# Supporting Information

## Synthesis of Potent Antifungal 3,4-Dichloroisothiazole-Based Strobilurins with Both Direct Fungicidal Activity and Systemic Acquired Resistance

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# $^1$H NMR spectra of intermediates6b-6d

Data for methyl 3,4-dichloro-N-methoxyisothiazole-5-carboxamide (**6b**). Yield 70%; white solid; mp125-126 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ 9.40 (s, 1H), 3.93 (s, 3H).

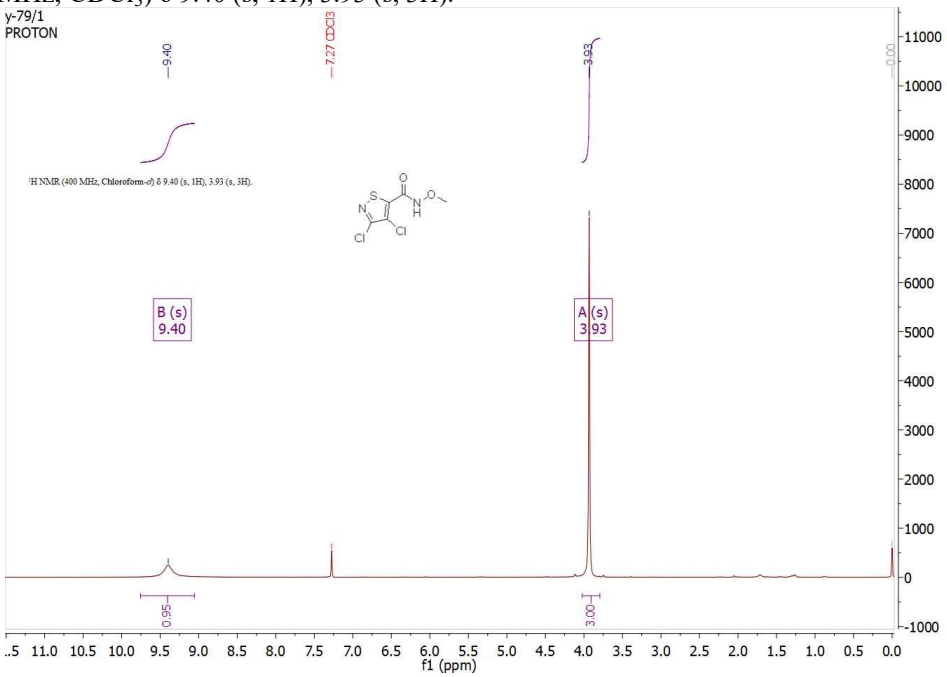


Figure S1. The $^1$H NMR (400 MHz, $CDCl_3$) of **6b**

Data for methyl 3,4-dichloro-N-(cyclopropylmethoxy)isothiazole-5-carboxamide (**6c**). Yield 59%; white solid; mp88-89 °C. $^1$H NMR (400 MHz, $CDCl_3$) δ3.87 – 3.66 (m, 2H), 1.28 (d, *J* = 18.5 Hz, 1H), 1.13 (s, 1H), 0.56 (s, 2H), 0.26 (s, 2H).

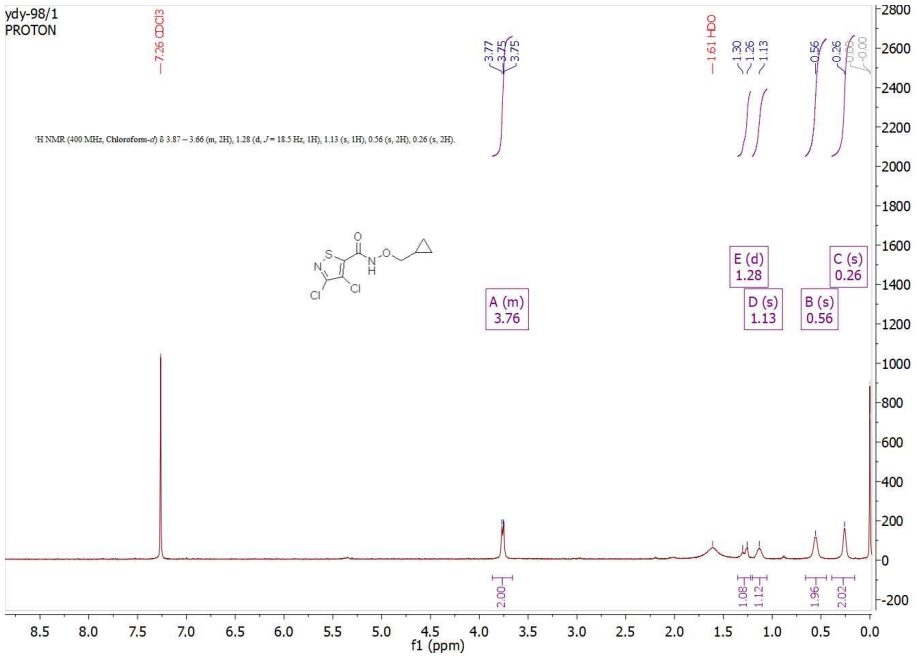


Figure S2. The $^1$H NMR (400 MHz, $CDCl_3$) of **6c**

Data for 3,4-dichloro-N-(prop-2-yn-1-yloxy)isothiazole-5-carboxamide (**6d**). Yield 60%; white solid; mp79-80°C. $^1$H NMR (400 MHz, $CDCl_3$) δ9.44 (s, 1H), 4.69 (d, $J$ = 2.4 Hz, 2H), 2.64 (t, $J$ = 2.4 Hz, 1H).

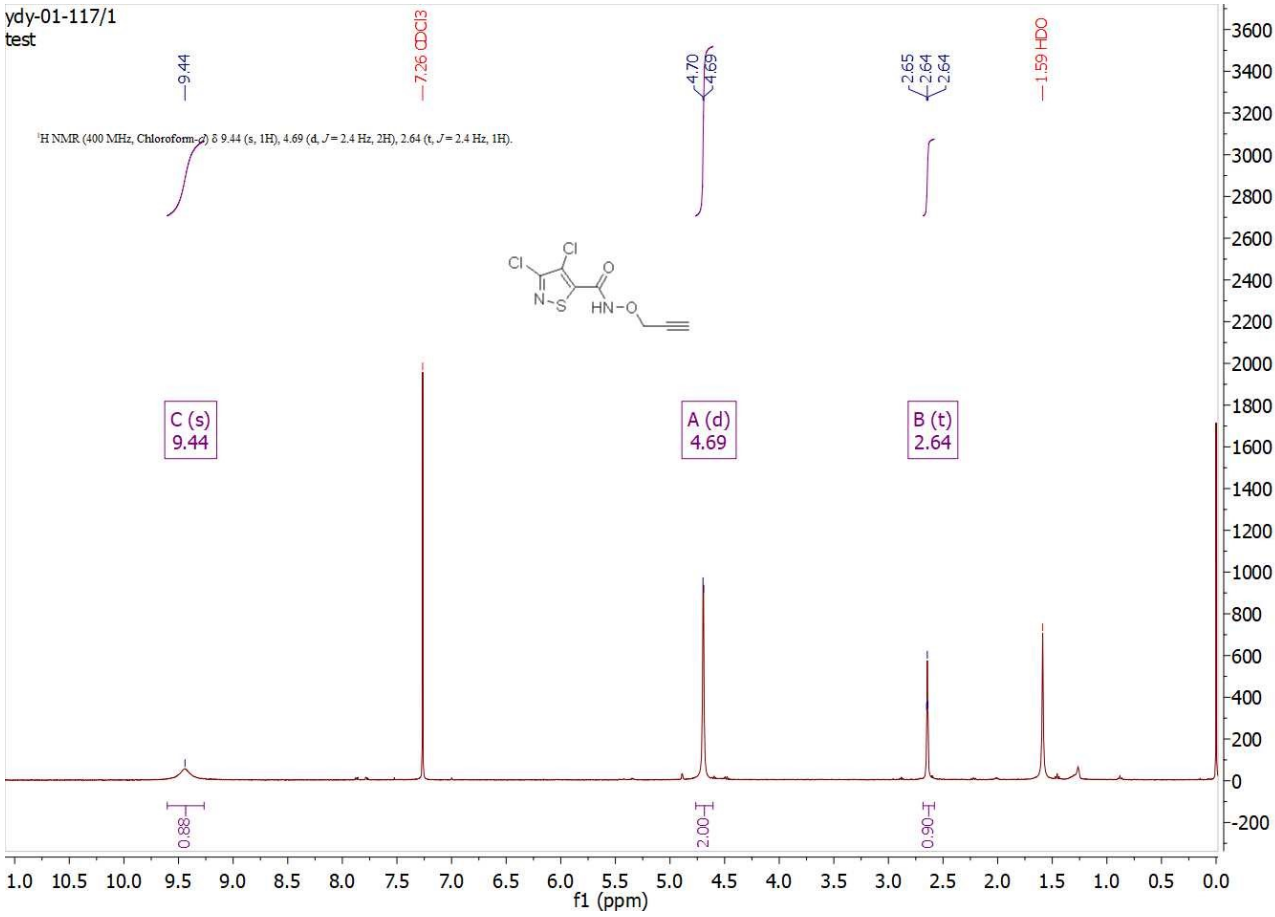


Figure S3. The $^1$H NMR (400 MHz, $CDCl_3$) of **6d**

## $^{1}$H NMR, $^{13}$C NMR and HRMS spectra of target compounds

Data for methyl (E)-2-(2-(((3,4-dichloroisothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**6a**). Yield 64%; white solid; mp108-109 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 7.53 – 7.31 (m, 3H), 7.20 (dd, *J* = 7.3, 1.6 Hz, 1H), 4.99 (s, 2H), 4.05 (s, 3H), 3.90 (s, 3H).$^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.52, 155.27, 154.45, 149.36, 149.13, 132.89, 131.29, 130.68, 129.62, 129.37, 128.45, 123.40, 76.95, 63.99, 53.37. HRMS (ESI) m/z calcd for $C_{15}H_{14}Cl_2N_3O_5S$ $(M+H)^+$418.0026, found 418.0027.

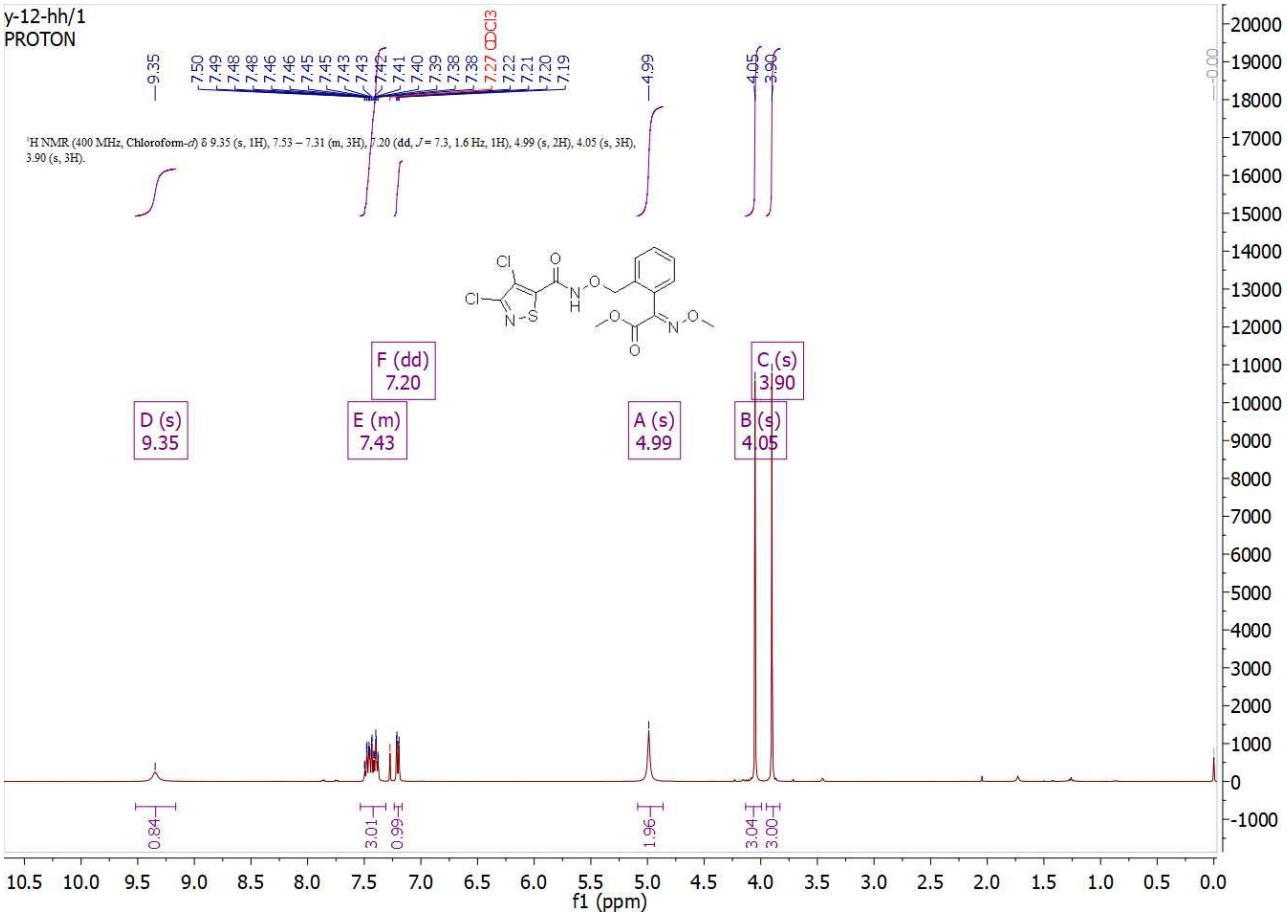


Figure S4. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **6a**

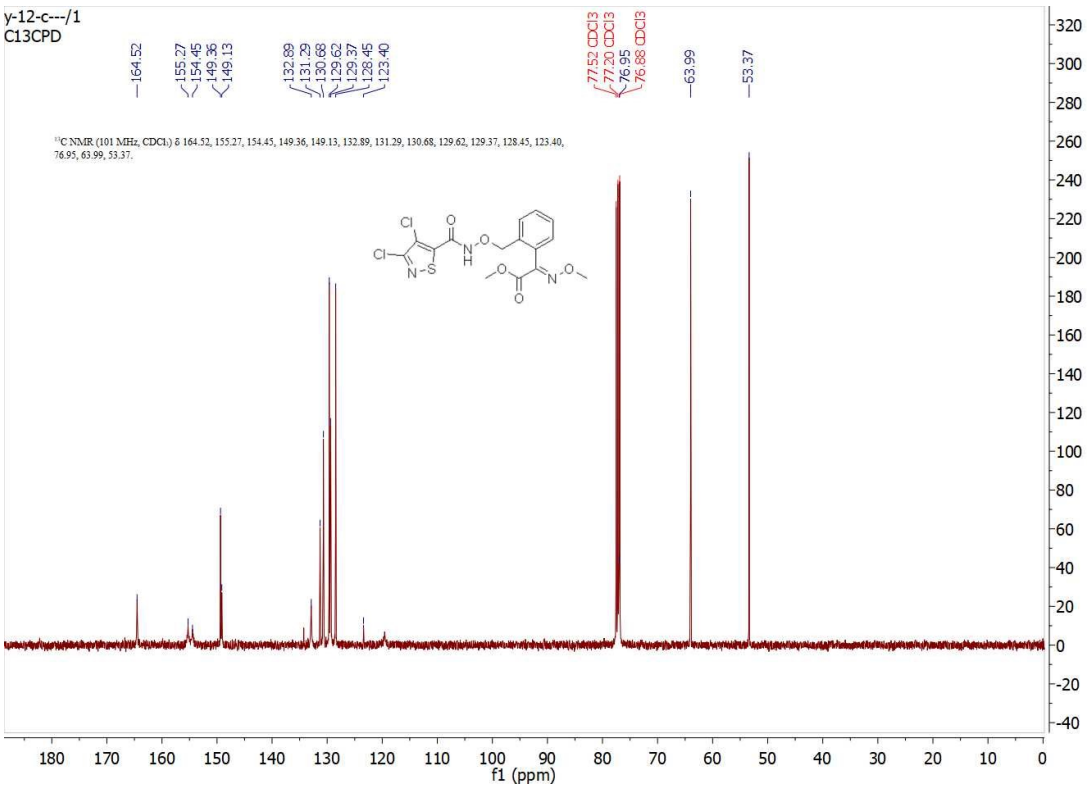


Figure S5. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **6a**

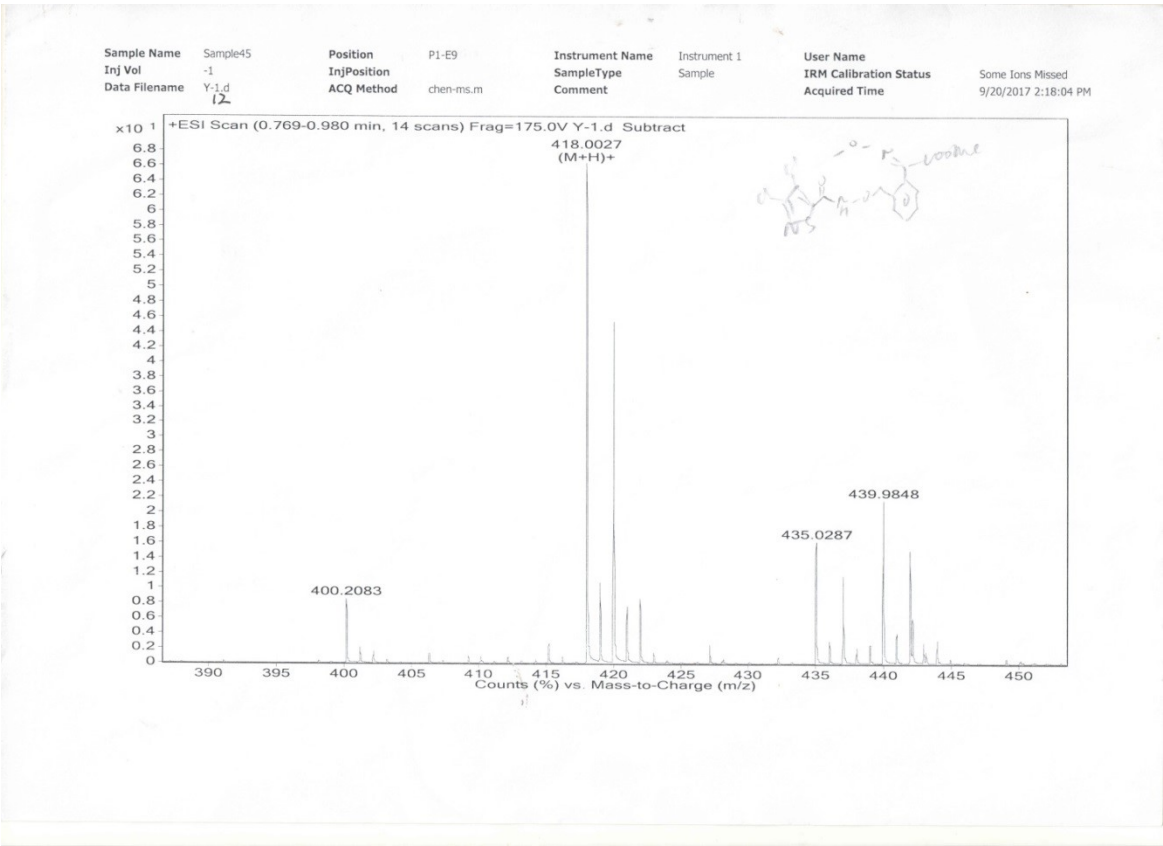


Figure S6. The HRMS spectra of **6a**

Data for methyl (E)-2-(2-(((3,4-dichloro-N-methylisothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**1a**). Yield 62%; white solid; mp79-80 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.36 (m, 3H), 7.26 – 7.22 (m, 1H), 4.76 (s, 2H), 4.04 (s, 3H), 3.88 (s, 3H), 3.26 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.08, 158.85, 149.28, 148.83, 147.82, 131.43, 130.90, 130.00, 129.77, 129.38, 128.92, 126.79,76.01, 64.05, 53.27, 34.33. HRMS (ESI) m/z calcd for $C_{16}H_{16}Cl_2N_3O_5S$ $(M+H)^+$432.0182, found 432.0186.

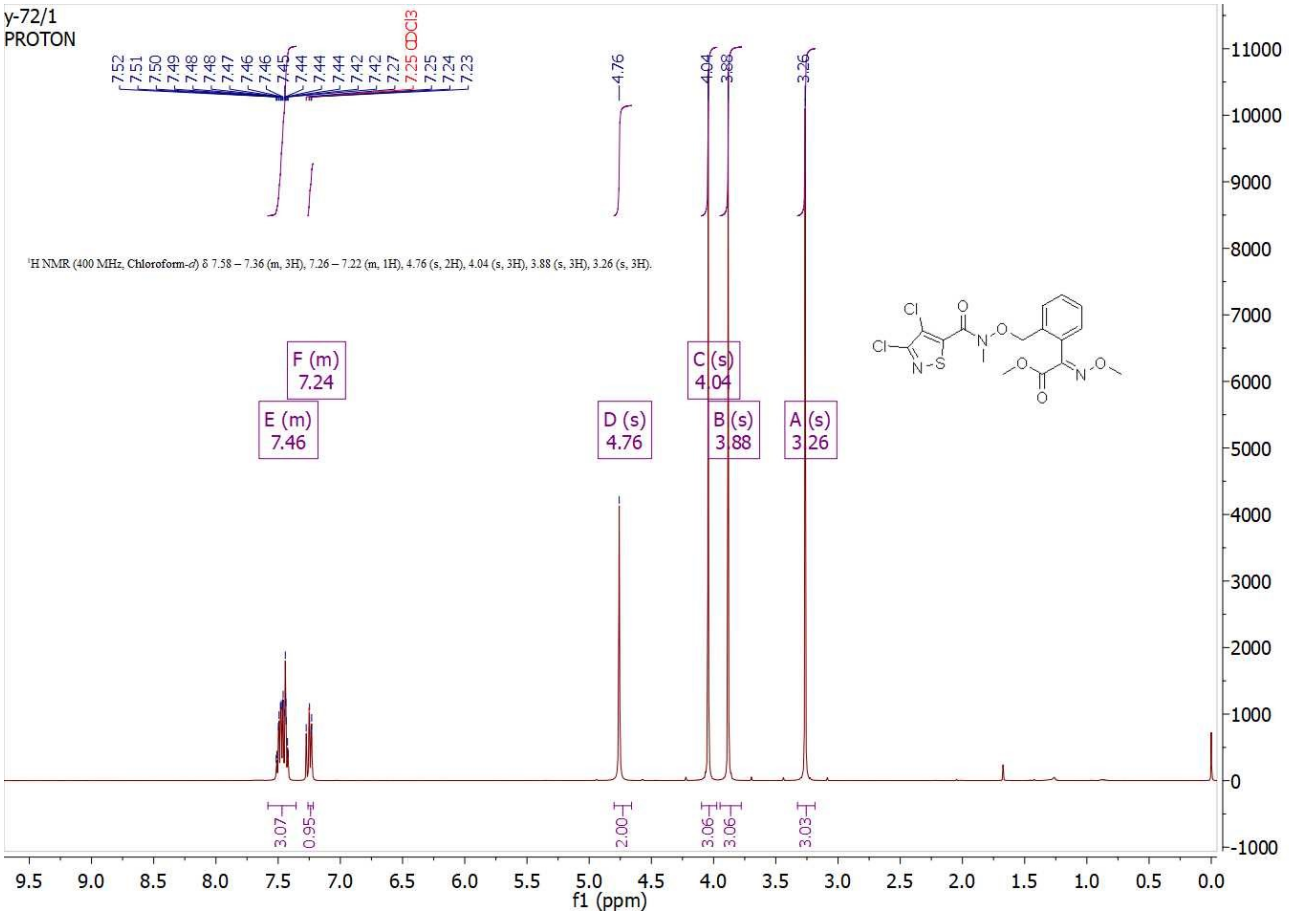


Figure S7. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **1a**

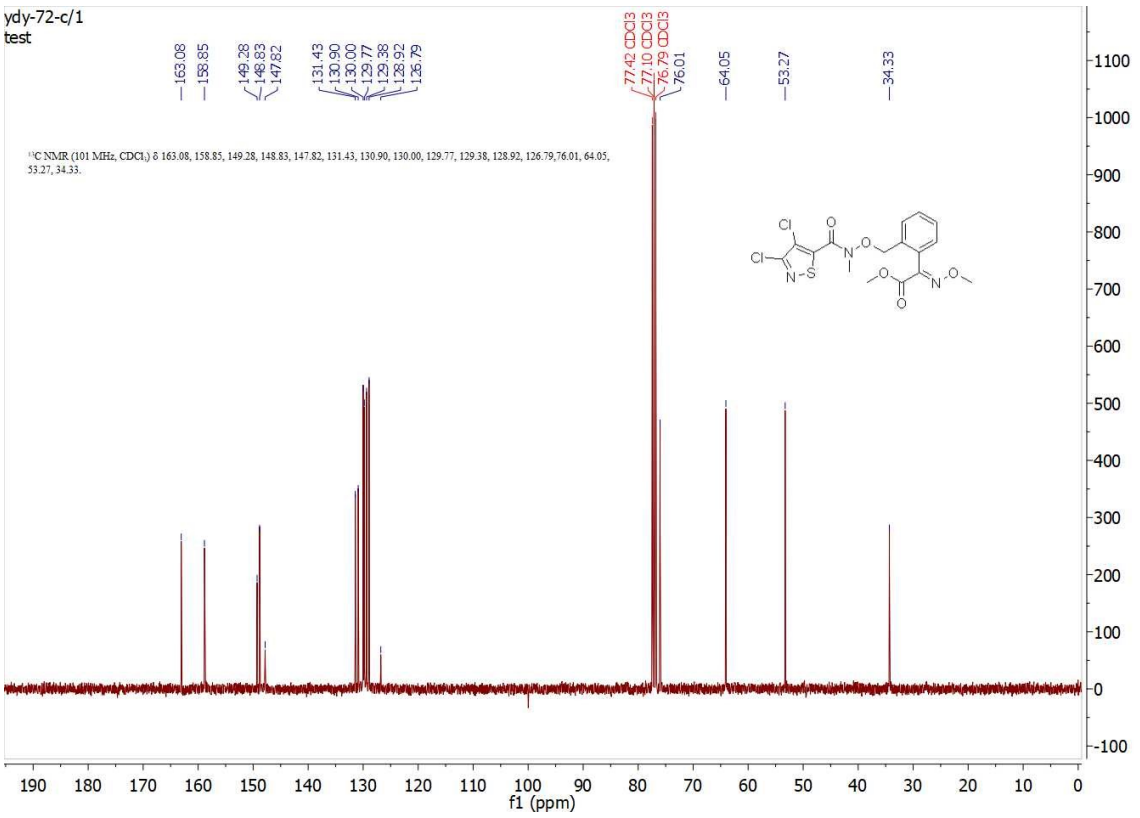


Figure S8. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **1a**

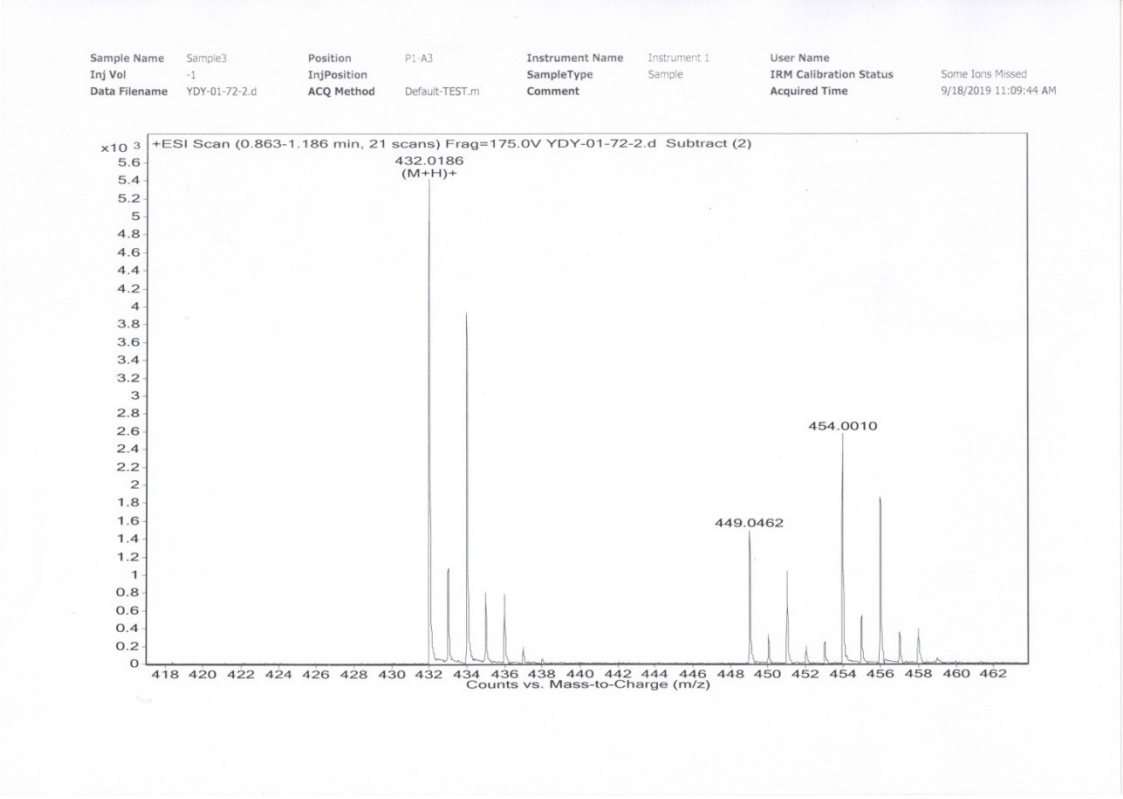


Figure S9. The HRMS spectra of **1a**

Data for methyl (E)-2-(2-(((N-allyl-3,4-dichloroisothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**1b**). Yield 54%; white crystal; mp107-108 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.39 (m, 3H), 7.25 (dd, *J* = 6.2, 2.5 Hz, 1H), 5.89 (ddt, *J* = 16.4, 10.2, 5.9 Hz, 1H), 5.39 – 5.22 (m, 2H), 4.80 (s, 2H), 4.32 (dt, *J* = 5.9, 1.4 Hz, 2H), 4.05 (s, 3H), 3.90 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.03, 158.81, 149.31, 148.70, 147.89, 131.51, 130.72, 130.58, 129.86, 129.75, 129.26, 128.84, 126.92, 119.39, 76.31, 64.05, 53.26, 50.06. HRMS (ESI) m/z calcd for $C_{18}H_{18}Cl_2N_3O_5S$ $(M+H)^+$458.0339, found 458.0340.

