-0.97494
C	0.71094	3.35064	-0.02391
C	-0.50794	3.99104	-0.24524
C	1.71809	4.03105	0.66738
C	-0.72848	5.28618	0.22127
H	-1.29471	3.47049	-0.78959
C	1.50025	5.32315	1.13181
H	2.67687	3.54241	0.82285
C	0.27581	5.95413	0.91316
H	-1.68461	5.76951	0.04423
H	2.29007	5.84187	1.66655
H	0.10822	6.96192	1.28015
O	3.20047	-0.18037	1.48621
O	3.8922	1.40783	0.03756
Cl	1.73728	-3.8358	1.75452
H	0.35315	-3.82251	0.67646
H	-2.41347	-2.53173	3.06452
H	1.94384	-1.58221	2.06542

- Transition state 1 (pathway 3)

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.16051	1.59564	0.76649
C	0.23767	1.51404	-0.24882
H	0.6404	1.54523	-1.25398
C	2.60516	1.56811	0.49249
H	3.21431	2.05084	1.25207
C	-1.1888	1.52284	-0.08294

H	-1.53974	1.75267	0.92522
C	3.16117	0.91483	-0.53802
H	2.50921	0.35919	-1.21328
O	0.9338	1.72994	2.06075
C	4.59459	0.81691	-0.83462
C	5.02966	-0.14592	-1.75399
C	5.55045	1.64571	-0.22958
C	6.38038	-0.29337	-2.0501
H	4.29601	-0.78701	-2.23706
C	6.89877	1.49998	-0.5254
H	5.23354	2.41904	0.46343
C	7.31948	0.52862	-1.43414
H	6.69854	-1.04725	-2.76324
H	7.62624	2.15159	-0.05172
H	8.37441	0.4201	-1.66511
C	-2.02734	2.17369	-1.11936
C	-3.1821	2.84688	-0.7039
C	-1.70523	2.14849	-2.48197
C	-3.9922	3.49362	-1.62986
H	-3.43865	2.85731	0.35353
C	-2.52244	2.78547	-3.40679
H	-0.8159	1.62761	-2.82542
C	-3.66542	3.4616	-2.98235
H	-4.88167	4.01647	-1.29425
H	-2.26677	2.75758	-4.46121
H	-4.30069	3.96034	-3.70749
C	-1.53352	-0.71901	1.21209
C	-1.83934	-0.40869	-0.15264
C	-3.29664	-0.16475	-0.1236
N	-2.58499	-0.40952	1.97653
C	-0.2872	-1.1189	1.84251
C	-0.1908	-1.16536	3.24544
C	0.84291	-1.39934	1.06321
C	1.02603	-1.4423	3.84471
H	-1.05881	-0.96433	3.86358
C	2.05983	-1.67978	1.67217
H	0.77338	-1.38867	-0.01568
C	2.15392	-1.69005	3.06
H	2.93481	-1.87753	1.06127
H	3.10687	-1.90002	3.53561
C	-1.29727	-1.0207	-1.42242
H	-1.93756	-0.63899	-2.22778
H	-0.28272	-0.657	-1.62171
C	-1.3156	-2.53675	-1.43655
C	-0.15745	-3.26148	-1.71774
C	-2.50227	-3.23403	-1.18876
C	-0.17364	-4.65447	-1.73835
H	0.76876	-2.73063	-1.93028
C	-2.52092	-4.62425	-1.20681
H	-3.42108	-2.68372	-1.00181
C	-1.35553	-5.33933	-1.4776
H	0.73818	-5.20162	-1.95694
H	-3.45018	-5.15116	-1.01387
H	-1.37168	-6.42453	-1.48971
O	-3.65597	0.00431	1.1965
O	-4.0915	-0.0733	-1.01498
Cl	-1.75256	1.92596	3.48001
H	-0.01393	1.81606	2.36157
H	1.09949	-1.45755	4.92656
H	-2.43787	0.30586	2.77694

- Molecular complex 2 (pathway 3)

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.47602	-1.18006	0.94605
C	-0.53222	-1.34159	0.00053
H	-0.88581	-1.50428	-1.01129
C	-2.91392	-1.10633	0.65104
H	-3.56089	-1.41788	1.46786
C	0.95039	-1.39616	0.23559
H	1.14367	-1.53852	1.30808
C	-3.4255	-0.61543	-0.48546
H	-2.74043	-0.2209	-1.23662
O	-1.26392	-1.03736	2.2772
C	-4.85147	-0.50298	-0.81826
C	-5.23739	0.33481	-1.87209
C	-5.84913	-1.19494	-0.11707
C	-6.57797	0.49669	-2.20533
H	-4.47215	0.86752	-2.43204
C	-7.18789	-1.03392	-0.44837
H	-5.57164	-1.87651	0.68131
C	-7.5588	-0.18569	-1.49156
H	-6.8558	1.15367	-3.02366
H	-7.94711	-1.57956	0.10344
H	-8.60603	-0.06552	-1.75035
C	1.58516	-2.59059	-0.46199
C	2.47968	-3.39544	0.24569
C	1.29437	-2.9207	-1.78844
C	3.07523	-4.50045	-0.35338
H	2.71767	-3.14804	1.27835
C	1.8922	-4.02237	-2.3929
H	0.59348	-2.31991	-2.36156
C	2.7838	-4.81629	-1.67696
H	3.76812	-5.11259	0.21511
H	1.65574	-4.26266	-3.42484

H	3.24694	-5.67749	-2.14813
C	1.37462	0.97808	0.97479
C	1.69192	-0.0217	-0.11876
C	3.17083	-0.23629	0.17623
N	2.35384	1.10067	1.80511
C	0.11253	1.68267	1.28379
C	-0.05097	2.2726	2.54639
C	-0.93377	1.77076	0.36057
C	-1.2339	2.91881	2.8743
H	0.75493	2.22099	3.27025
C	-2.12003	2.41729	0.69162
H	-0.83582	1.31255	-0.61515
C	-2.27462	2.98941	1.94979
H	-2.92844	2.45791	-0.032
H	-3.20369	3.48567	2.2116
C	1.5452	0.40395	-1.59064
H	2.00563	-0.39683	-2.17912
H	0.48689	0.44139	-1.86614
C	2.2362	1.7144	-1.90695
C	1.5713	2.93725	-1.78087
C	3.57295	1.71692	-2.3187
C	2.2275	4.13469	-2.05118
H	0.52969	2.95929	-1.47374
C	4.23019	2.91389	-2.58812
H	4.09908	0.7724	-2.42316
C	3.56009	4.12656	-2.45349
H	1.69394	5.07467	-1.94916
H	5.26775	2.8963	-2.90683
H	4.0721	5.0602	-2.66461
O	3.45251	0.34671	1.38071
O	3.99769	-0.81676	-0.46017
Cl	1.55421	-0.83166	4.16297
H	-0.32419	-1.1078	2.51161
H	-1.34734	3.36148	3.85843
H	2.0717	0.17018	3.50932