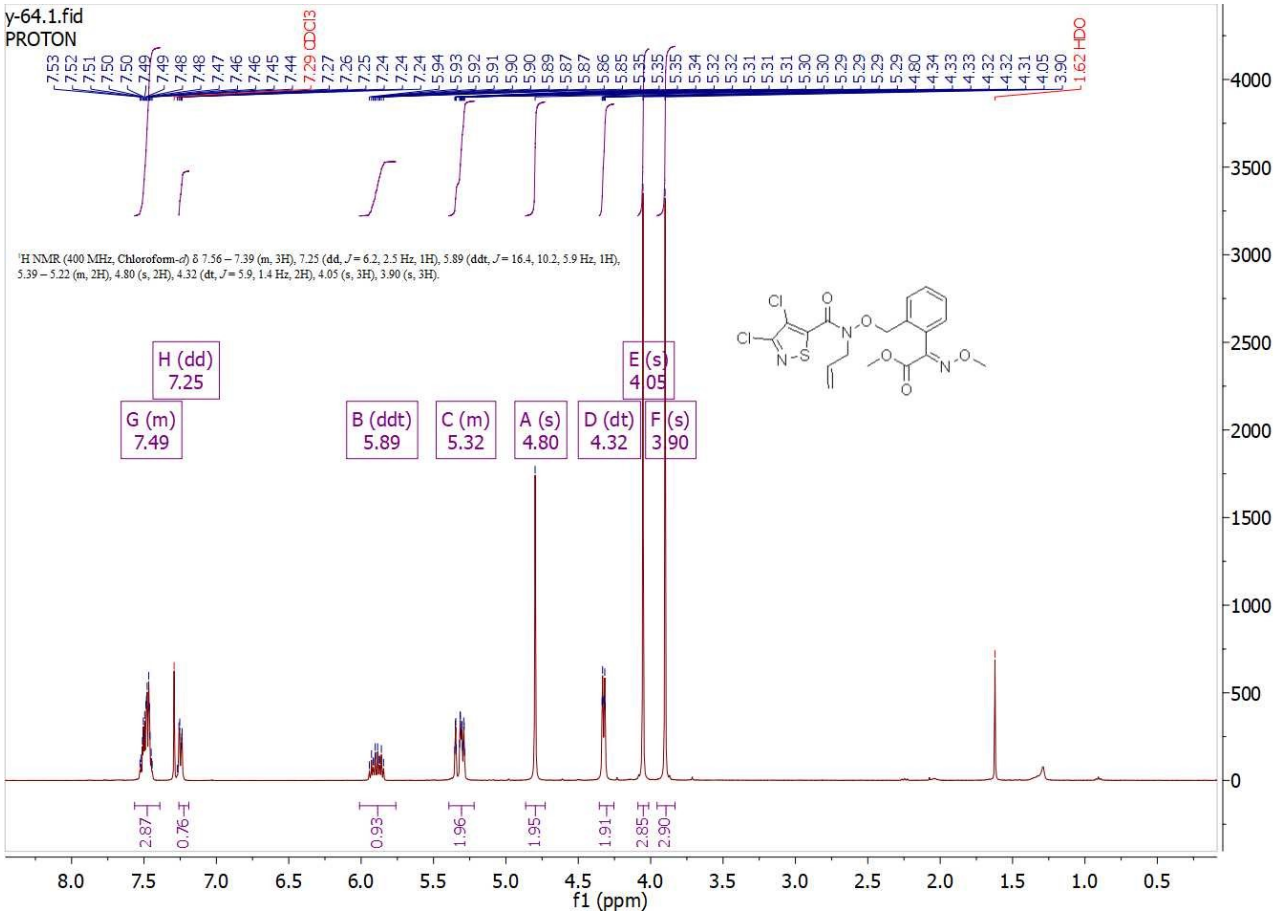


Figure S10. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **1b**

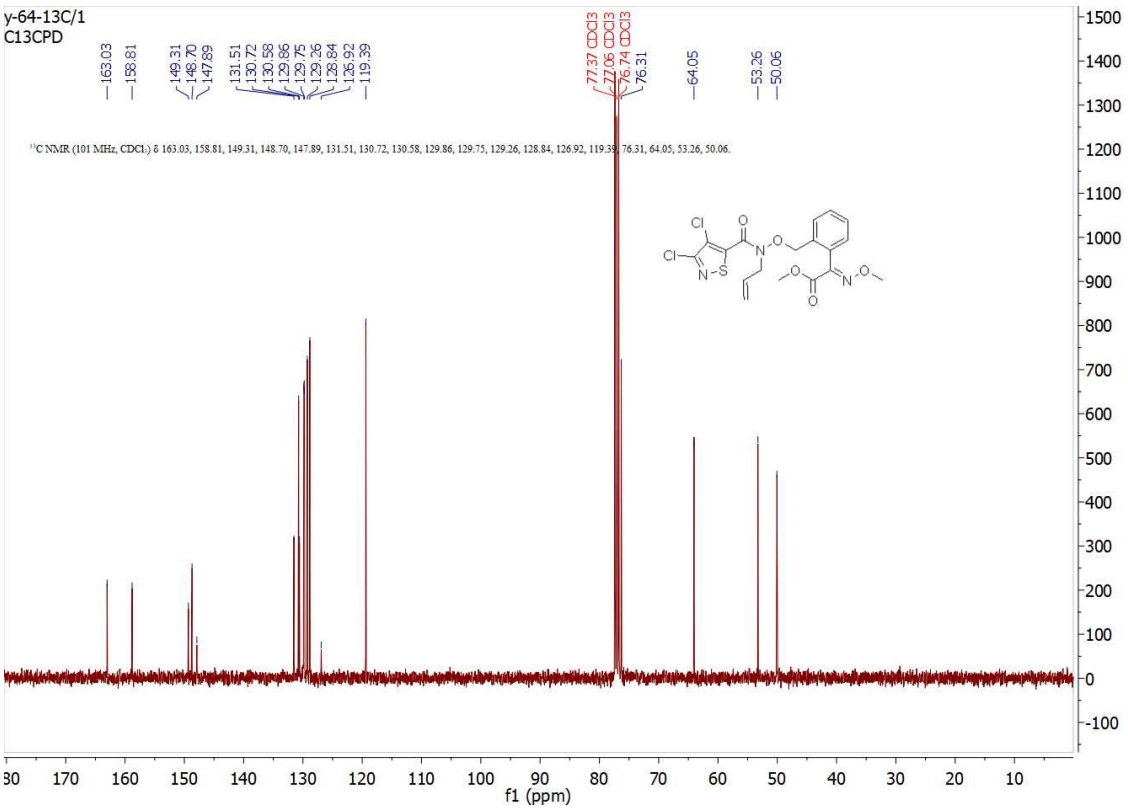


Figure S11. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **1b**

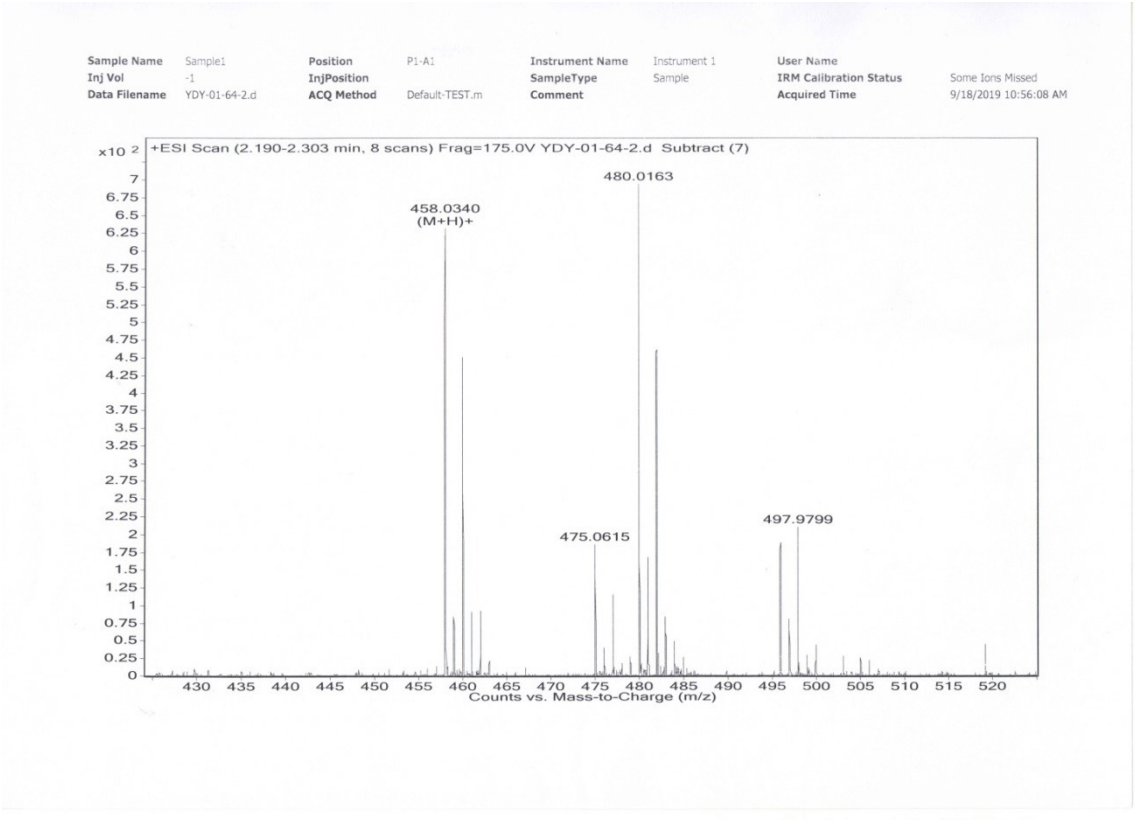


Figure S12. The HRMS spectra of **1b**

Data for methyl (E)-2-(2-(((3,4-dichloro-N-(prop-2-yn-1-yl)isothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**1c**). Yield 70%; white solid; mp140-140 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 7.53 – 7.31 (m, 3H), 7.20 (dd, *J* = 7.3, 1.6 Hz, 1H), 4.99 (s, 2H), 4.05 (s, 3H), 3.90 (s, 3H).$^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.52, 155.27, 154.45, 149.36, 149.13, 132.89, 131.29, 130.68, 129.62, 129.37, 128.45, 123.40, 76.95, 63.99, 53.37. HRMS (ESI) m/z calcd for $C_{18}H_{16}Cl_2N_3O_5S$ $(M+H)^+$456.0182, found 456.0182.

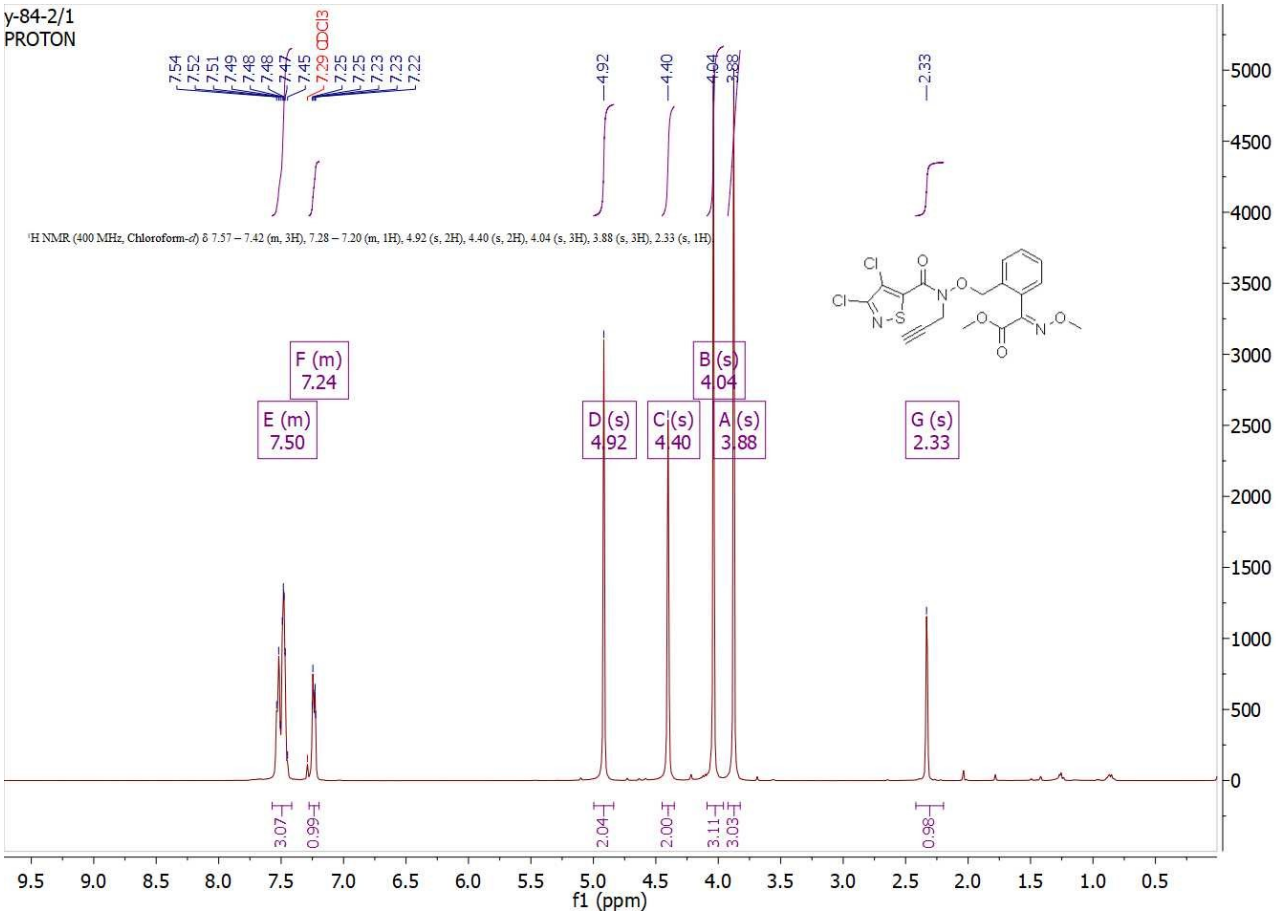


Figure S13. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **1c**

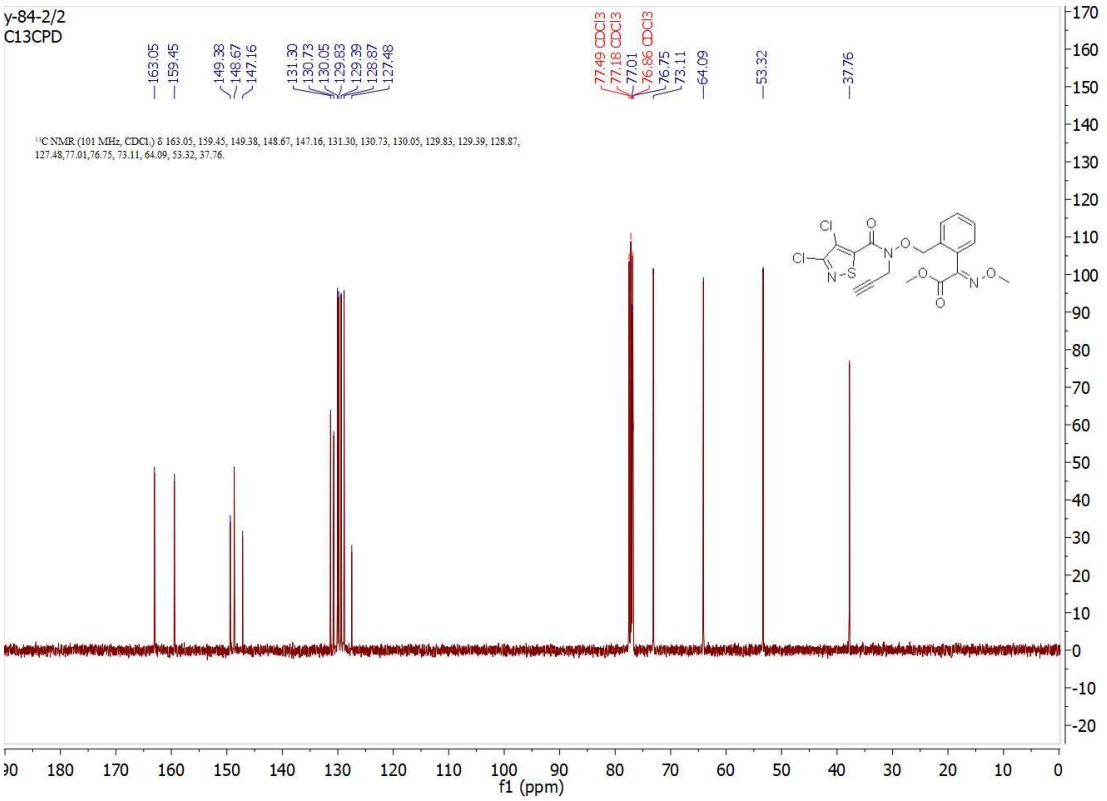


Figure S14. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **1c**

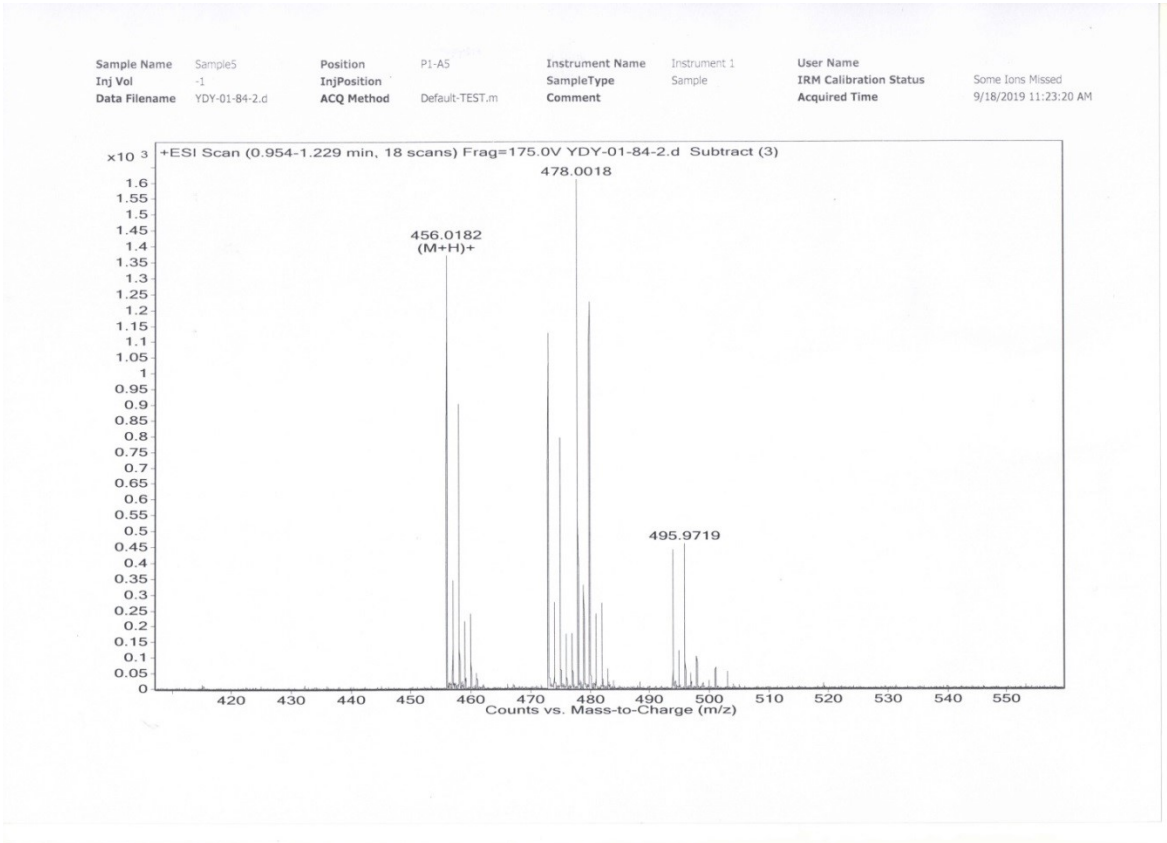


Figure S15. The HRMS spectra of **1c**

Data for methyl (E)-2-(2-(((N-(but-2-yn-1-yl)-3,4-dichloroisothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**1d**). Yield 44%; white solid; mp91-92 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.40 (m, 3H), 7.26 – 7.18 (m, 1H), 4.91 (s, 2H), 4.38 (s, 2H), 4.04 (s, 3H), 3.88 (s, 3H), 1.82 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.03, 159.17, 149.26, 148.70, 147.50, 131.47, 130.66, 129.96, 129.75, 129.26, 128.80, 127.20, 80.83, 76.79, 72.07, 64.02, 53.26, 38.10, 3.66. HRMS (ESI) m/z calcd for $C_{19}H_{18}Cl_2N_3O_5S$ $(M+H)^+$470.0339, found 470.0343.

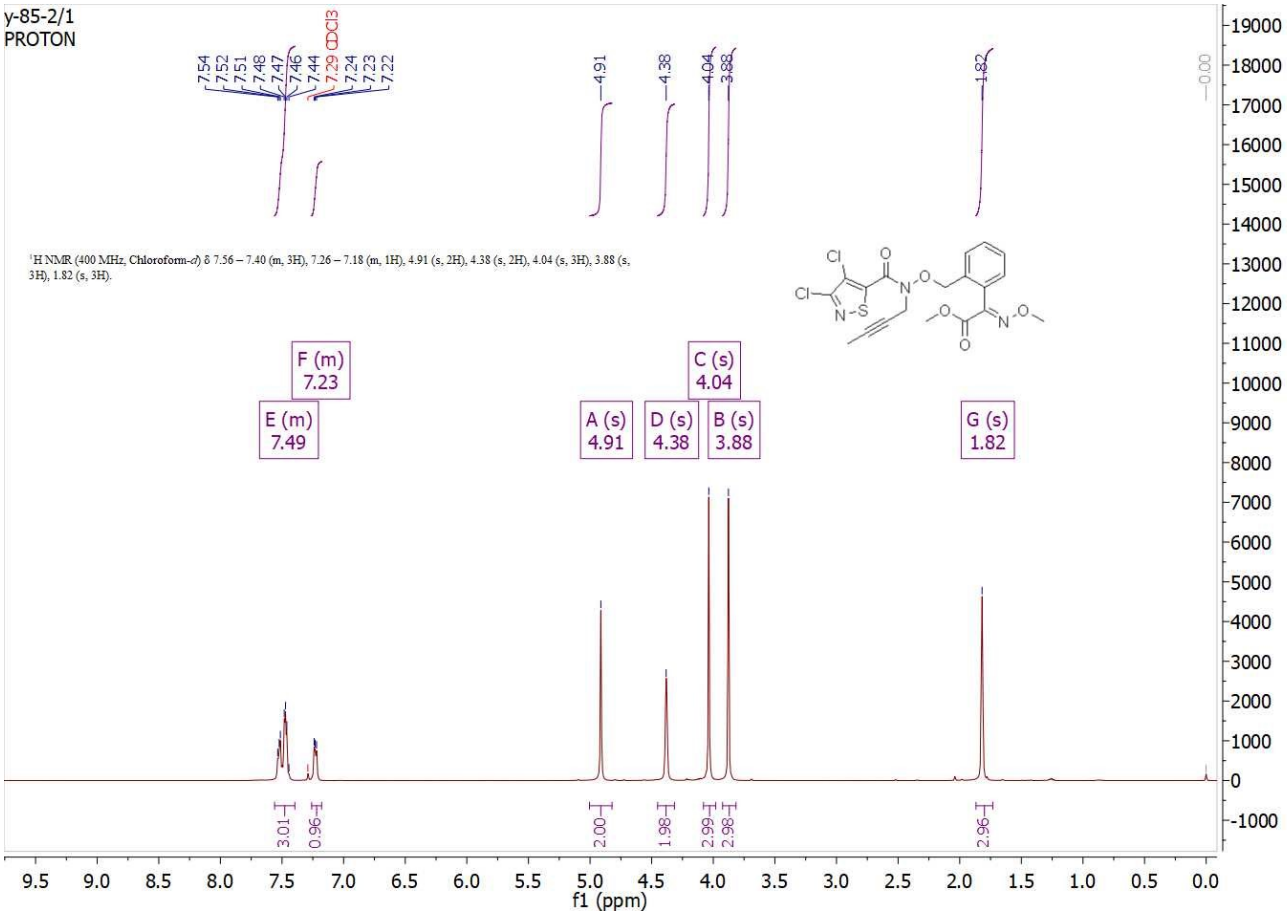


Figure S16. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **1d**

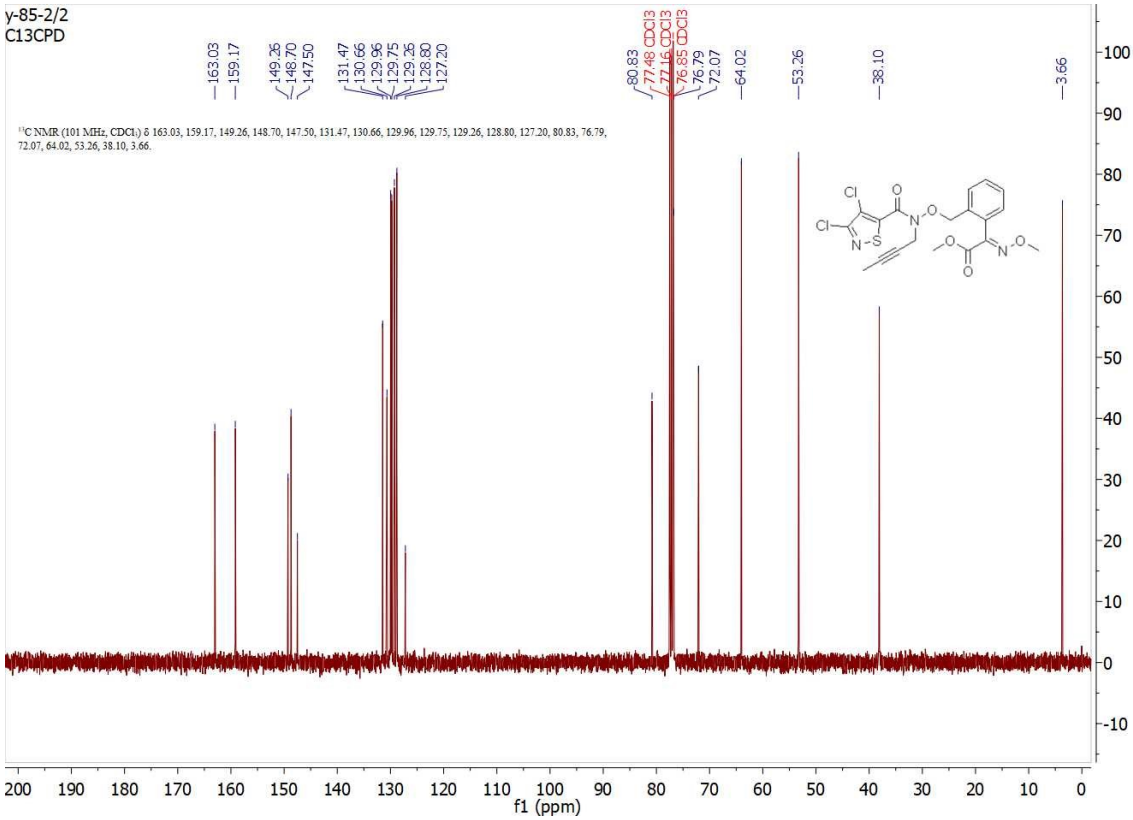


Figure S17. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **1d**

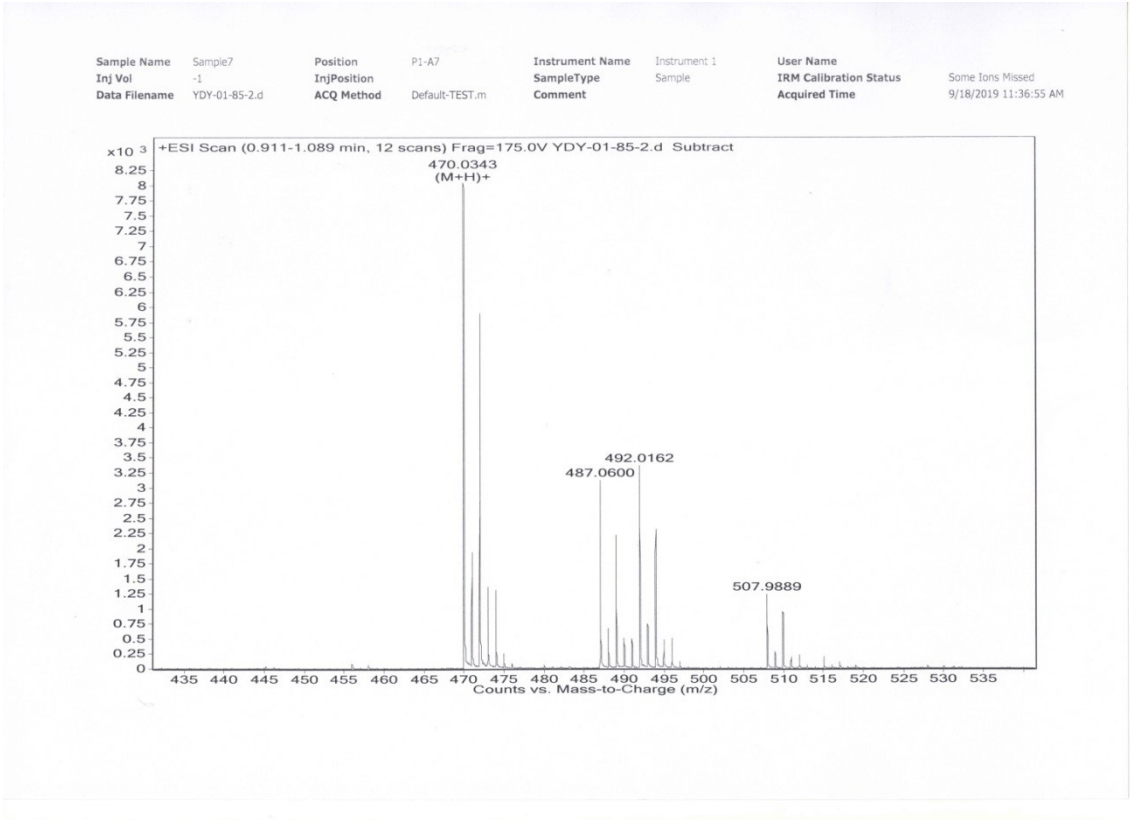


Figure S18. The HRMS spectra of **1d**

Data for methyl (E)-2-(2-(((3,4-dichloro-N-(cyclopropylmethyl)isothiazole-5-carboxamido)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**1e**). Yield 16%; white crystal; mp77-78 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.46 (tq, *J* = 5.4, 3.1 Hz, 3H), 7.23 (dt, *J* = 5.8, 2.6 Hz, 1H), 4.77 (s, 2H), 4.02 (s, 3H), 3.87 (s, 3H), 3.58 (d, *J* = 7.1 Hz, 2H), 1.30 – 1.13 (m, 1H), 0.64 – 0.49 (m, 2H), 0.43 – 0.27 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.04, 159.03, 149.15, 148.70, 148.48, 131.66, 130.37, 129.78, 129.59, 129.15, 128.84, 126.49, 76.00, 64.04, 53.28, 51.99, 9.33, 4.02. HRMS (ESI) m/z calcd for $C_{19}H_{20}Cl_2N_3O_5S$ $(M+H)^+$472.0495, found 472.0493.

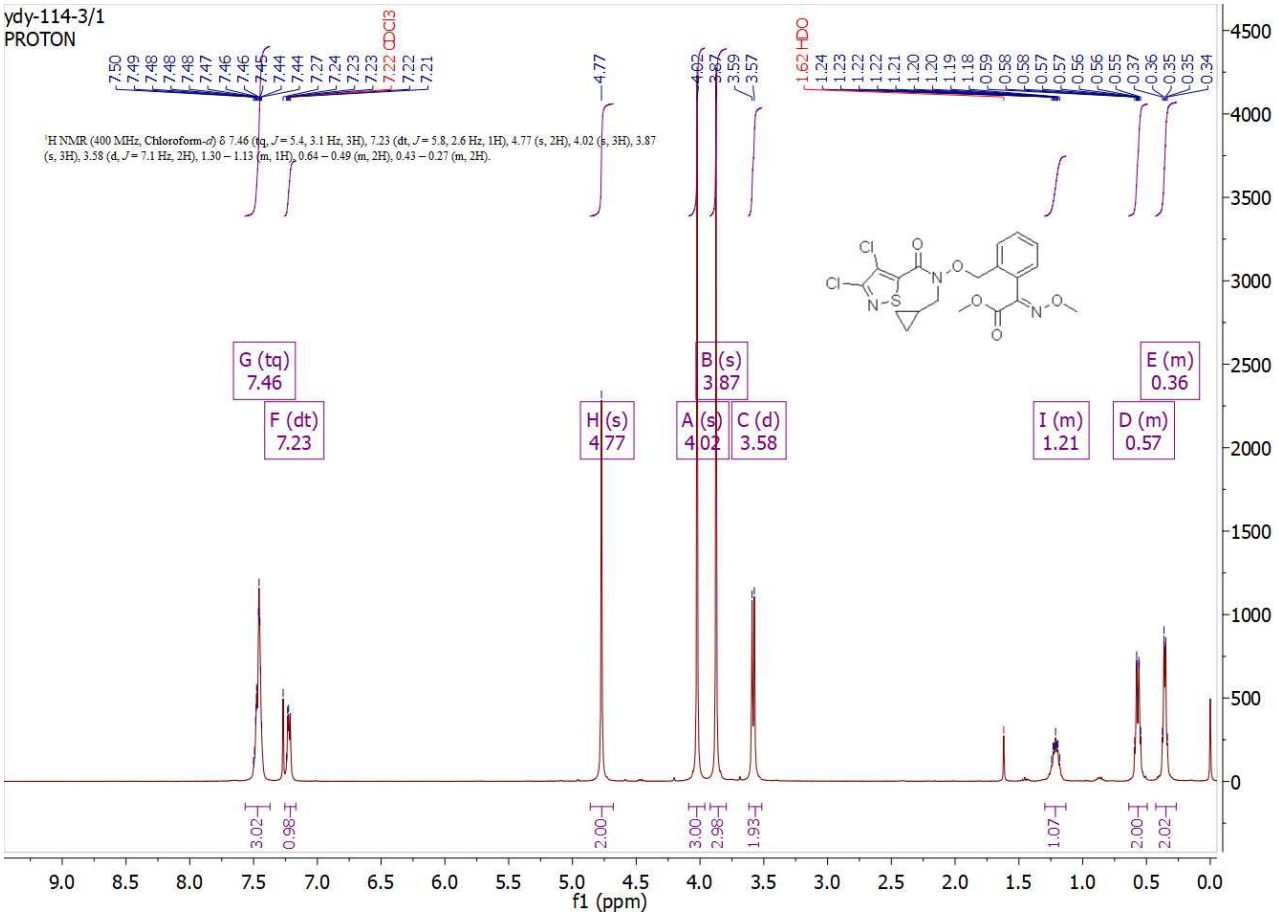


Figure S19. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **1e**

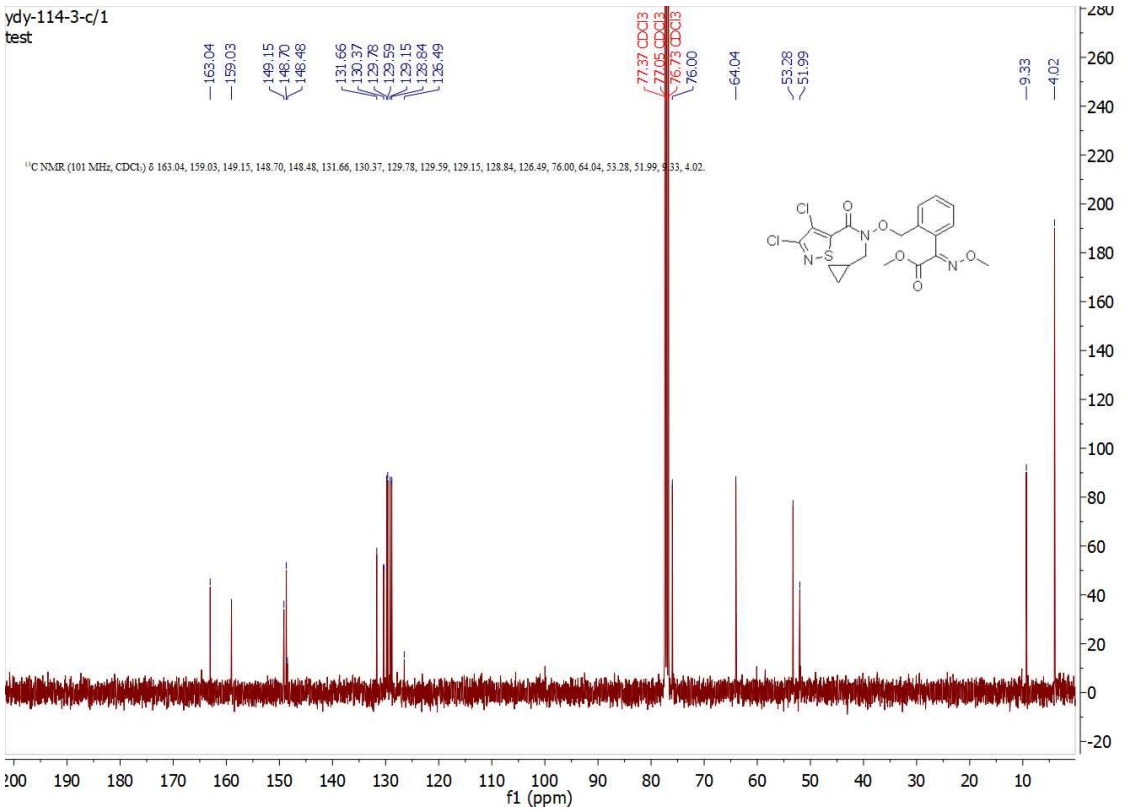


Figure S20. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **1e**

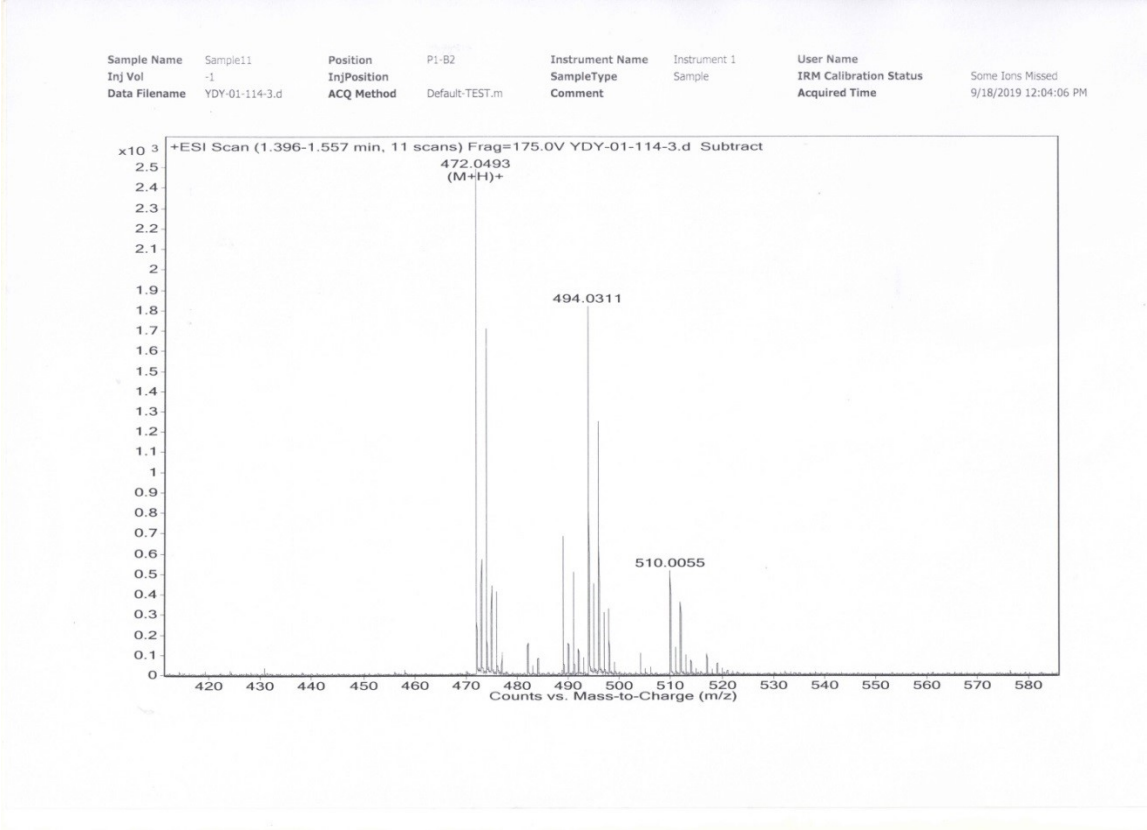


Figure S21. The HRMS spectra of **1e**

Data for methyl (E)-2-(2-(((((Z)-(3,4-dichloroisothiazol-5-yl)(methoxy)methylene)amino)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**2a**). Yield 21%; white solid; mp136-137 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 1H), 7.46 – 7.36 (m, 2H), 7.23 – 7.16 (m, 1H), 5.00 (s, 2H), 4.05 (s, 6H), 3.84 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.25, 151.67, 149.38, 149.35, 147.20, 134.86, 130.23, 129.41, 129.30, 128.55, 128.24, 120.85, 75.98, 63.81, 60.74, 52.95. HRMS (ESI) m/z calcd for $C_{16}H_{16}Cl_2N_3O_5S$ $(M+H)^+$432.0182, found 432.0181.

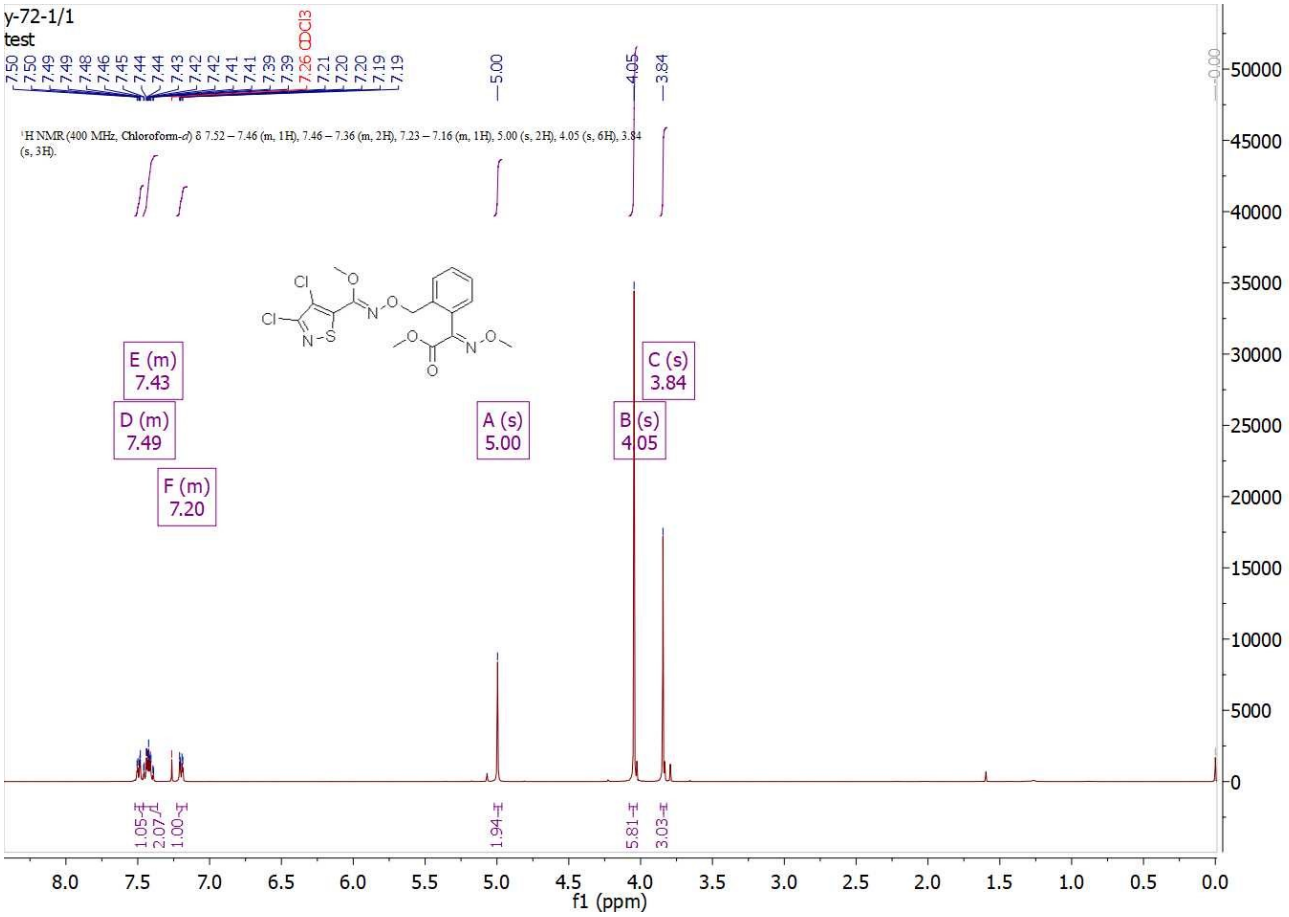


Figure S22. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **2a**

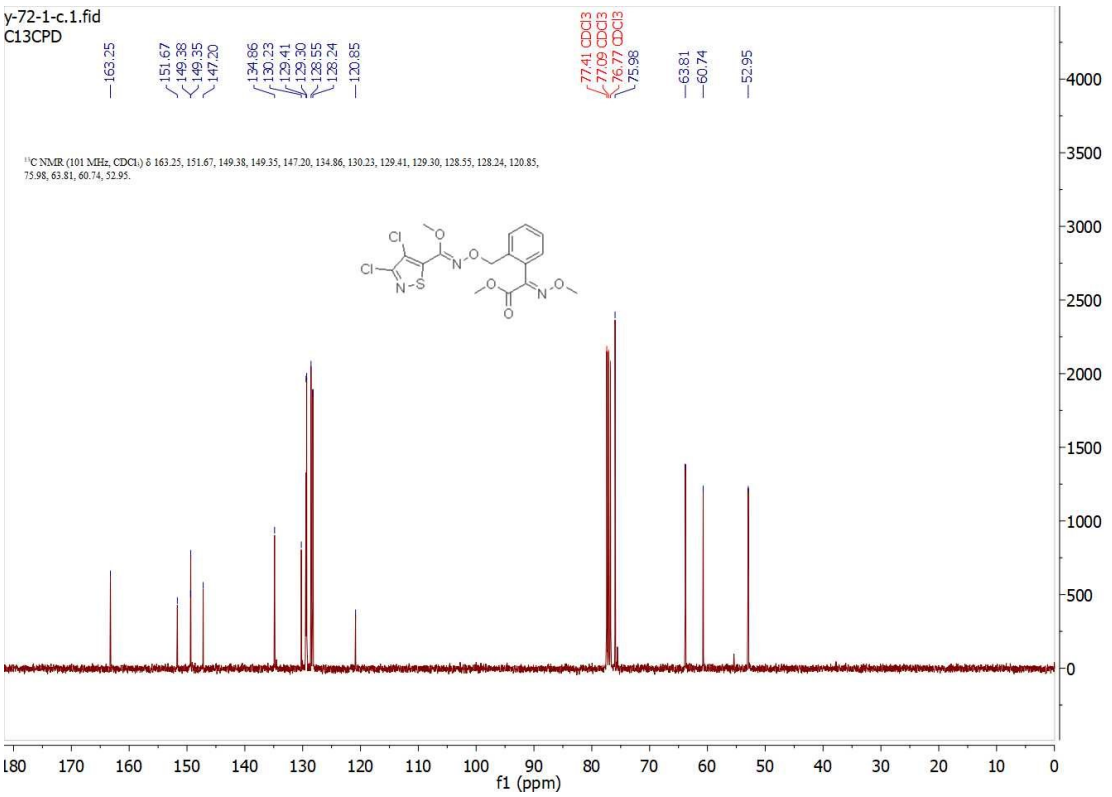


Figure S23. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **2a**

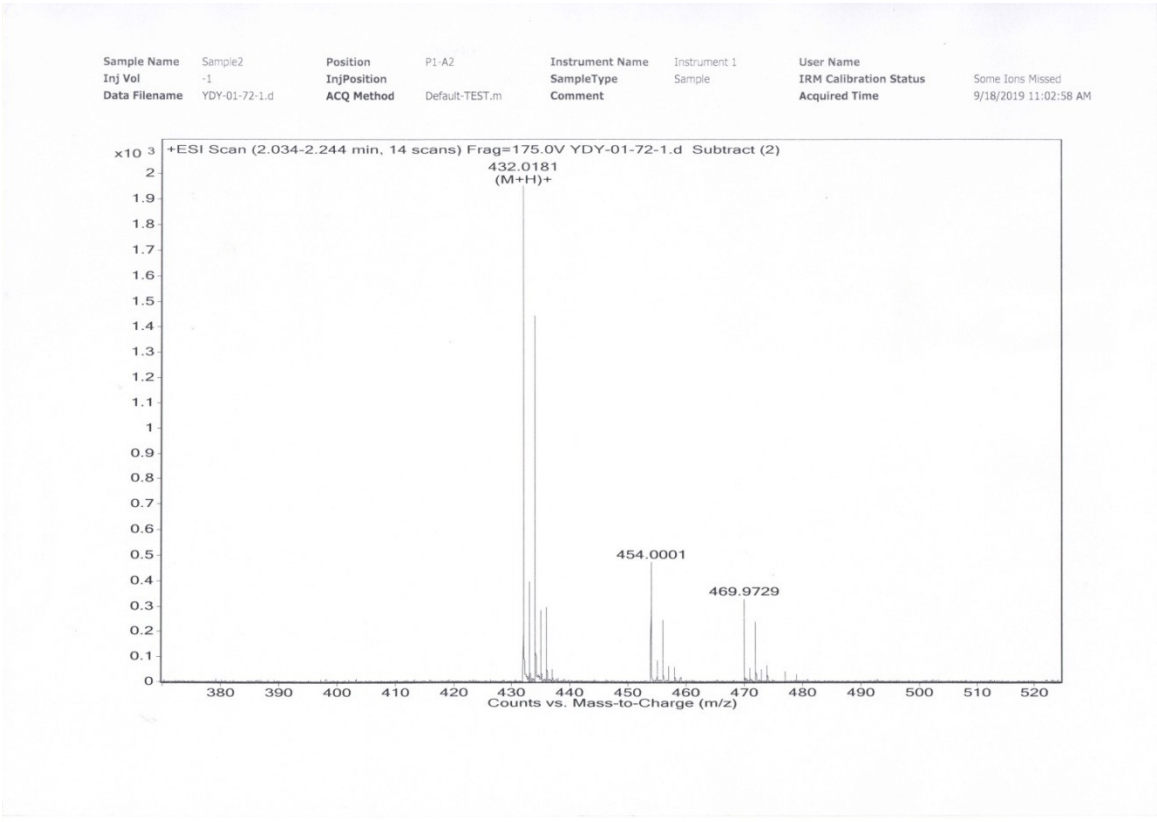


Figure S24. The HRMS spectra of **2a**

Data for methyl methyl (E)-2-(2-(((((Z)-(allyloxy)(3,4-dichloroisothiazol-5-yl)methylene)amino)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**2b**). Yield 31%; white crystal; mp65-66 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.48 (m, 1H), 7.47 – 7.39 (m, 2H), 7.24 – 7.16 (m, 1H), 5.96 (ddt, *J* = 16.5, 10.3, 6.1 Hz, 1H), 5.44 – 5.16 (m, 2H), 5.00 (s, 2H), 4.82 (dt, *J* = 6.0, 1.2 Hz, 2H), 4.05 (s, 3H), 3.84 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.27, 152.16, 149.47, 149.31, 146.17, 134.77, 132.15, 130.24, 129.44, 129.41, 128.52, 128.31, 120.62, 119.79, 75.99, 73.90, 63.89, 53.07. HRMS (ESI) m/z calcd for $C_{18}H_{18}Cl_2N_3O_5S$ $(M+H)^+$458.0339, found 458.0332.

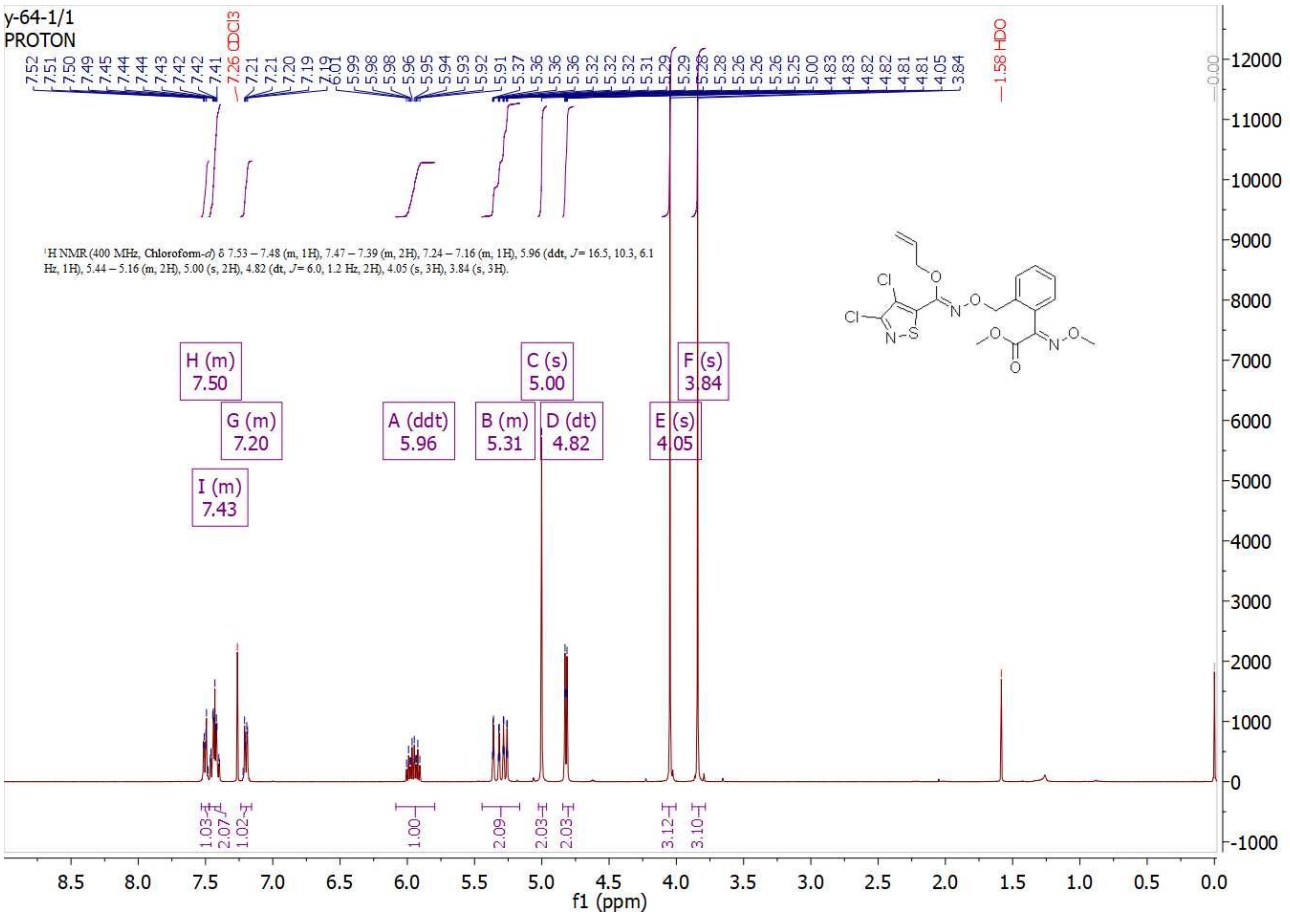


Figure S25. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **2b**

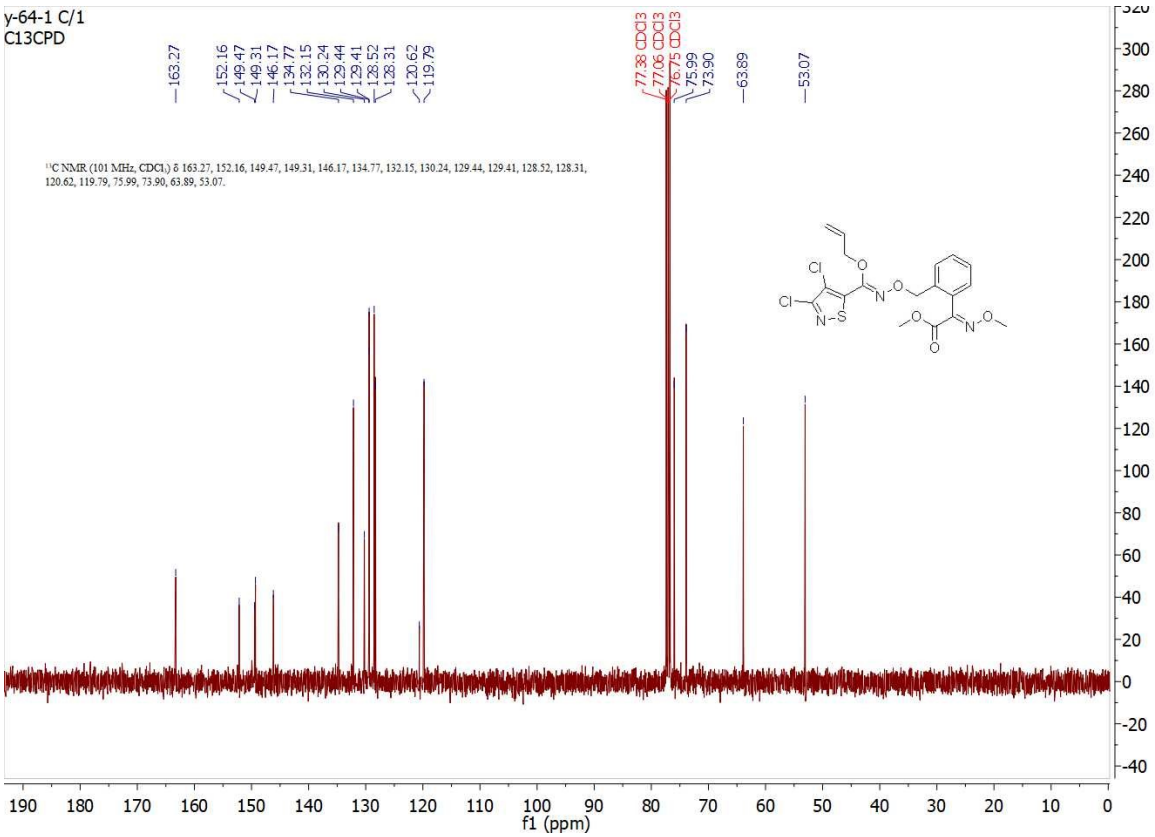


Figure S26. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **2b**

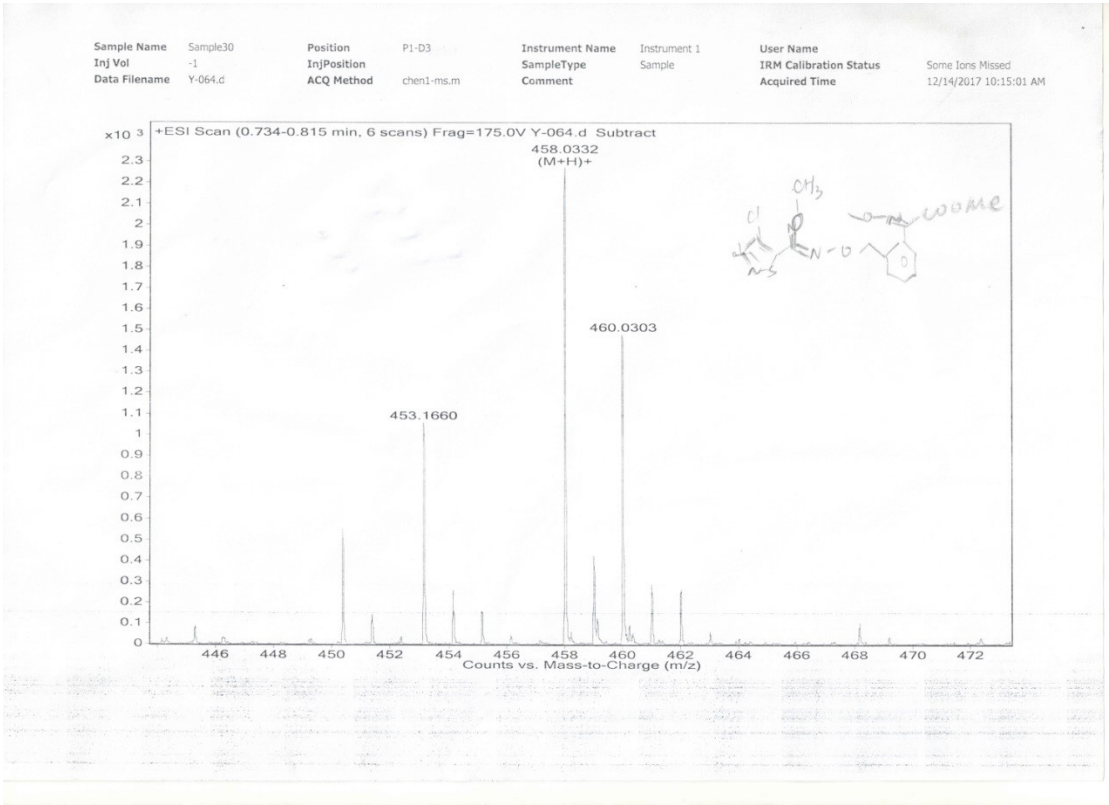


Figure S27. The HRMS spectra of **2b**

Data for methyl (E)-2-(2-(((((Z)-(3,4-dichloroisothiazol-5-yl)(prop-2-yn-1-yloxy)methylene)amino)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**2c**). Yield 56%; white powder; mp70-71 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, $J$ = 5.9 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.22 – 7.16 (m, 1H), 5.03 (s, 2H), 4.98 (s, 2H), 4.04 (s, 3H), 3.84 (s, 3H), 2.58 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.28, 151.70, 149.52, 149.27, 145.33, 134.43, 130.34, 129.54, 129.48, 128.53, 128.44, 120.88, 77.28, 77.13,76.29, 63.91, 60.50, 53.11. HRMS (ESI) m/z calcd for $C_{18}H_{16}Cl_2N_3O_5S$ $(M+H)^+$456.0182, found 456.0190.

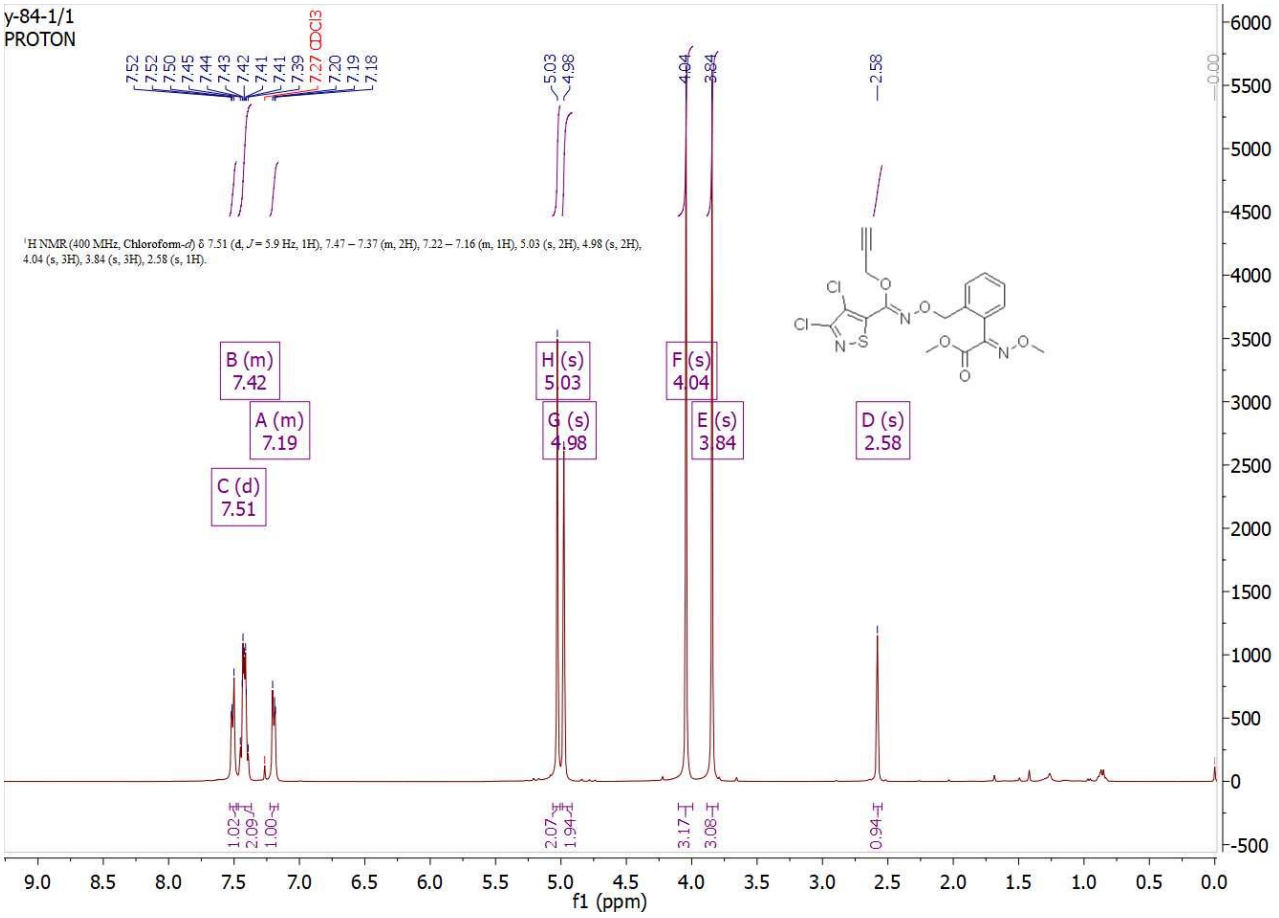


Figure S28. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **2c**

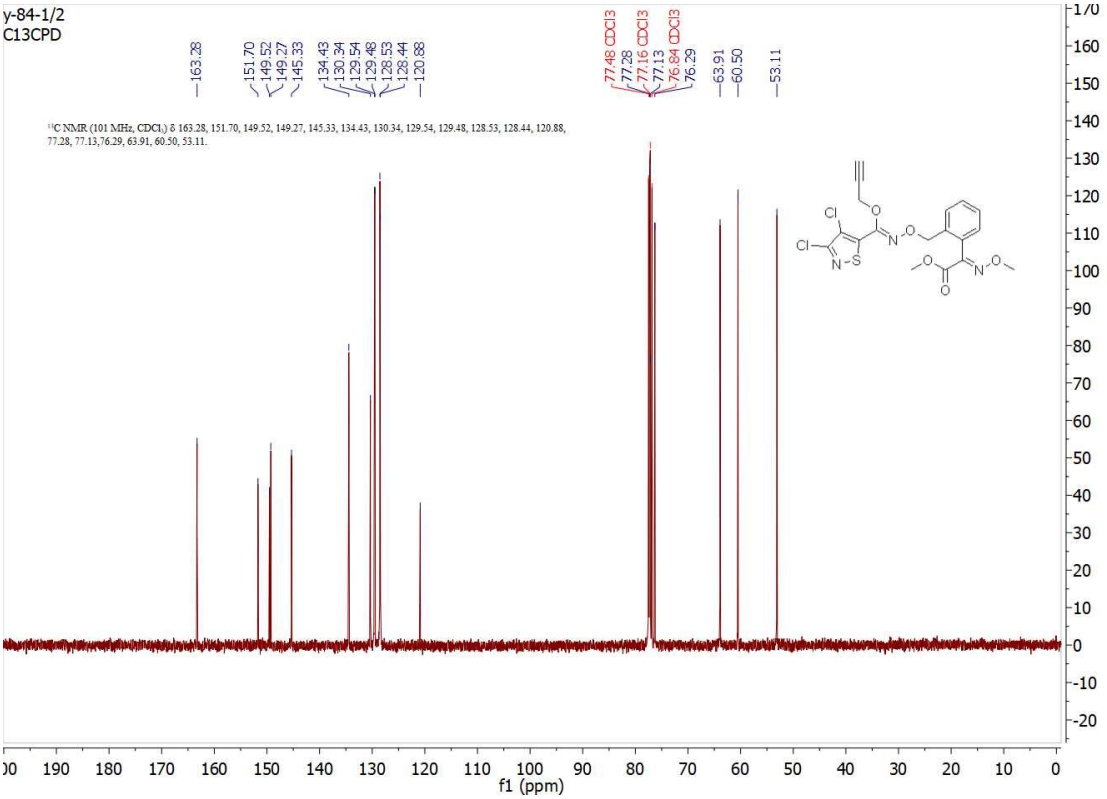


Figure S29. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **2c**

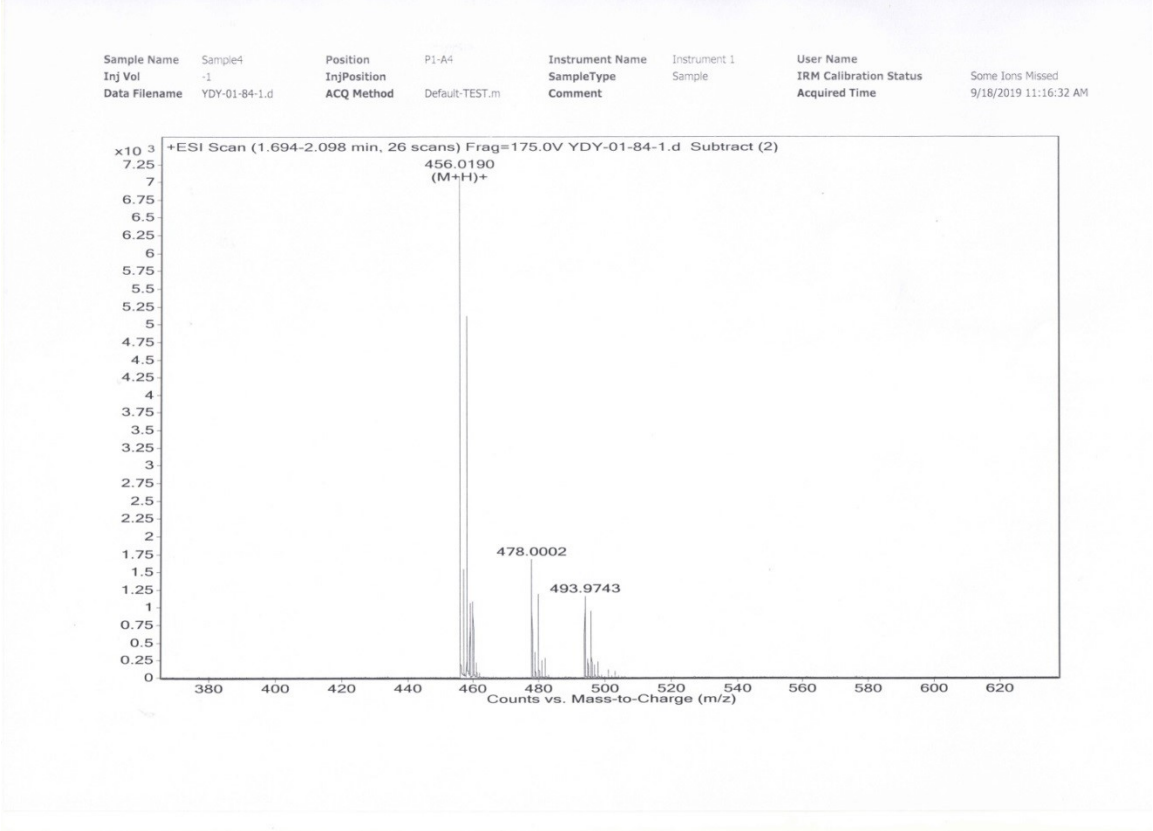


Figure S30. The HRMS spectra of **2c**

Data for methyl (E)-2-(2-(((((Z)-(but-2-yn-1-yloxy)(3,4-dichloroisothiazol-5-yl)methylene)amino)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**2d**). Yield 48%; white powder; mp68-69 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, $J$ = 6.5 Hz, 1H), 7.48 – 7.36 (m, 2H), 7.19 (d, $J$ = 6.5 Hz, 1H), 5.02 (s, 2H), 4.92 (s, 2H), 4.04 (s, 3H), 3.84 (s, 3H), 1.81 (d, $J$ = 2.7 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.25, 152.15, 149.40, 149.27, 145.68, 134.67, 130.23, 129.43, 129.39, 128.47, 128.29, 120.75, 85.74, 76.07, 72.98, 63.88, 61.27, 53.06, 3.68. HRMS (ESI) m/z calcd for $C_{19}H_{18}Cl_2N_3O_5S$ $(M+H)^+$470.0339, found 470.0344.

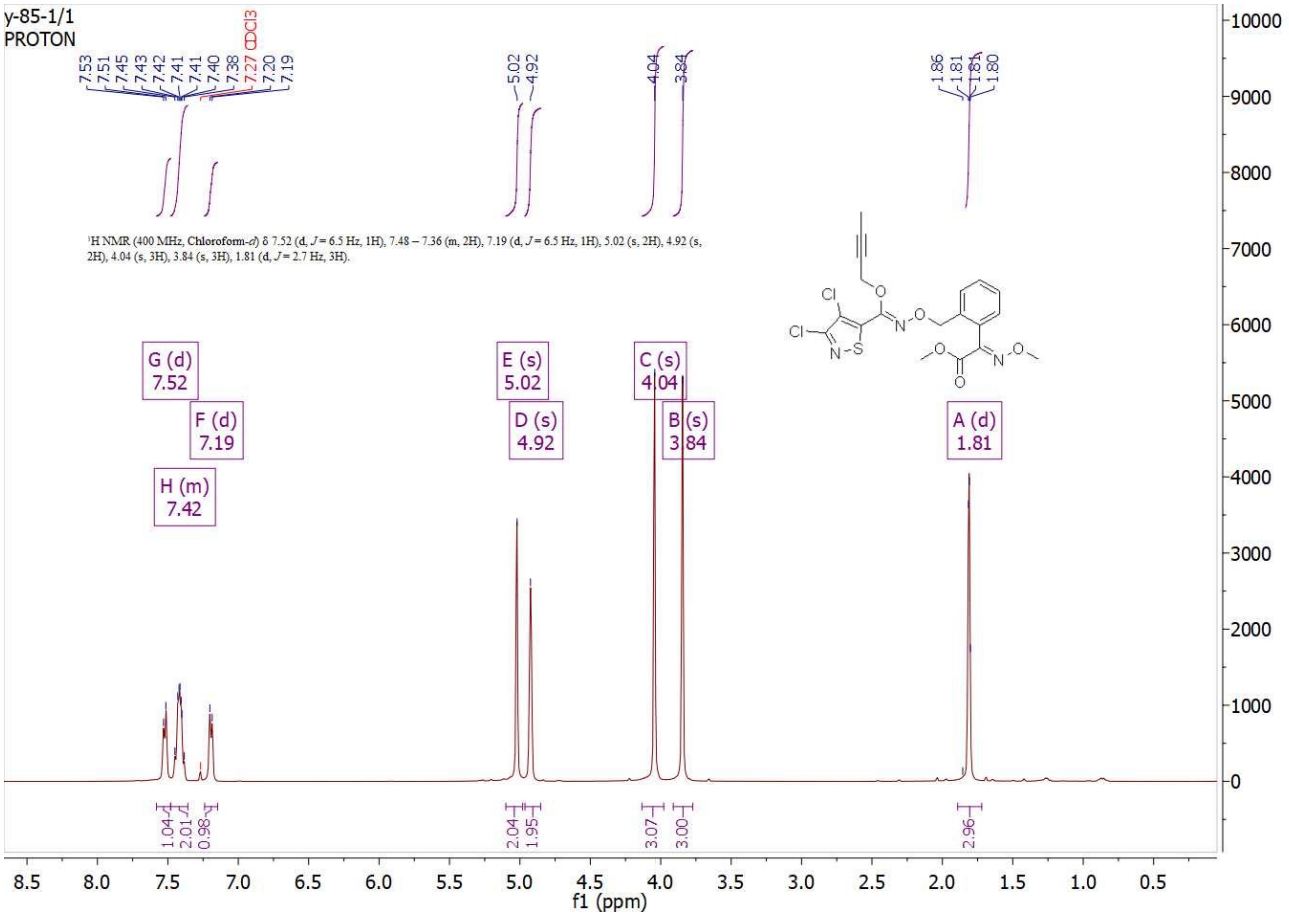


Figure S31. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **2d**

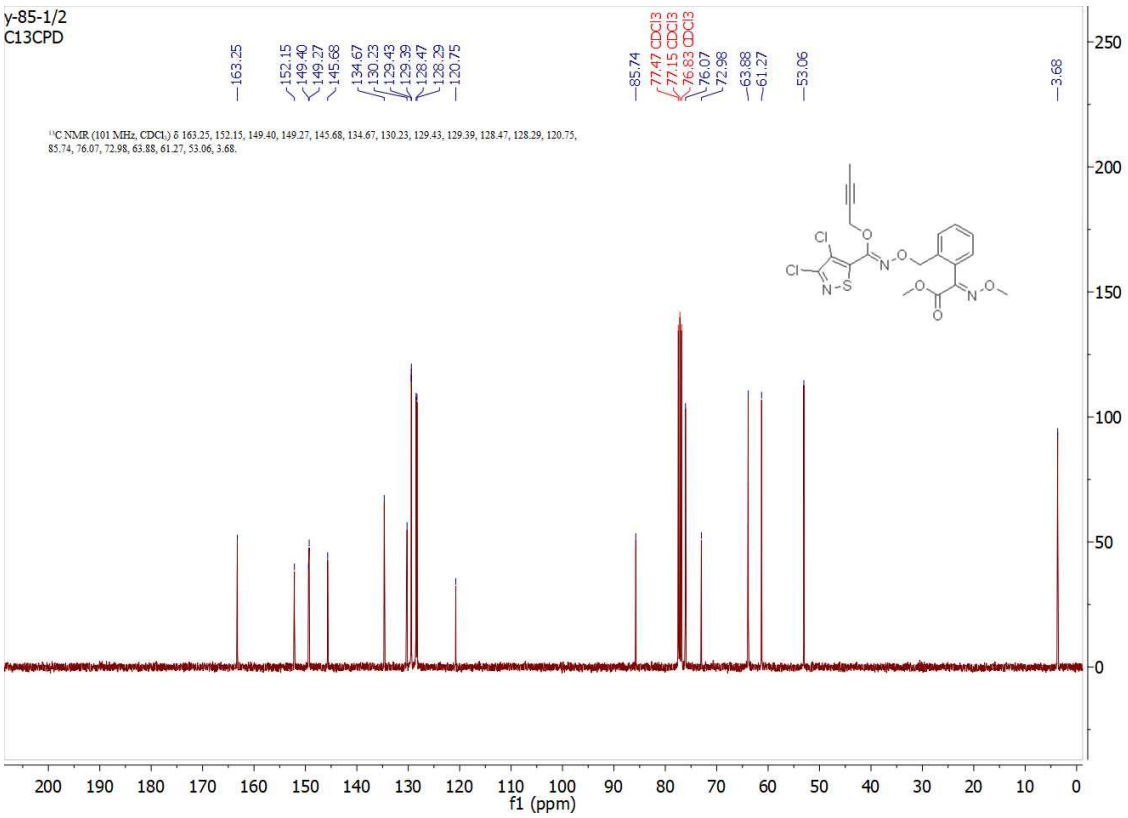


Figure S32. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of 2**d**

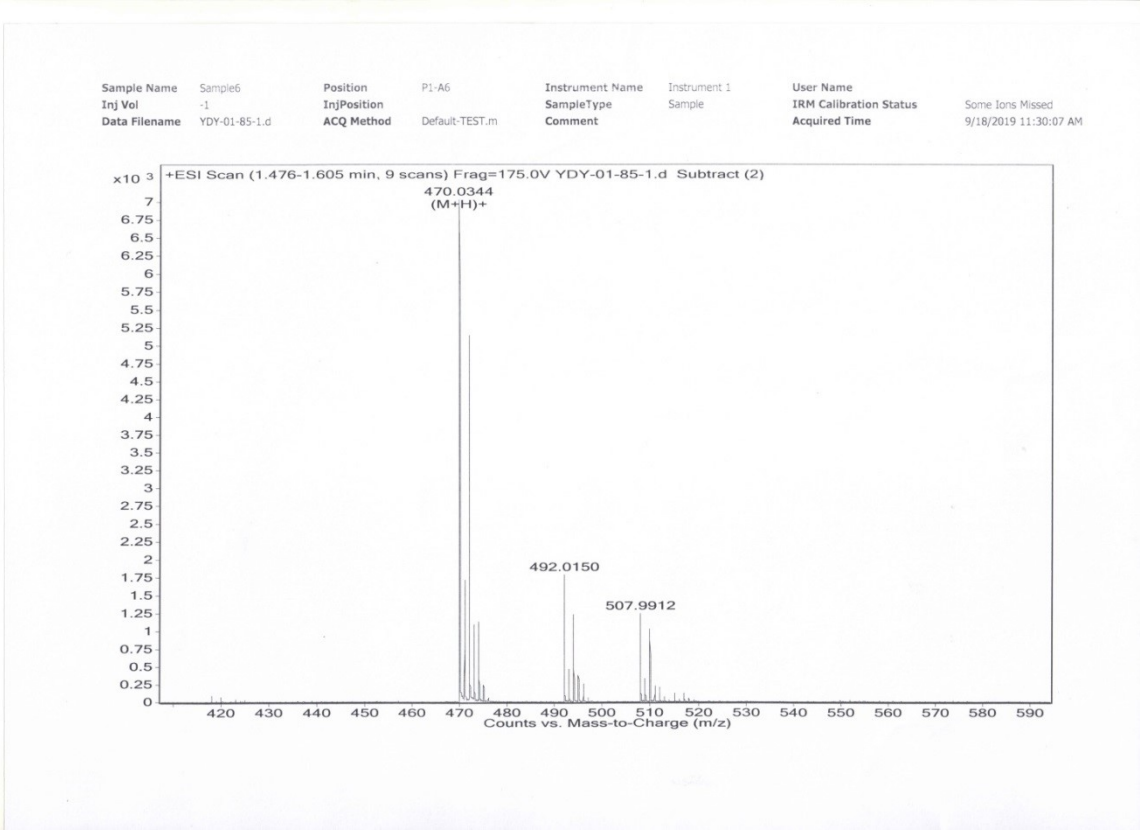


Figure S33. The HRMS spectra of **2d**

Data for methyl (E)-2-(2-(((((Z)-(cyclopropylmethoxy)(3,4-dichloroisothiazol-5-yl)methylene)amino)oxy)methyl)phenyl)-2-(methoxyimino)acetate (**2e**). Yield 48%; white solid; mp69-70 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.46 (m, 1H), 7.42 (tt, *J* = 7.5, 5.6 Hz, 2H), 7.22 – 7.13 (m, 1H), 5.00 (s, 2H), 4.17 (d, *J* = 7.4 Hz, 2H), 4.04 (s, 3H), 3.84 (s, 3H), 1.28 – 1.05 (m, 1H), 0.68 – 0.50 (m, 2H), 0.30 (q, *J* = 5.0 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.24, 152.66, 149.44, 149.31, 146.76, 134.94, 130.18, 129.41, 129.32, 128.49, 128.24, 120.40, 78.54, 75.87, 63.87, 53.05, 10.90, 3.39. HRMS (ESI) m/z calcd for $C_{19}H_{20}Cl_2N_3O_5S$ $(M+H)^+$472.0495, found 472.0500.

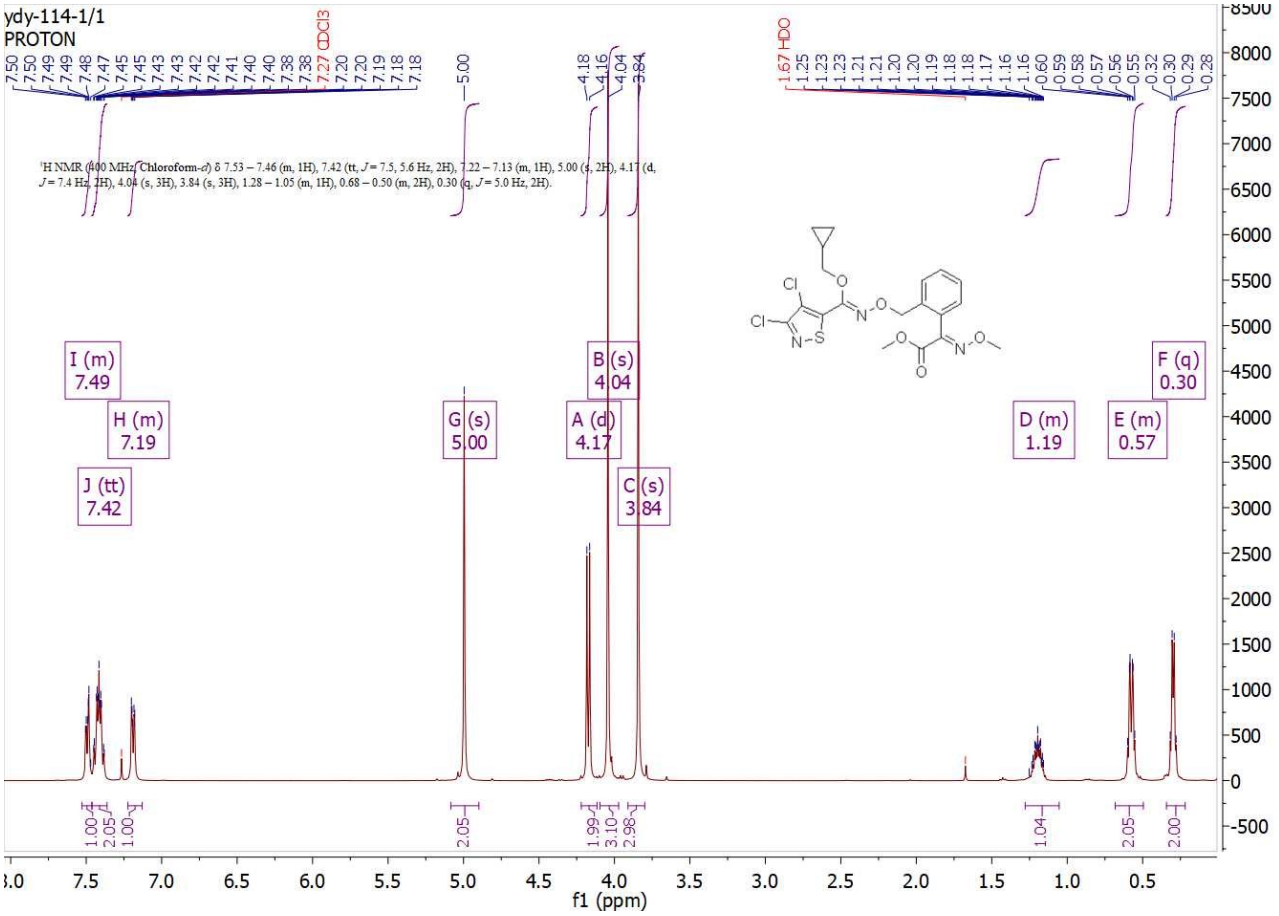


Figure S34. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **2e**

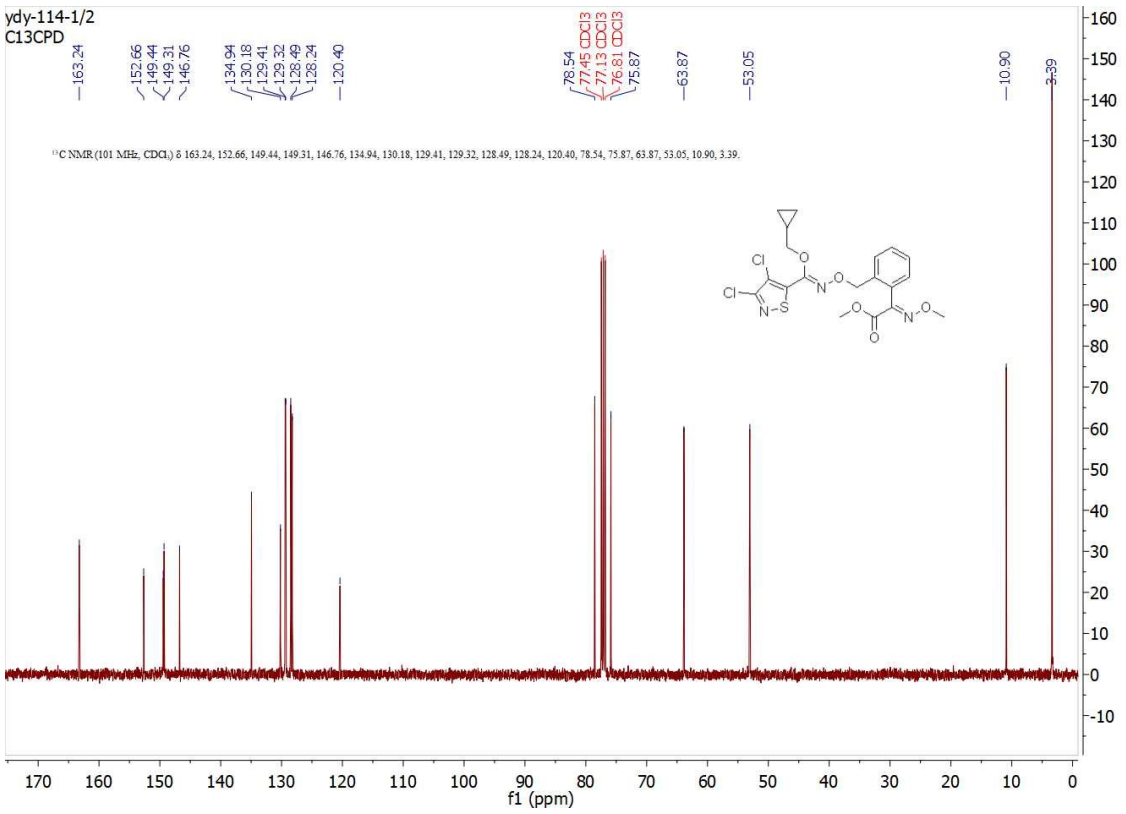


Figure S35. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **2e**

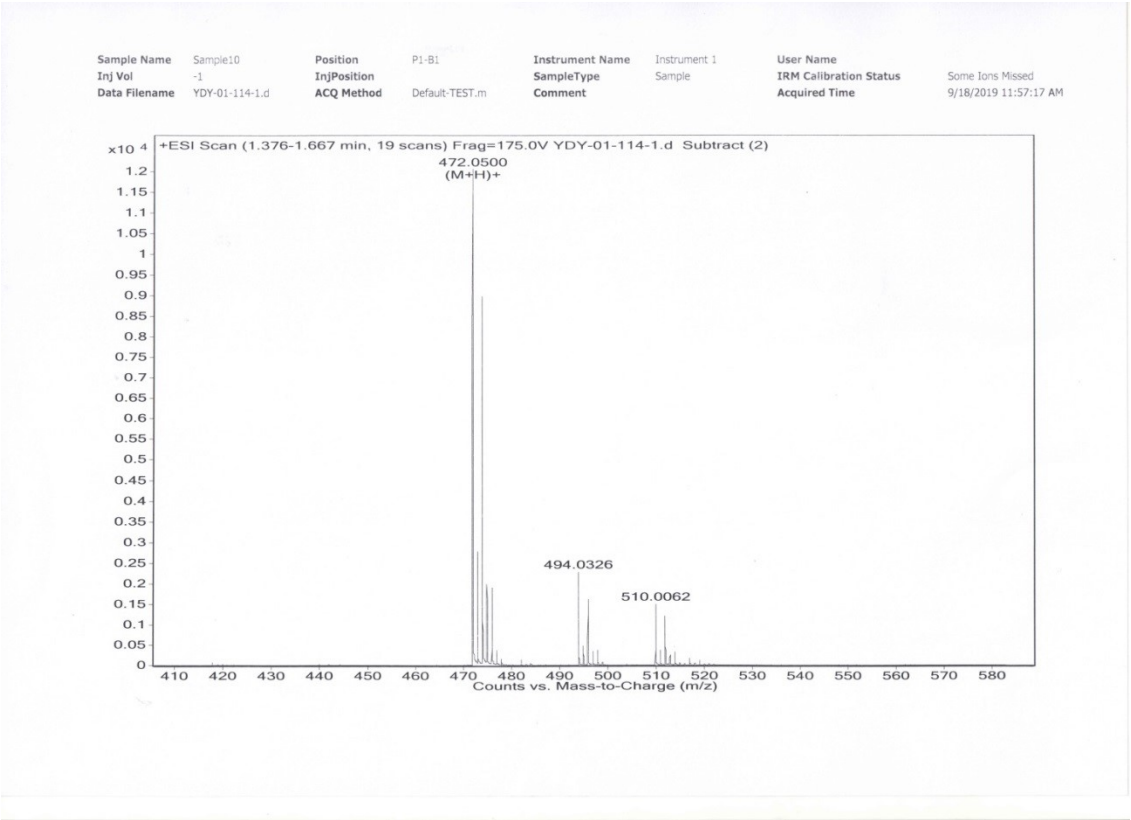


Figure S36. The HRMS spectra of **2e**

Data for methyl (E)-2-(2-((3,4-dichloro-N-methoxyisothiazole-5-carboxamido)methyl)phenyl)-2-(methoxyimino)acetate (**3a**). Yield 28%; white solid; mp113-114 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.33 (m, 3H), 7.24 – 7.11 (m, 1H), 4.83 (s, 2H), 4.07 (s, 3H), 3.88 (s, 3H), 3.62 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.27, 158.07, 149.58, 149.10, 146.94, 133.06, 130.24, 129.86, 129.46, 128.65, 128.24, 127.67,64.01, 63.37, 53.17, 47.61. HRMS (ESI) m/z calcd for $C_{16}H_{16}Cl_2N_3O_5S$ $(M+H)^+$432.0182, found 432.0181.

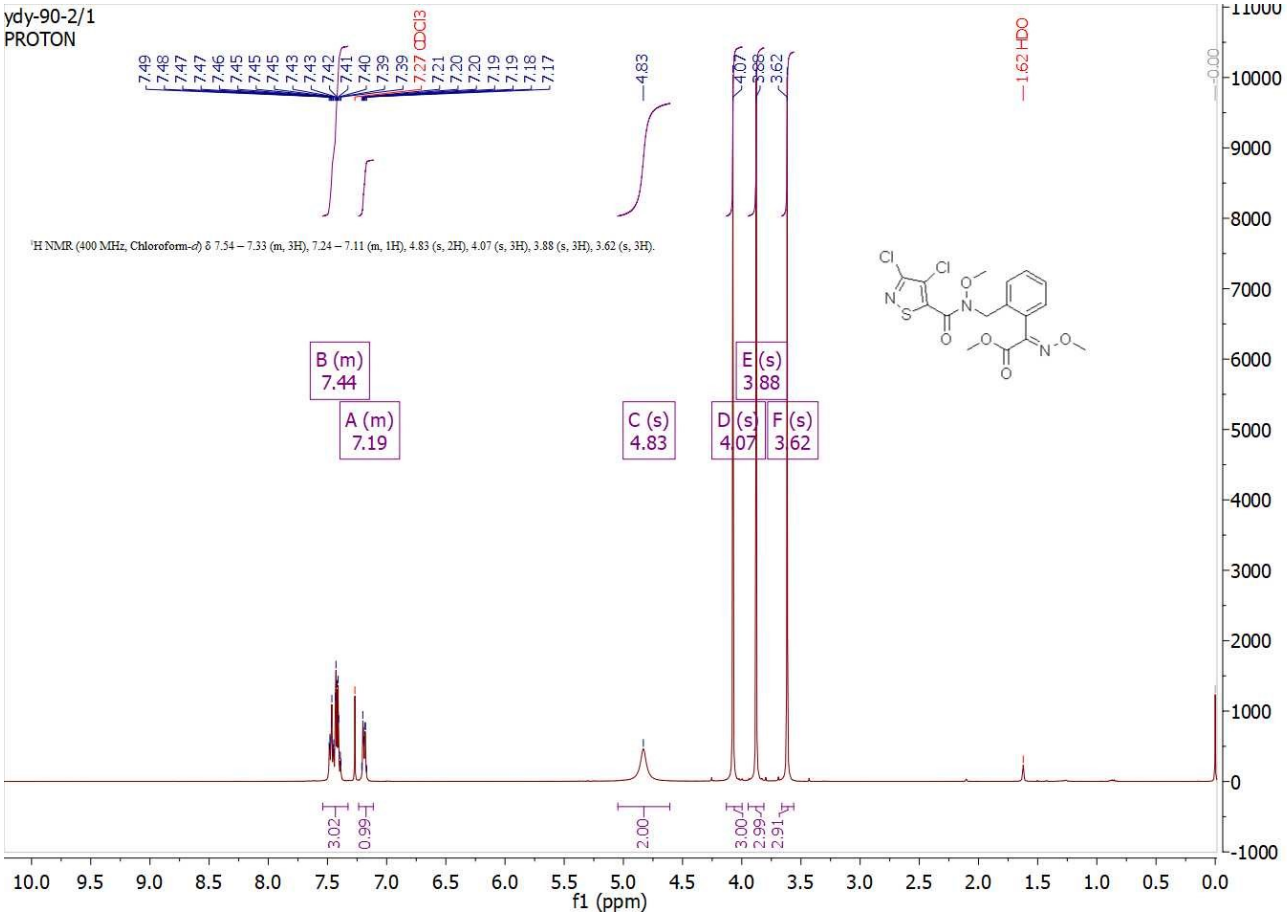


Figure S37. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **3a**

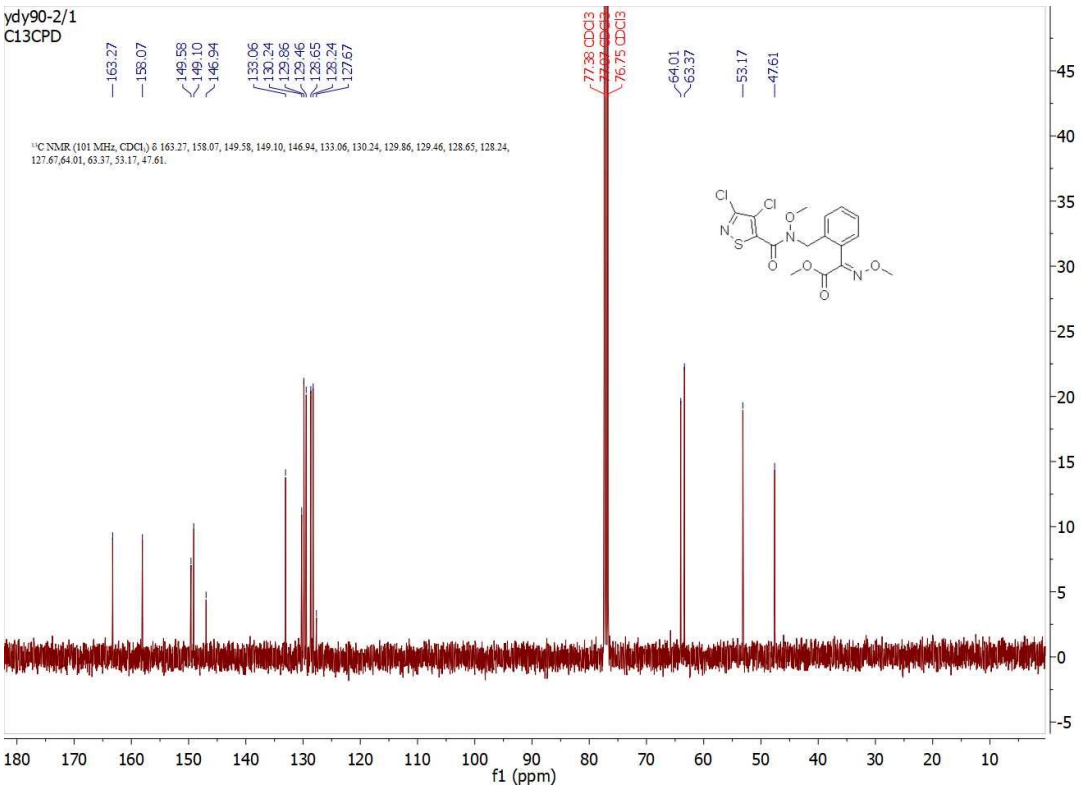


Figure S38. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **3a**

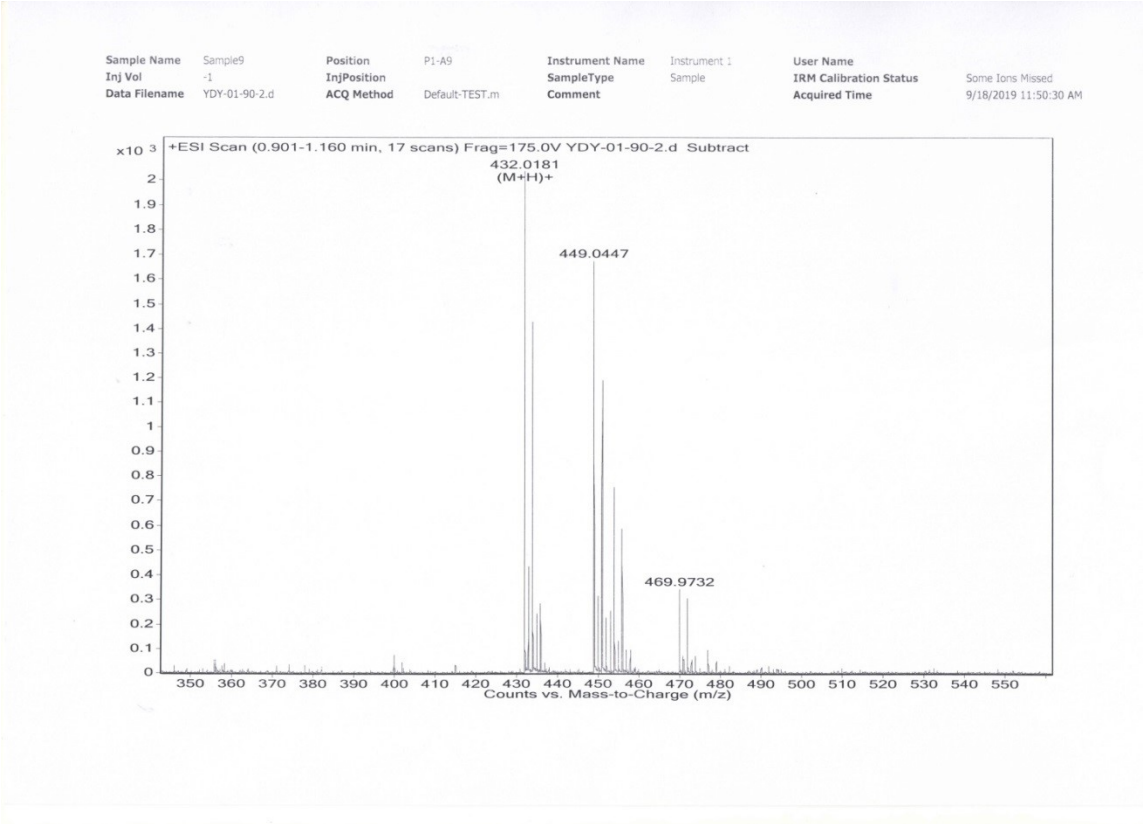


Figure S39. The HRMS spectra of **3a**

Data for methyl (E)-2-(2-((3,4-dichloro-N-(cyclopropylmethoxy)isothiazole-5-carboxamido)methyl)phenyl)-2-(methoxyimino)acetate (**3b**). Yield 17%; white solid; mp114-115 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.33 (m, 3H), 7.20 – 7.07 (m, 1H), 4.84 (s, 2H), 4.06 (s, 3H), 3.87 (s, 3H), 3.59 (d, $J$ = 7.3 Hz, 2H), 1.00 (tt, $J$ = 7.7, 4.8 Hz, 1H), 0.65 – 0.47 (m, 2H), 0.16 (dt, $J$ = 6.2, 4.7 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 186.12, 163.26, 158.35, 149.35, 149.06, 147.71, 133.26, 129.98, 129.73, 129.21, 128.62, 128.05, 81.15, 63.95, 53.10, 48.53, 8.68, 3.86. HRMS (ESI) m/z calcd for $C_{19}H_{20}Cl_2N_3O_5S$ $(M+H)^+$472.0495, found 472.0497.

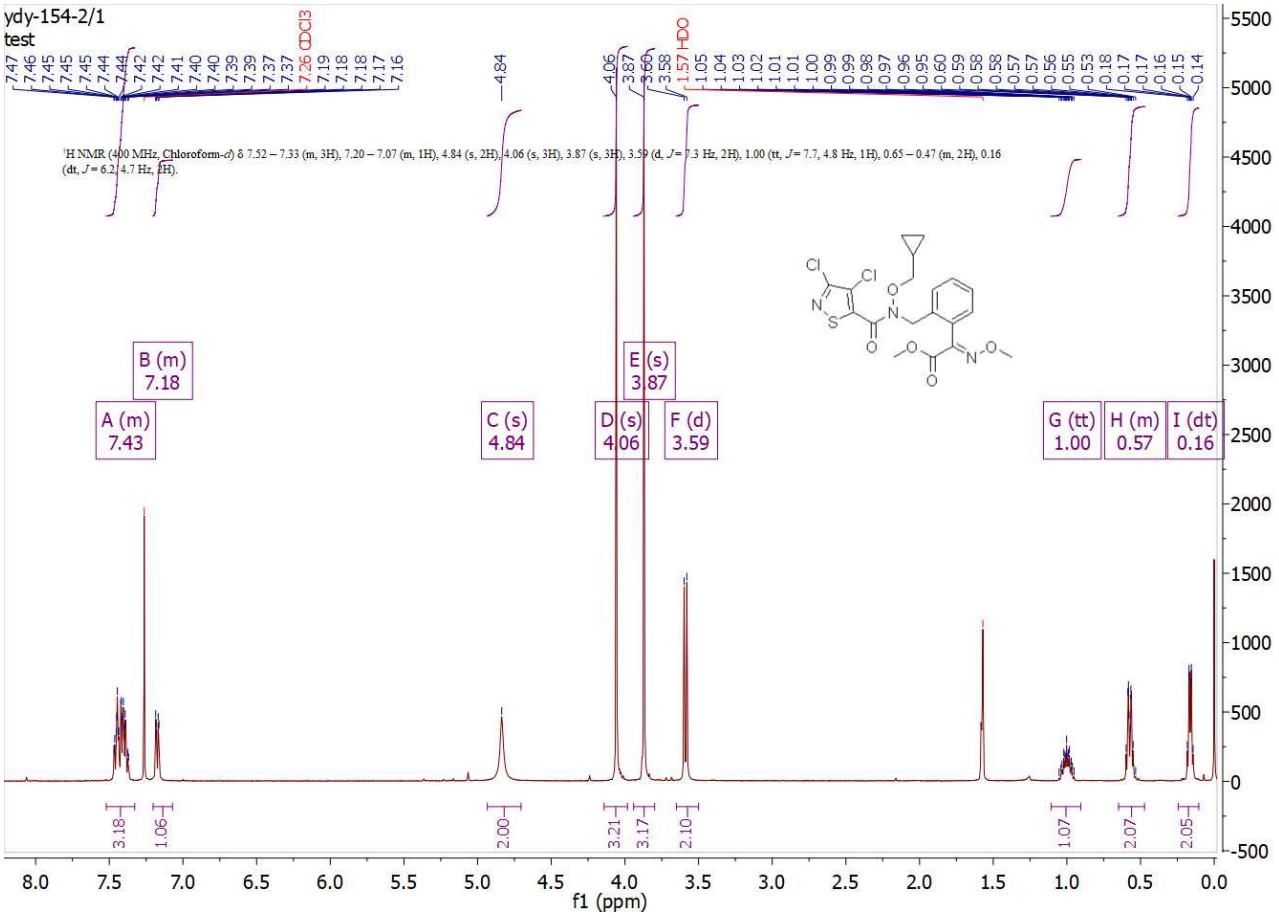


Figure S40. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **3b**

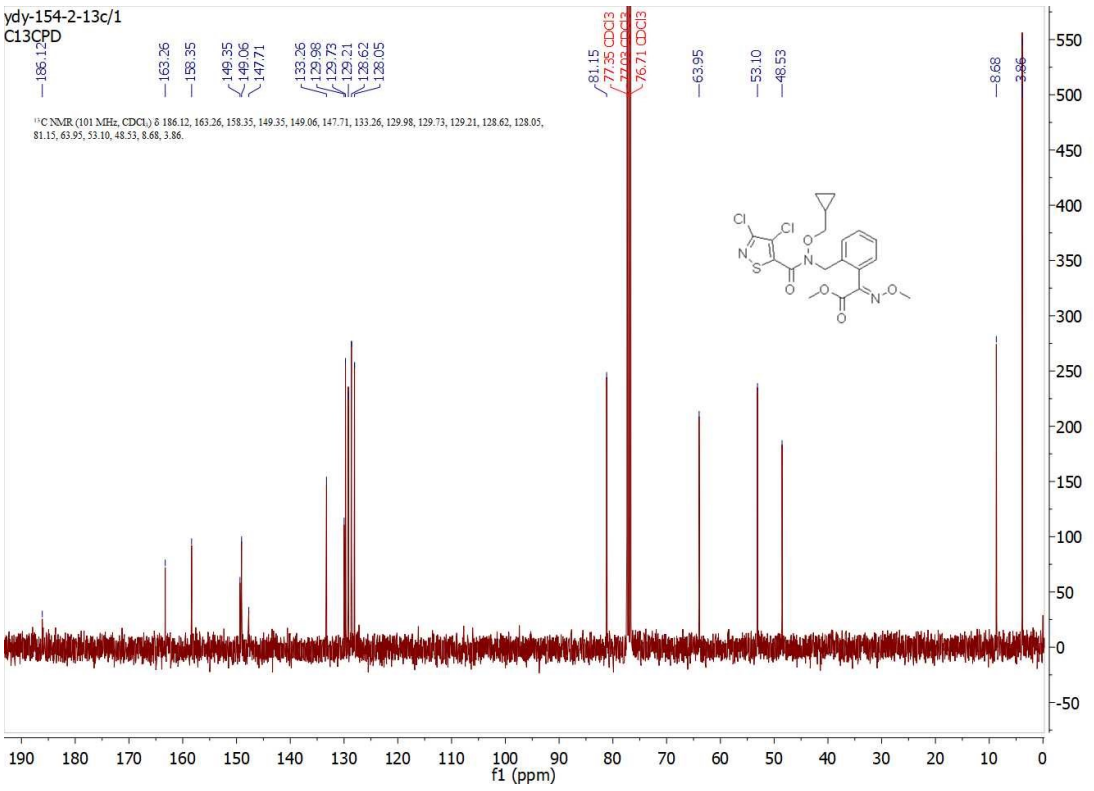


Figure S41. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **3b**

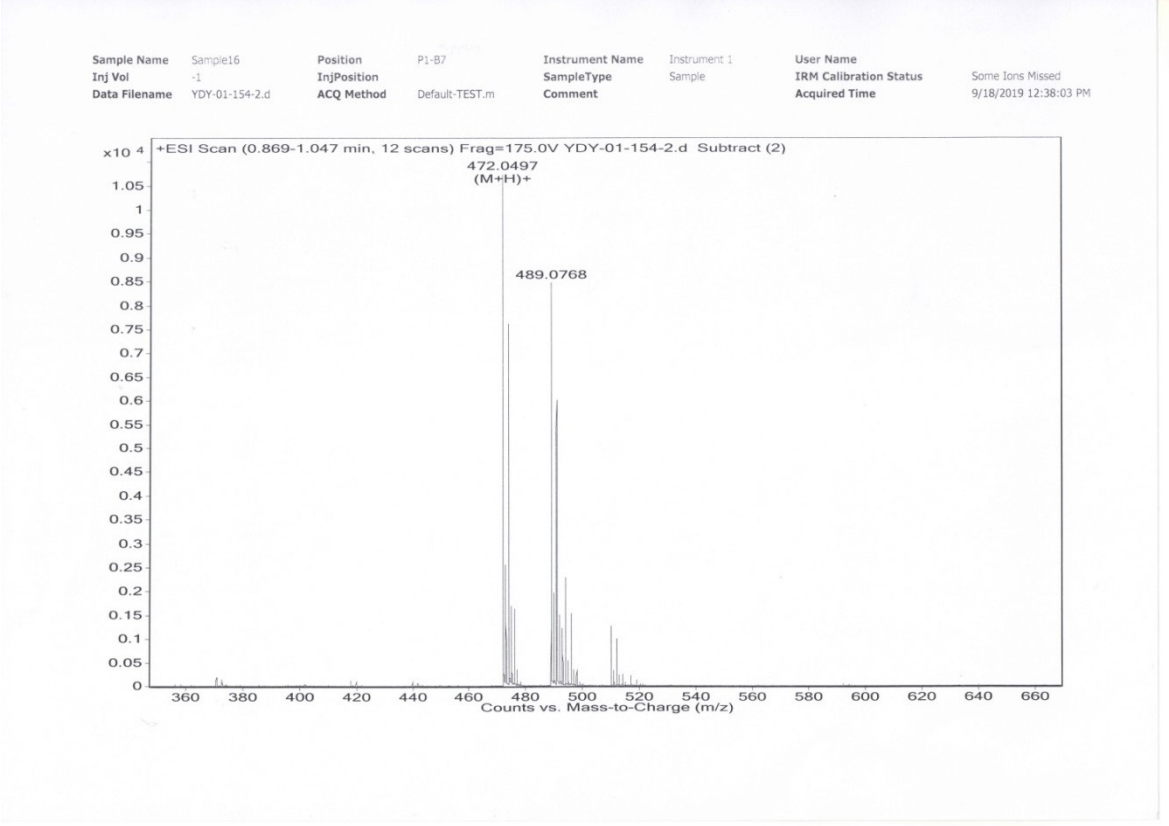


Figure S42. The HRMS spectra of **3b**

Data for methyl (E)-2-(2-(((Z)-(3,4-dichloroisothiazol-5-yl)(methoxyimino)methoxy)methyl)phenyl)-2-(methoxyimino)acetate (**4a**). Yield 42%; white solid; mp103-104 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.44 (dtd, *J* = 18.0, 7.5, 1.5 Hz, 2H), 7.19 (dd, *J* = 7.5, 1.6 Hz, 1H), 5.24 (s, 2H), 4.02 (s, 3H), 3.94 (s, 3H), 3.85 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.13, 151.78, 149.34, 148.72, 145.71, 134.13, 129.76, 129.34, 128.61, 128.48, 120.68, 72.22, 72.20, 63.89, 63.37, 53.11. HRMS (ESI) m/z calcd for $C_{16}H_{16}Cl_2N_3O_5S$ $(M+H)^+$432.0182, found 432.0182.

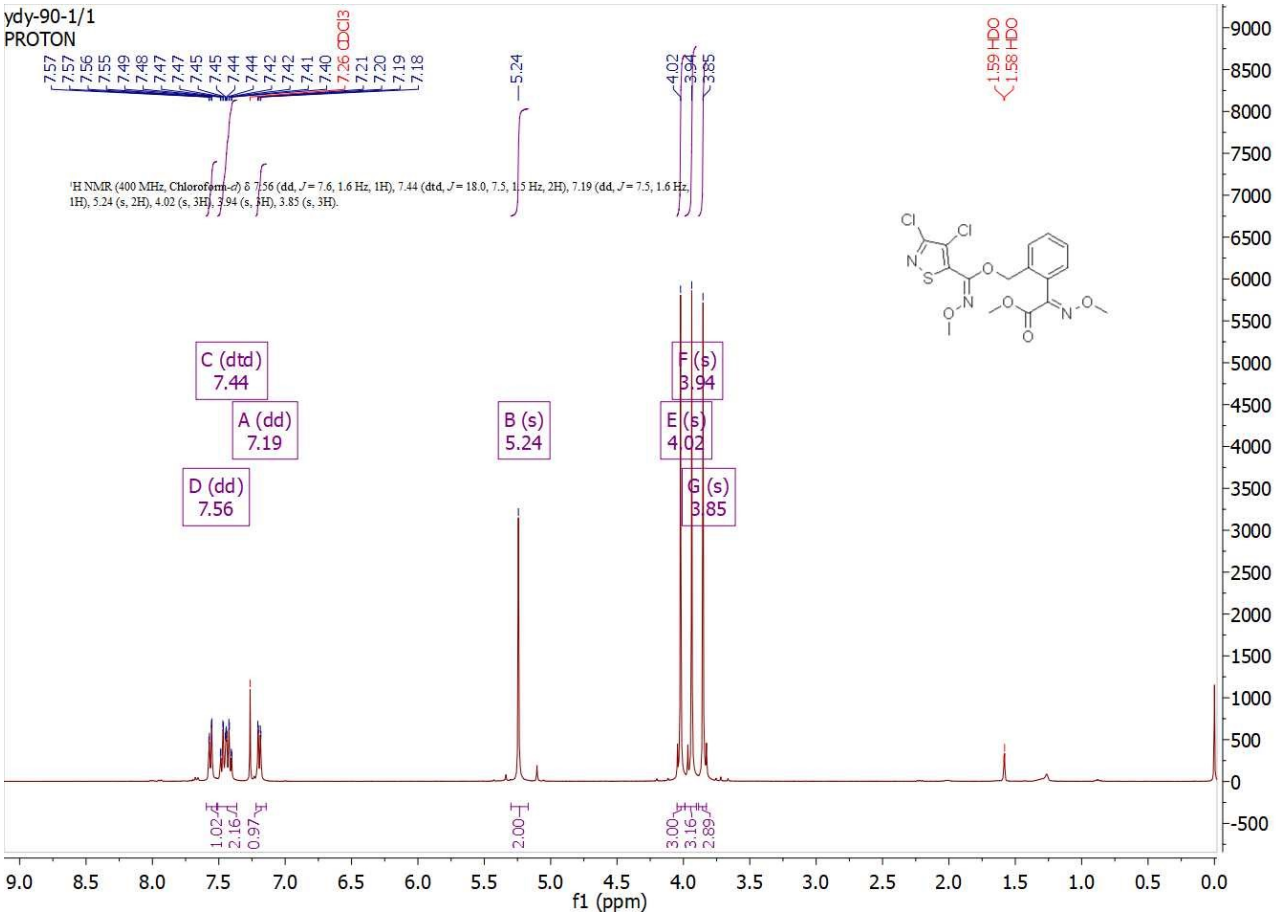


Figure S43. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **4a**

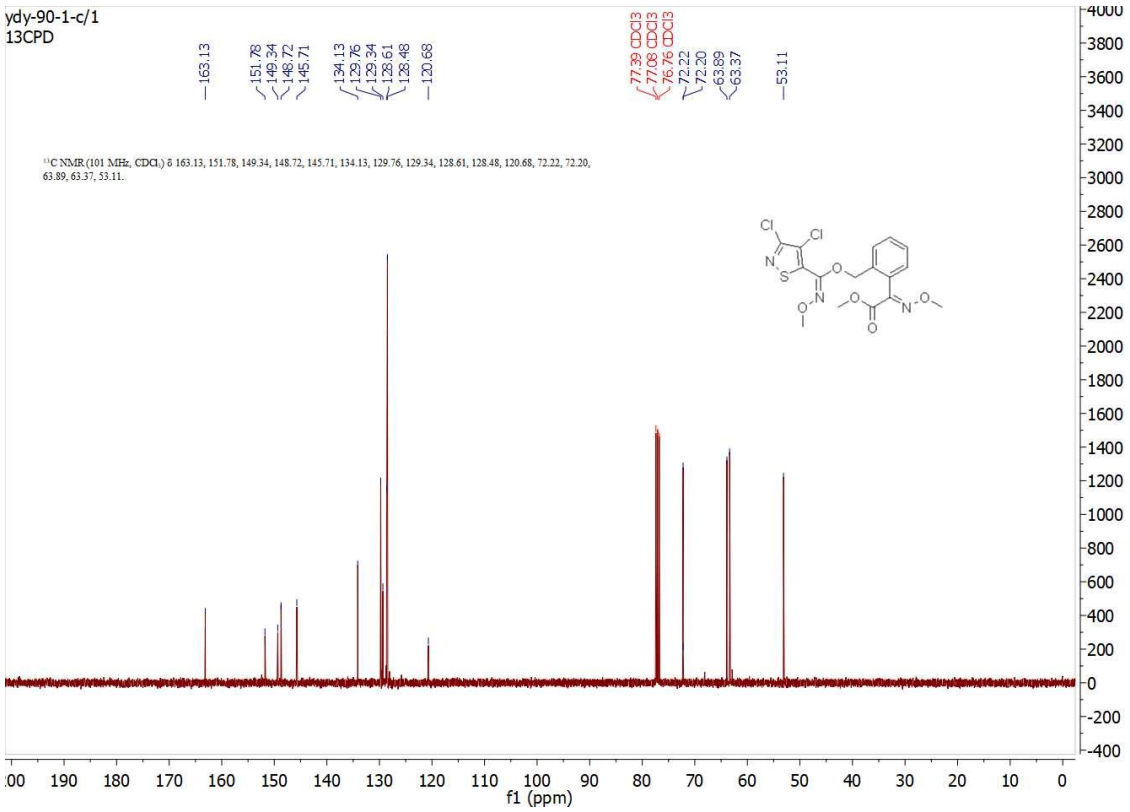


Figure S44. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **4a**

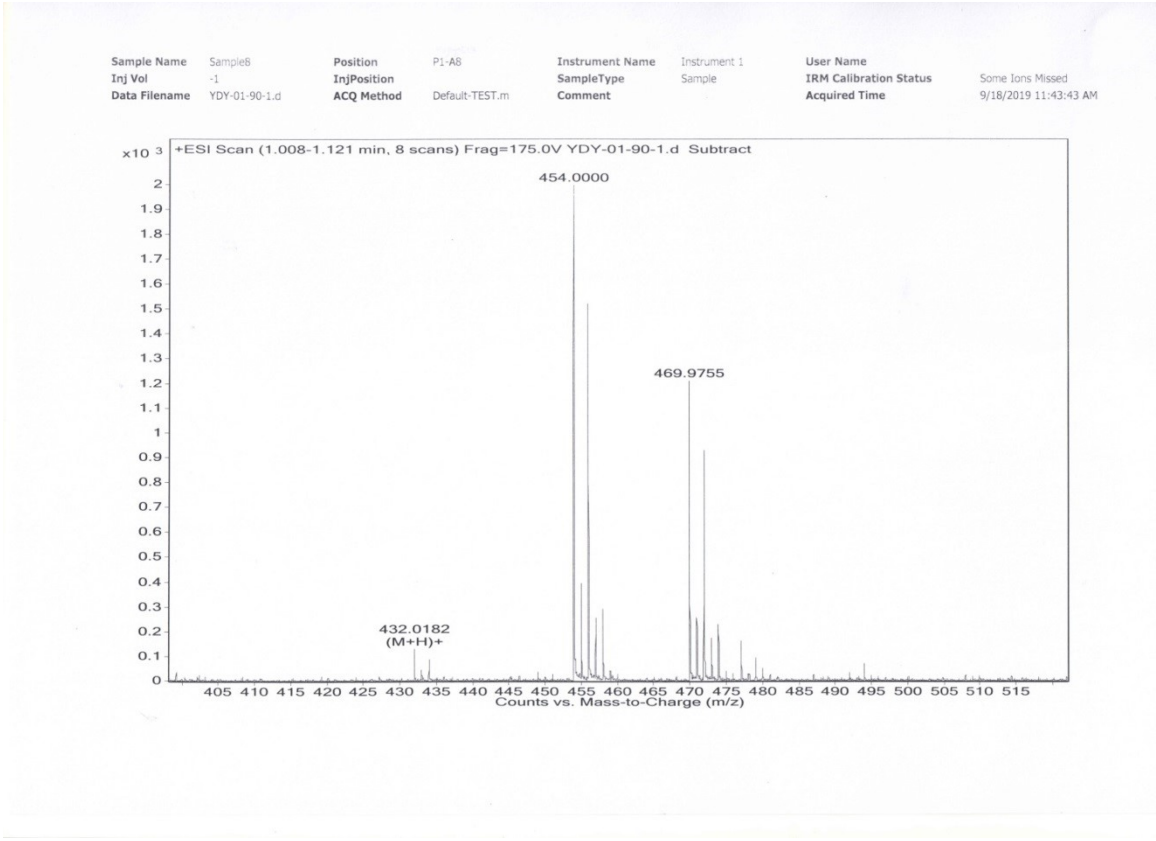


Figure S45. The HRMS spectra of **4a**

Data for methyl (E)-2-(2-(((Z)-(3,4-dichloroisothiazol-5-yl)(methoxyimino)methoxy)methyl)phenyl)-3-methoxyacrylate (**4b**). Yield 55%; white solid; mp100-101 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.55 – 7.50 (m, 1H), 7.40 – 7.30 (m, 2H), 7.20 – 7.12 (m, 1H), 5.27 (s, 2H), 3.94 (s, 3H), 3.78 (s, 3H), 3.67 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 167.64, 160.35, 152.03, 149.13, 146.10, 134.92, 131.49, 131.20, 128.27, 128.22, 128.12, 120.61, 109.61, 72.27, 63.30, 62.01, 51.71. HRMS (ESI) m/z calcd for $C_{17}H_{17}Cl_2N_2O_5S$ $(M+H)^+$431.0230, found 431.0235.

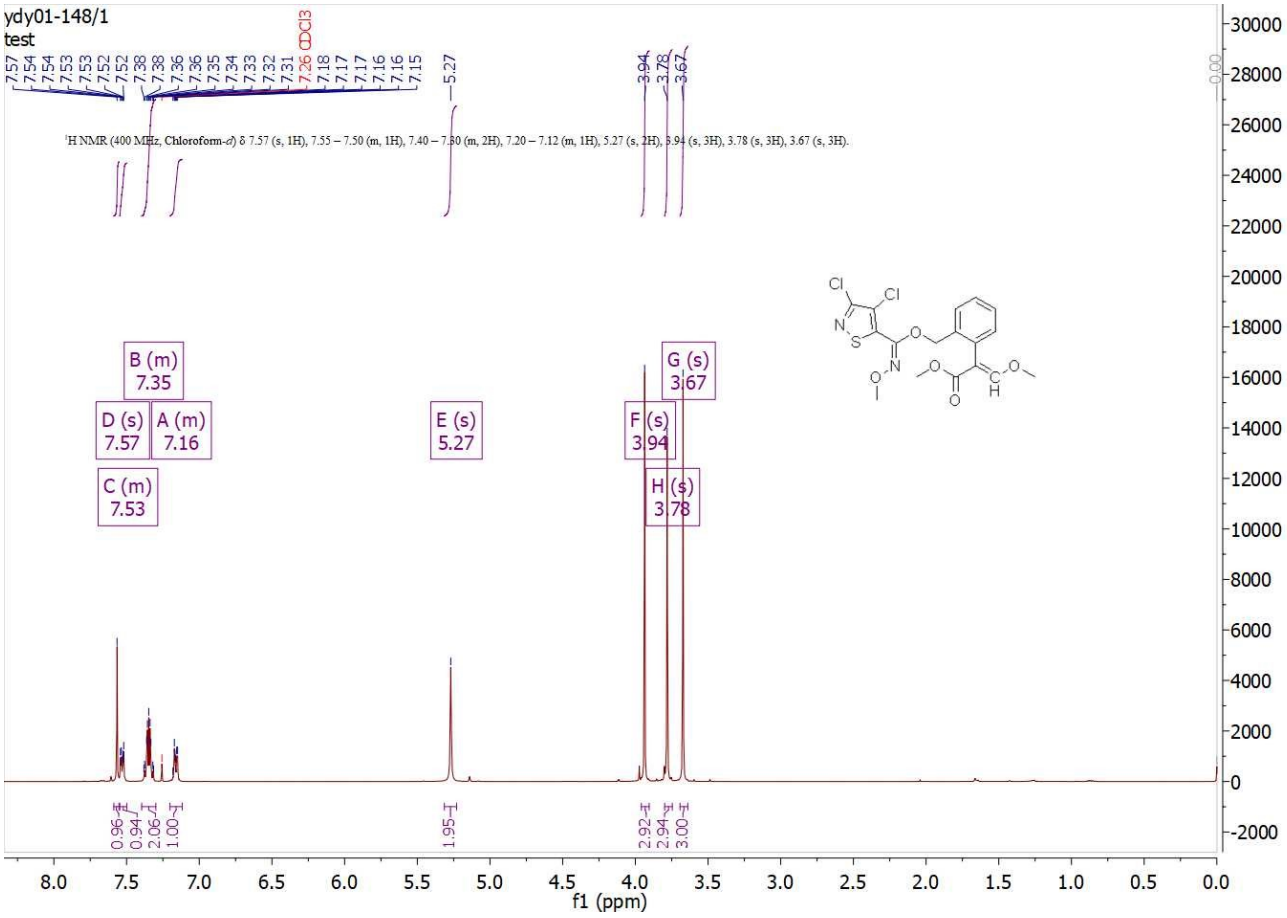


Figure S46. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **4b**

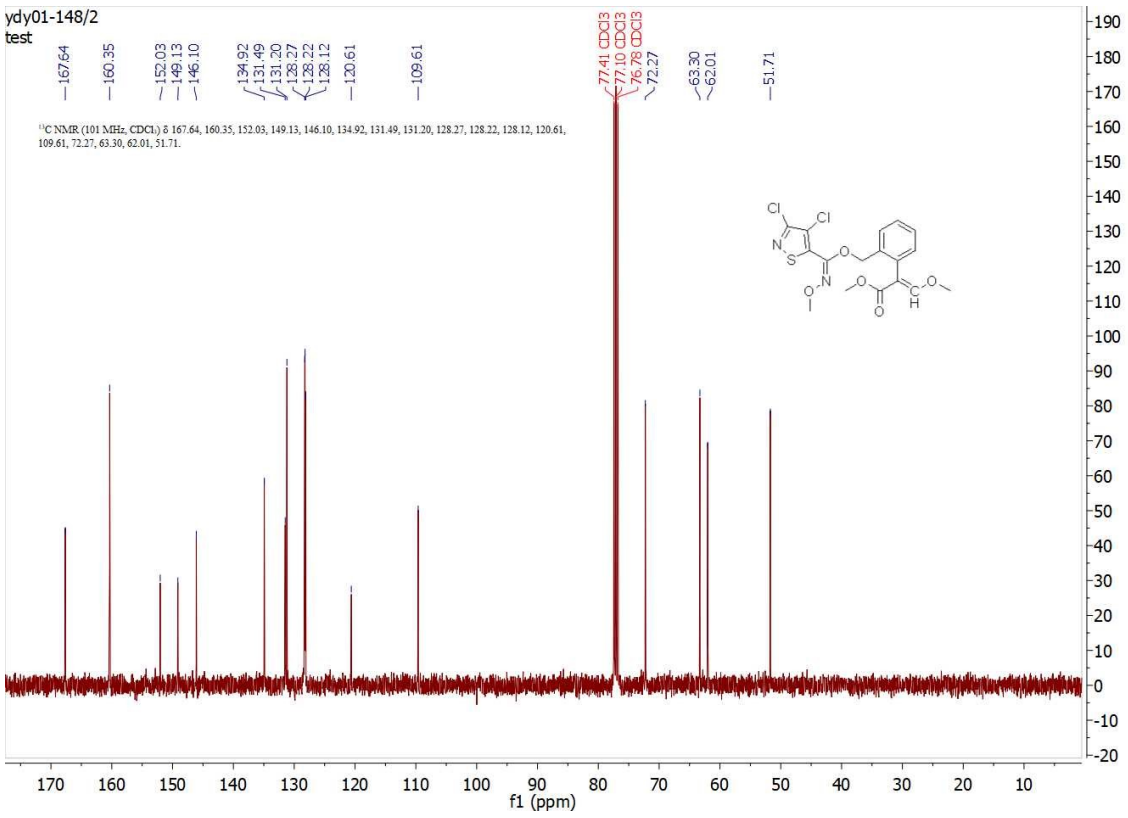


Figure S47. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **4b**

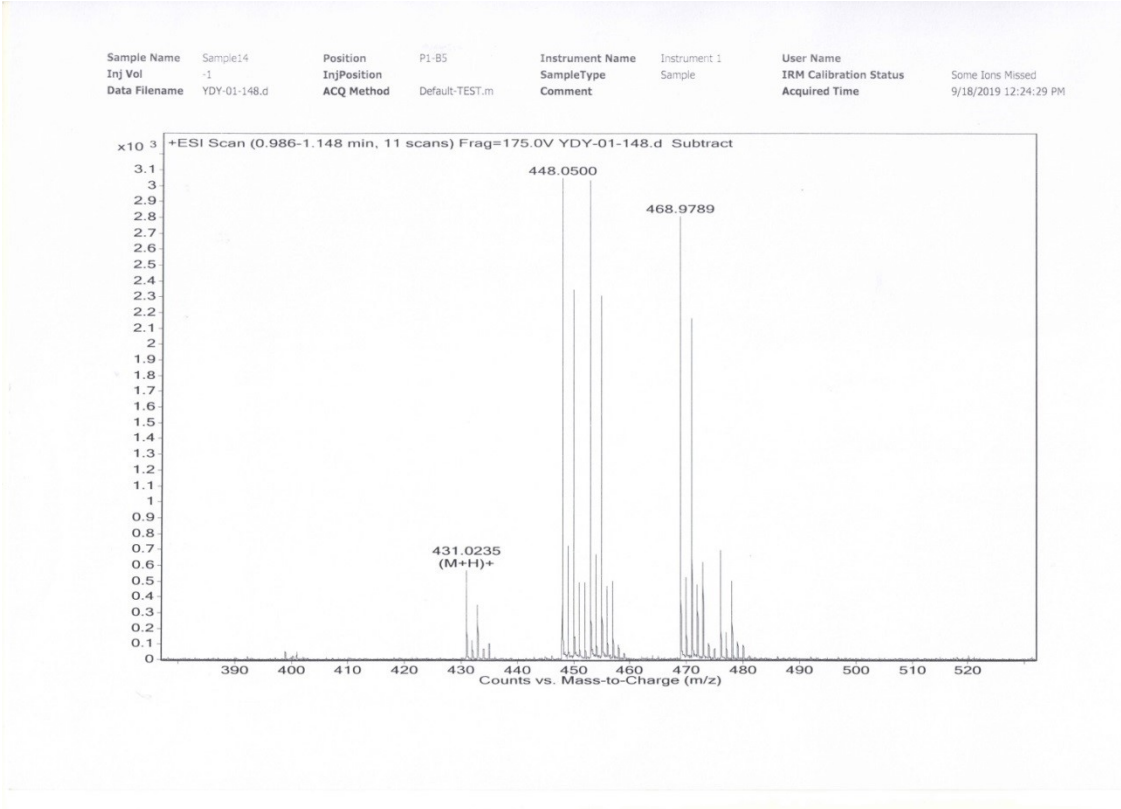


Figure S48. The HRMS spectra of **4b**

Data for methyl (E)-2-(2-(((Z)-((cyclopropylmethoxy)imino)(3,4-dichloroisothiazol-5-yl)methoxy)methyl)phenyl)-2-(methoxyimino)acetate (**4c**). Yield 61%; white solid; mp99-100 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) 7.68 – 7.55 (m, 1H), 7.44 (dtd, $J$ = 20.4, 7.5, 1.4 Hz, 2H), 7.19 (dd, $J$ = 7.5, 1.5 Hz, 1H), 5.31 (s, 2H), 4.02 (s, 3H), 3.95 (d, $J$ = 7.2 Hz, 2H), 3.84 (s, 3H), 1.30 – 1.12 (m, 1H), 0.66 – 0.49 (m, 2H), 0.34 (dt, $J$ = 6.1, 4.6 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.13, 152.27, 149.35, 148.78, 145.63, 134.32, 129.68, 129.36, 128.53, 128.50, 128.36, 120.32, 80.50, 72.20, 63.83, 53.02, 10.14, 3.17. HRMS (ESI) m/z calcd for $C_{19}H_{20}Cl_2N_3O_5S$ $(M+H)^+$472.0495, found 472.0503.

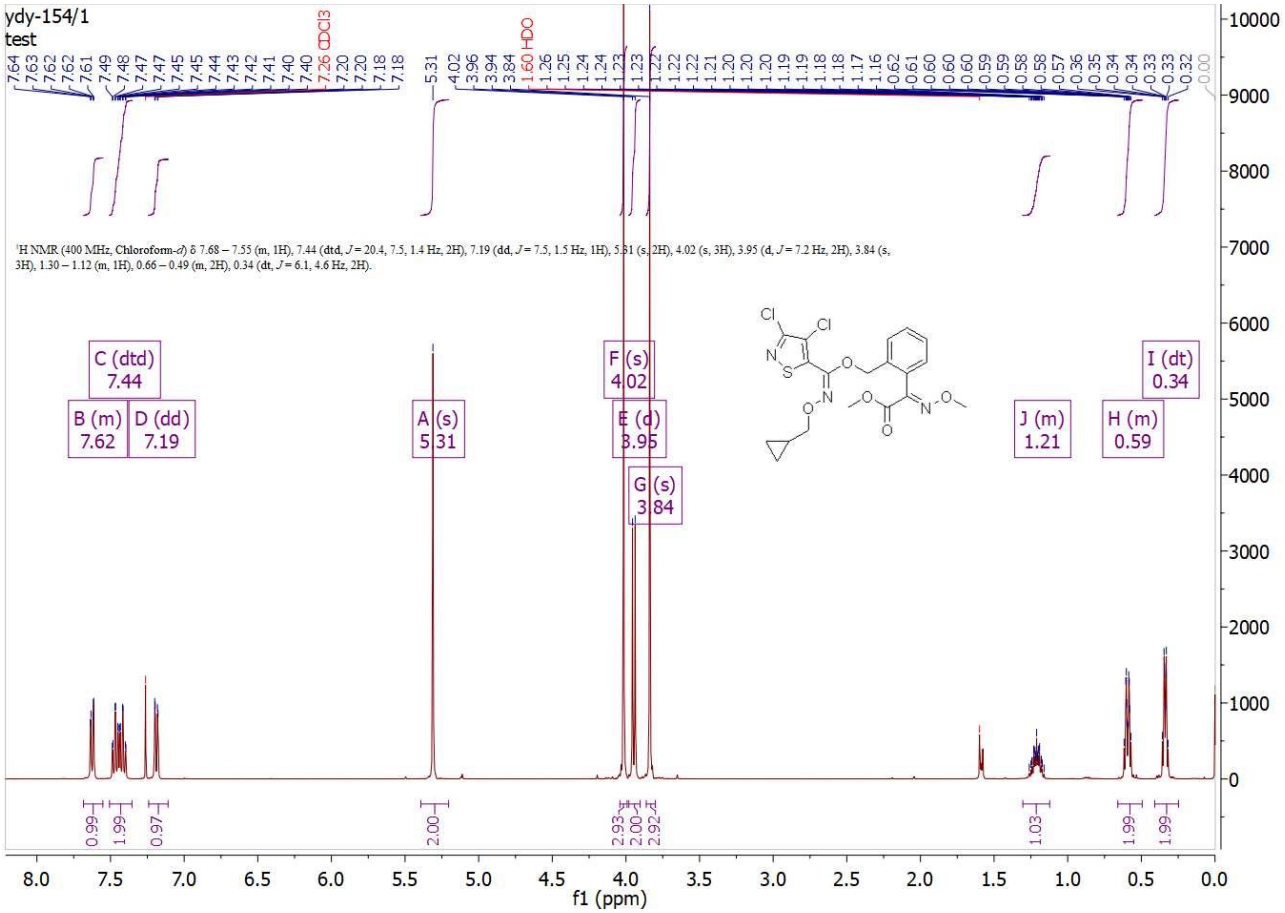


Figure S49. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **4c**

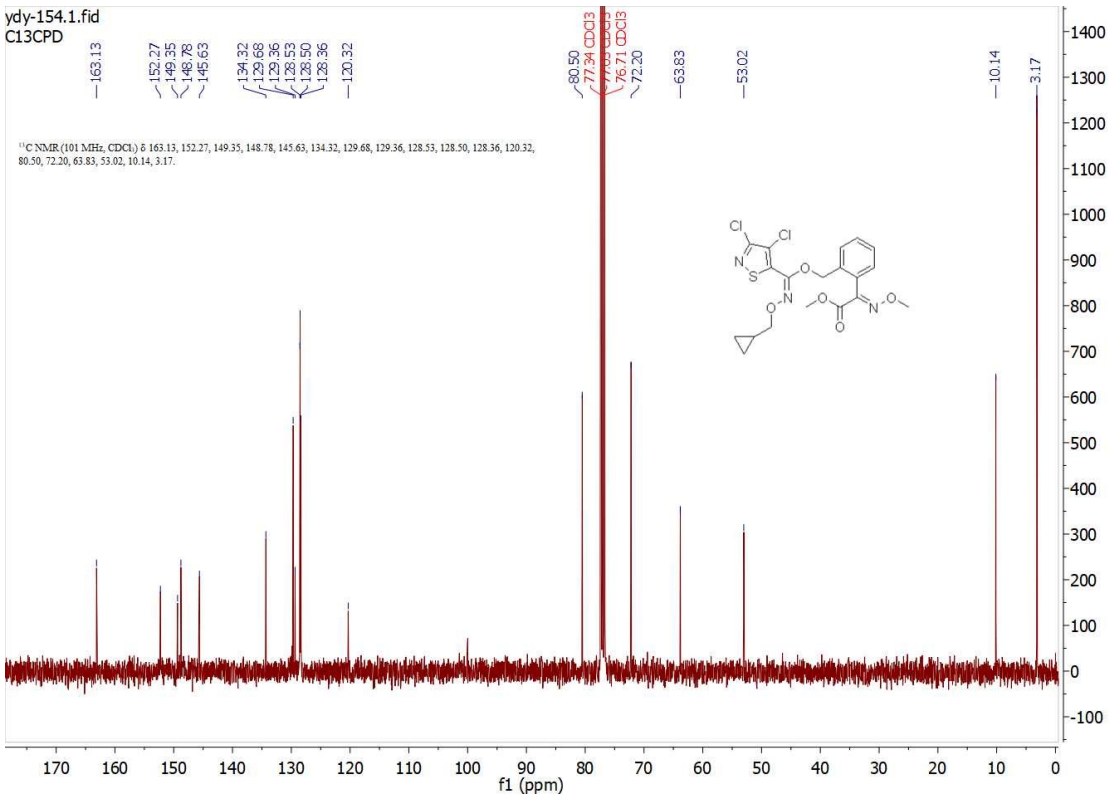


Figure S50. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **4c**

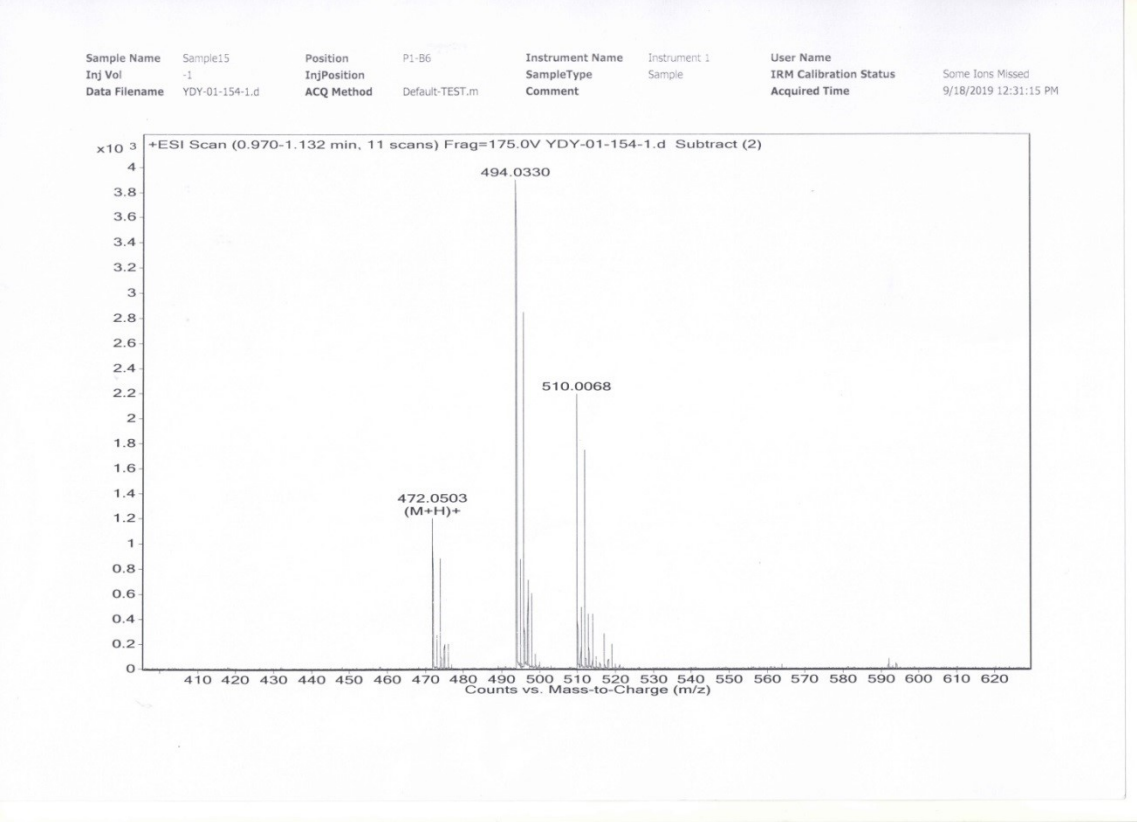


Figure S51. The HRMS spectra of **4c**

Data for methyl (E)-2-(2-(((Z)-((cyclopropylmethoxy)imino)(3,4-dichloroisothiazol-5-yl)methoxy)methyl)phenyl)-3-methoxyacrylate (**4d**). Yield 53%; white solid; mp78-79 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, $J$ = 6.8 Hz, 1H), 7.58 (s, 1H), 7.36 (tt, $J$ = 9.2, 4.6 Hz, 2H), 7.17 (d, $J$ = 7.0 Hz, 1H), 5.35 (s, 2H), 3.96 (d, $J$ = 7.2 Hz, 2H), 3.80 (s, 3H), 3.68 (s, 3H), 1.35 – 1.11 (m, 1H), 0.61 (d, $J$ = 7.7 Hz, 2H), 0.35 (d, $J$ = 5.0 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 167.64, 160.37, 152.56, 149.15, 145.99, 135.13, 131.50, 131.15, 131.02, 128.33, 128.21, 128.09, 120.22, 109.65, 80.40, 72.26, 62.00, 51.69, 10.19, 3.21. HRMS (ESI) m/z calcd for $C_{20}H_{21}Cl_2N_2O_5S$ $(M+H)^+$471.0543, found 471.0549.

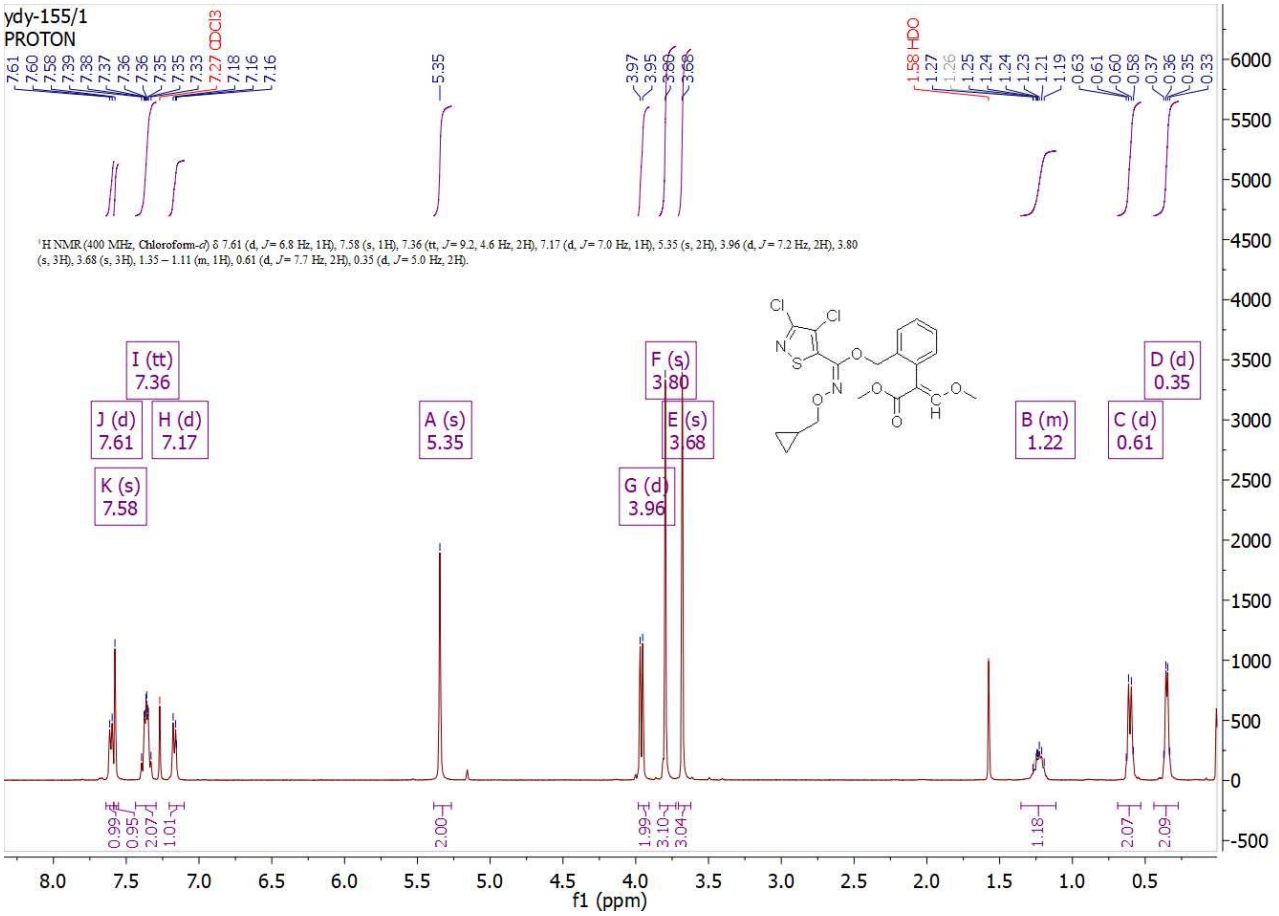


Figure S52. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **4d**

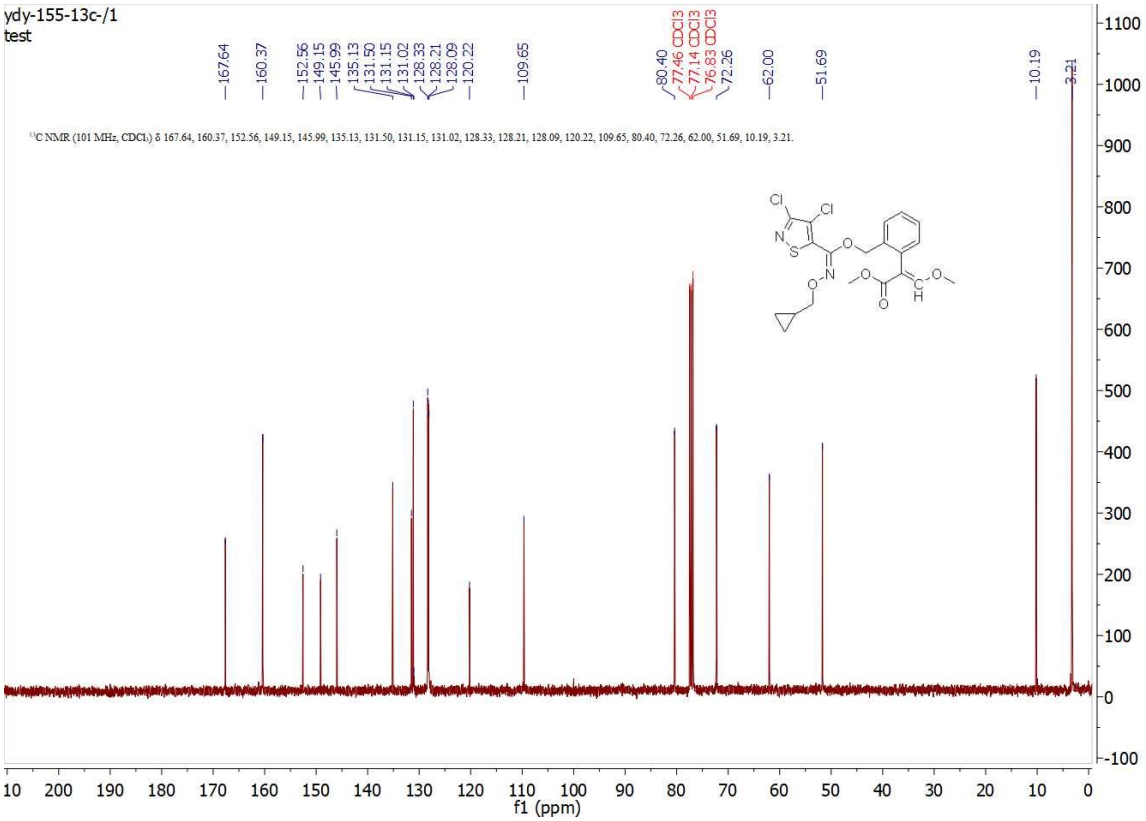


Figure S53. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **4d**

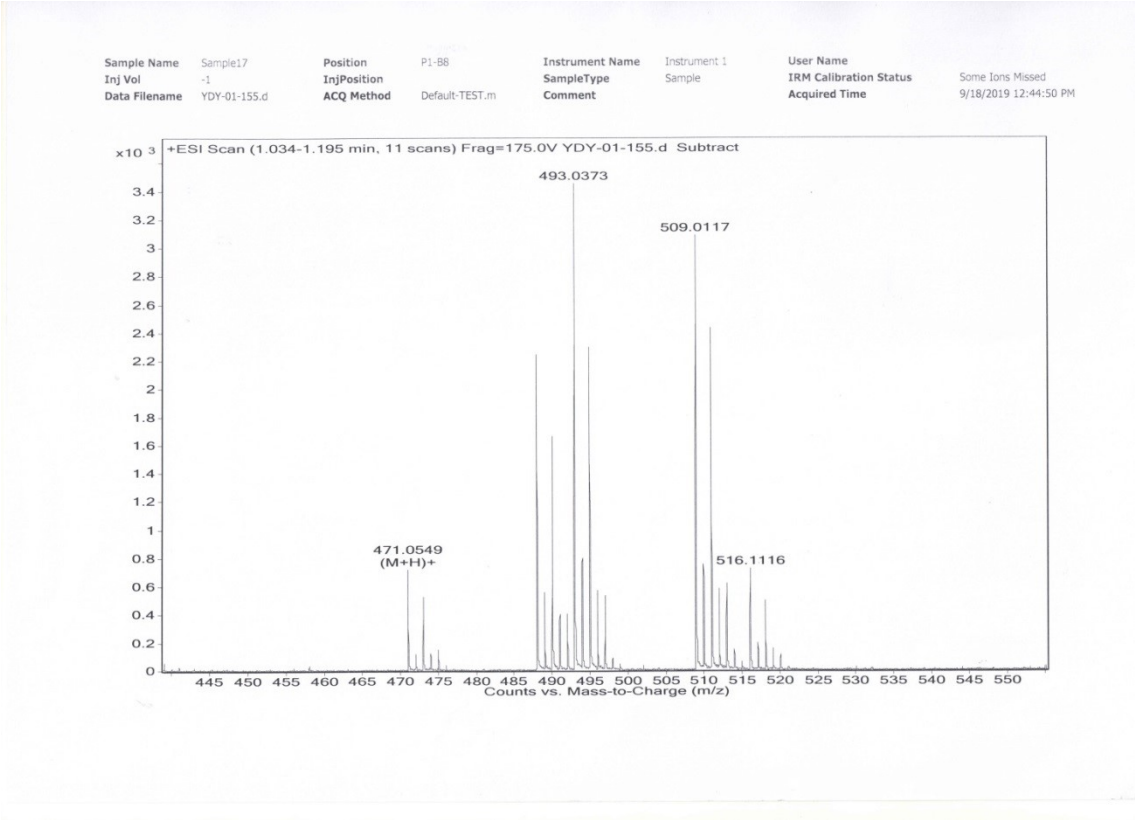


Figure S54. The HRMS spectra of **4d**

Data for methyl (E)-2-(2-(((E)-(3,4-dichloroisothiazol-5-yl)((prop-2-yn-1-yloxy)imino)methoxy)methyl)phenyl)-2-(methoxyimino)acetate (**4e**). Yield 28%; white solid; mp77-78 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.5 Hz, 1H), 7.45 (dddd, *J* = 16.1, 8.7, 6.8, 3.7 Hz, 2H), 7.24 – 7.15 (m, 1H), 5.29 (s, 2H), 4.75 – 4.66 (m, 2H), 4.03 (s, 3H), 3.85 (s, 3H), 2.54 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.13, 151.36, 149.41, 148.66, 146.86, 133.98, 129.77, 129.38, 128.62, 128.54, 121.24, 78.61, 75.55, 72.69, 63.92, 62.99, 53.14. HRMS (ESI) m/z calcd for $C_{18}H_{16}Cl_2N_3O_5S$ $(M+H)^+$456.0182, found 456.0188.

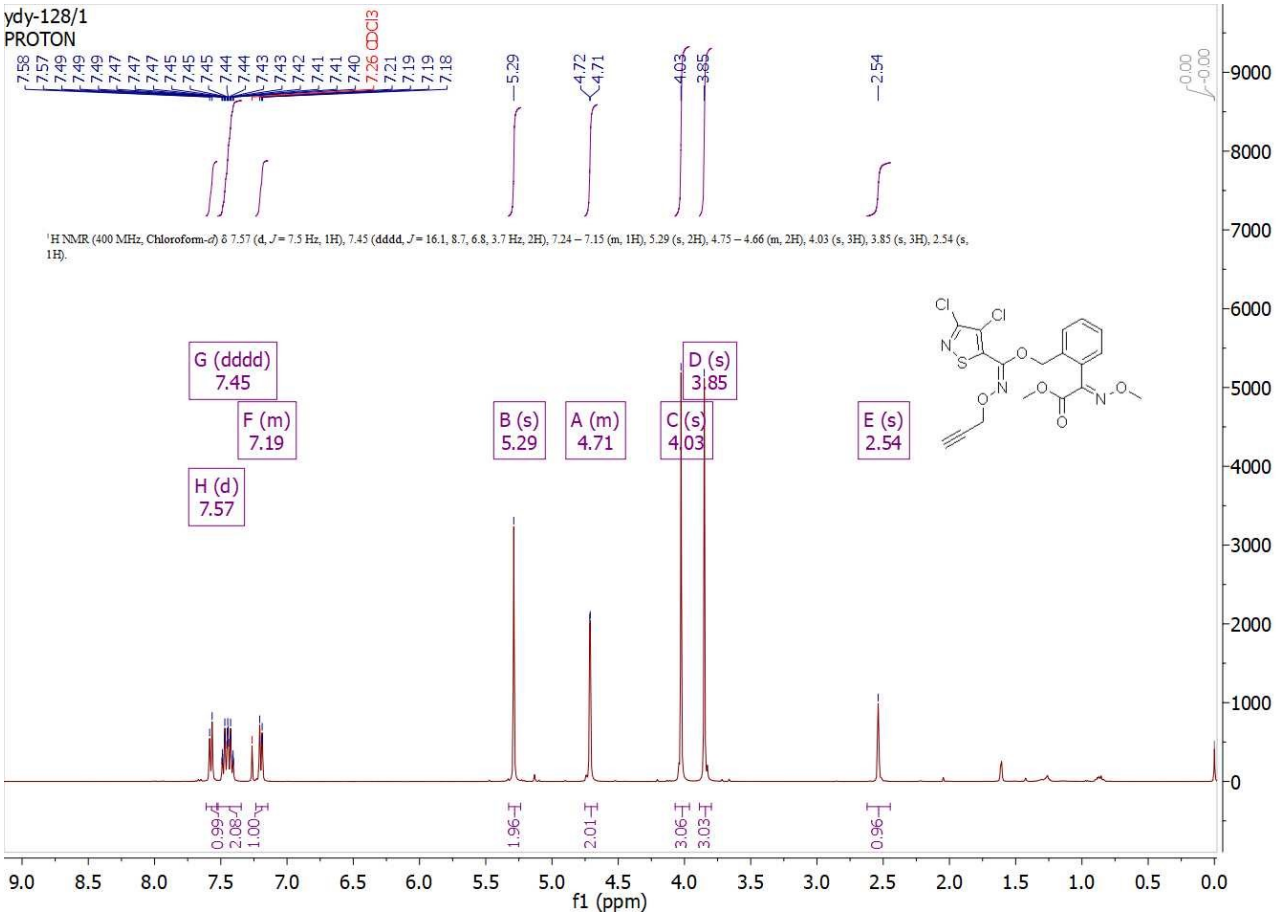


Figure S55. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **4e**

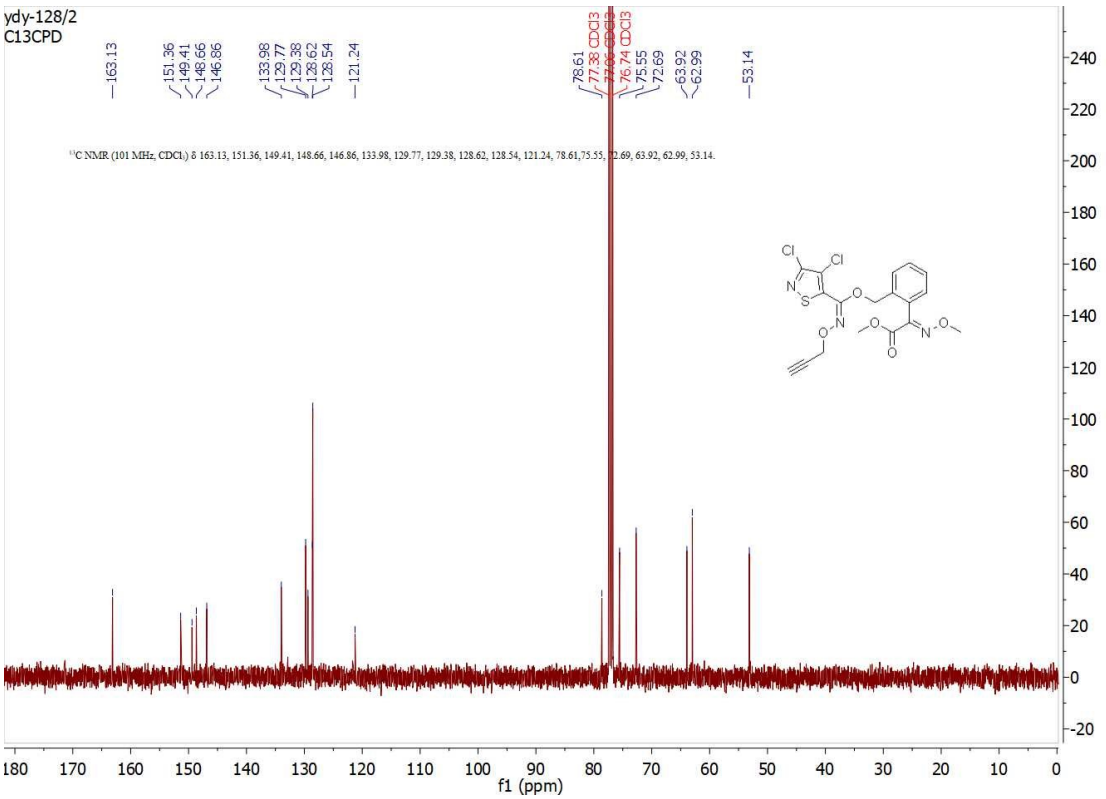


Figure S56. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **4e**

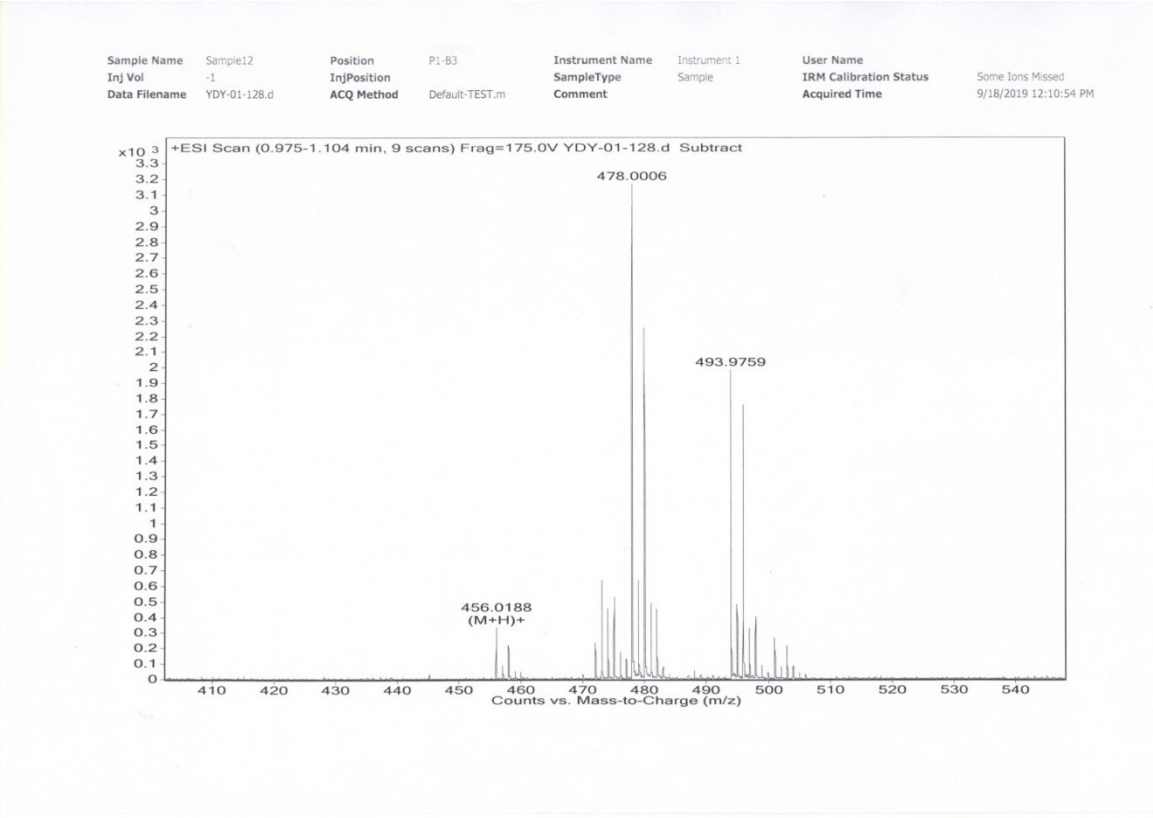


Figure S57. The HRMS spectra of **4e**

Data for methyl (E)-2-(2-(((E)-(3,4-dichloroisothiazol-5-yl)((prop-2-yn-1-yloxy)imino)methoxy)methyl)phenyl)-3-methoxyacrylate (**4f**). Yield 27%; white solid; mp120-140 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.56 – 7.51 (m, 1H), 7.42 – 7.30 (m, 2H), 7.17 (dd, *J* = 6.4, 2.6 Hz, 1H), 5.32 (s, 2H), 4.71 (d, *J* = 1.9 Hz, 2H), 3.80 (s, 3H), 3.68 (s, 3H), 2.54 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 167.63, 160.38, 151.65, 149.22, 147.22, 134.77, 131.53, 131.20, 128.33, 128.29, 128.12, 121.15, 109.57, 78.75, 75.40, 72.73, 62.92, 62.04, 51.73. HRMS (ESI) m/z calcd for $C_{19}H_{17}Cl_2N_2O_5S$ $(M+H)^+$455.0230, found 455.0219.

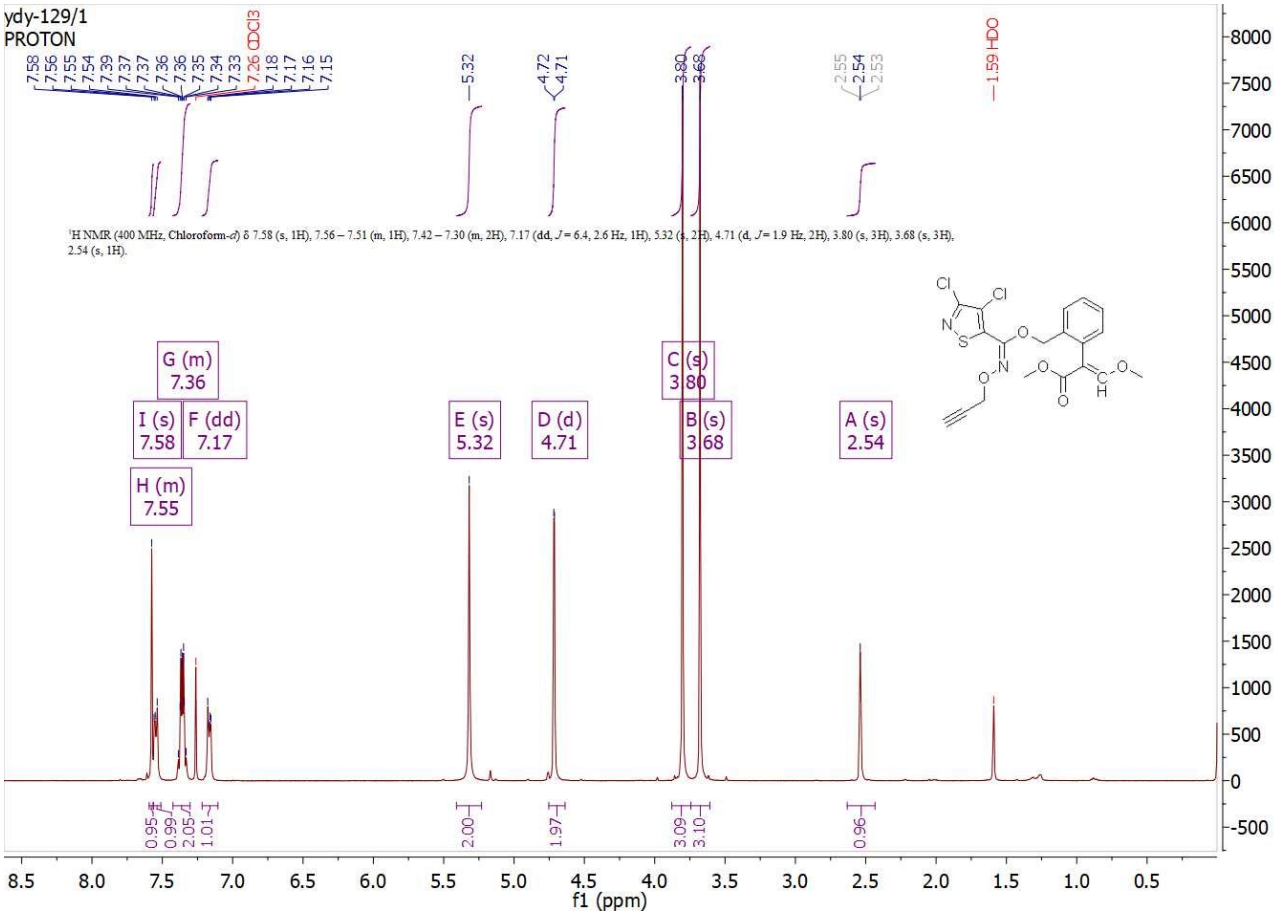


Figure S58. The $^{1}$H NMR (400 MHz, $CDCl_3$) of 4**f**

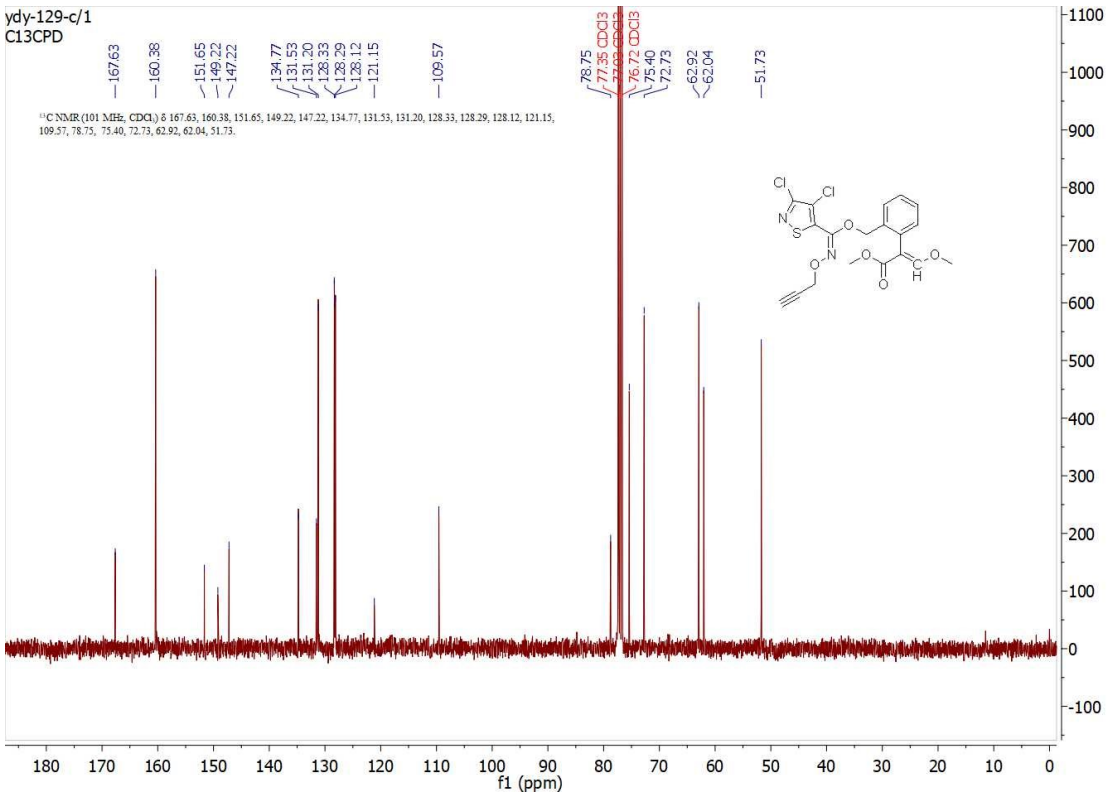


Figure S59. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of 4**f**

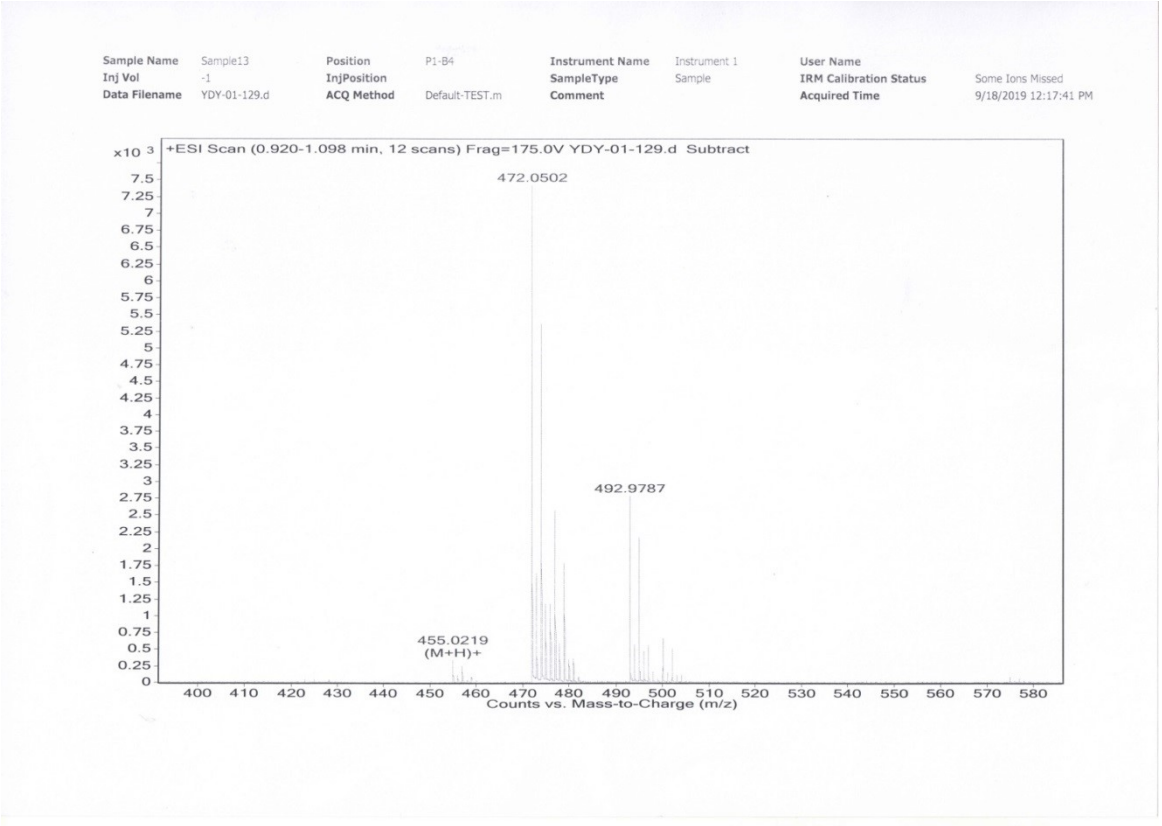


Figure S60. The HRMS spectra of **4f**

Data for methyl (Z)-3,4-dichloro-N-((2-((E)-1-(methoxyimino)-2-(methylamino)-2-oxoethyl)benzyl)oxy)isothiazole-5-carbimidate (**7a**). Yield 76%; white solid; mp93-94 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.48 (m, 1H), 7.44 (qd, *J* = 7.6, 3.8 Hz, 2H), 7.26 – 7.20 (m, 1H), 6.83 (d, *J* = 5.7 Hz, 1H), 5.04 (s, 2H), 4.06 (s, 3H), 3.98 (s, 3H), 2.92 (d, *J* = 5.0 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.79, 151.80, 150.92, 149.39, 147.13, 134.92, 129.85, 129.37, 129.26, 128.86, 128.16, 120.77, 76.24, 63.33, 60.84, 26.23. HRMS (ESI) m/z calcd for $C_{16}H_{17}Cl_2N_4O_4S$ $(M+H)^+$431.0342, found 431.0349.

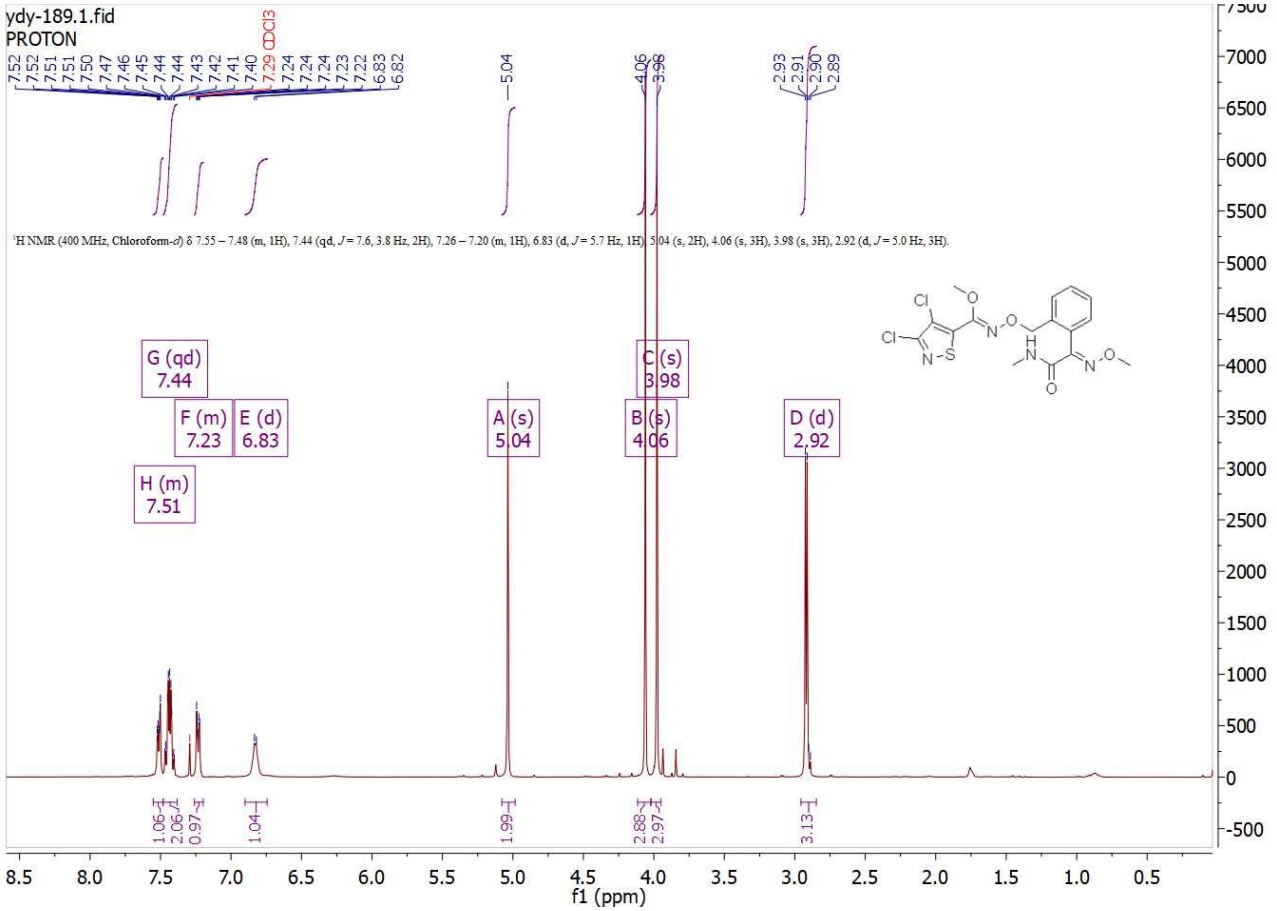


Figure S61. The $^{1}$H NMR (400 MHz, $CDCl_3$) of 7**a**

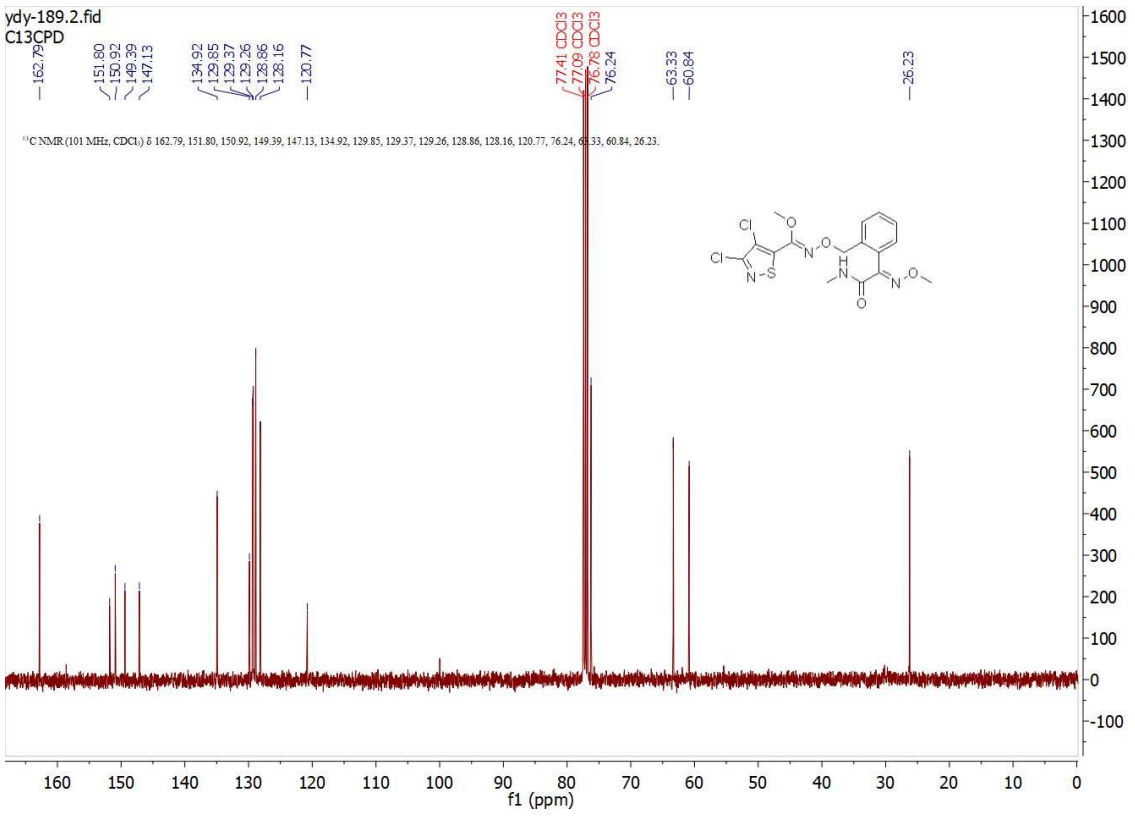


Figure S62. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **7a**

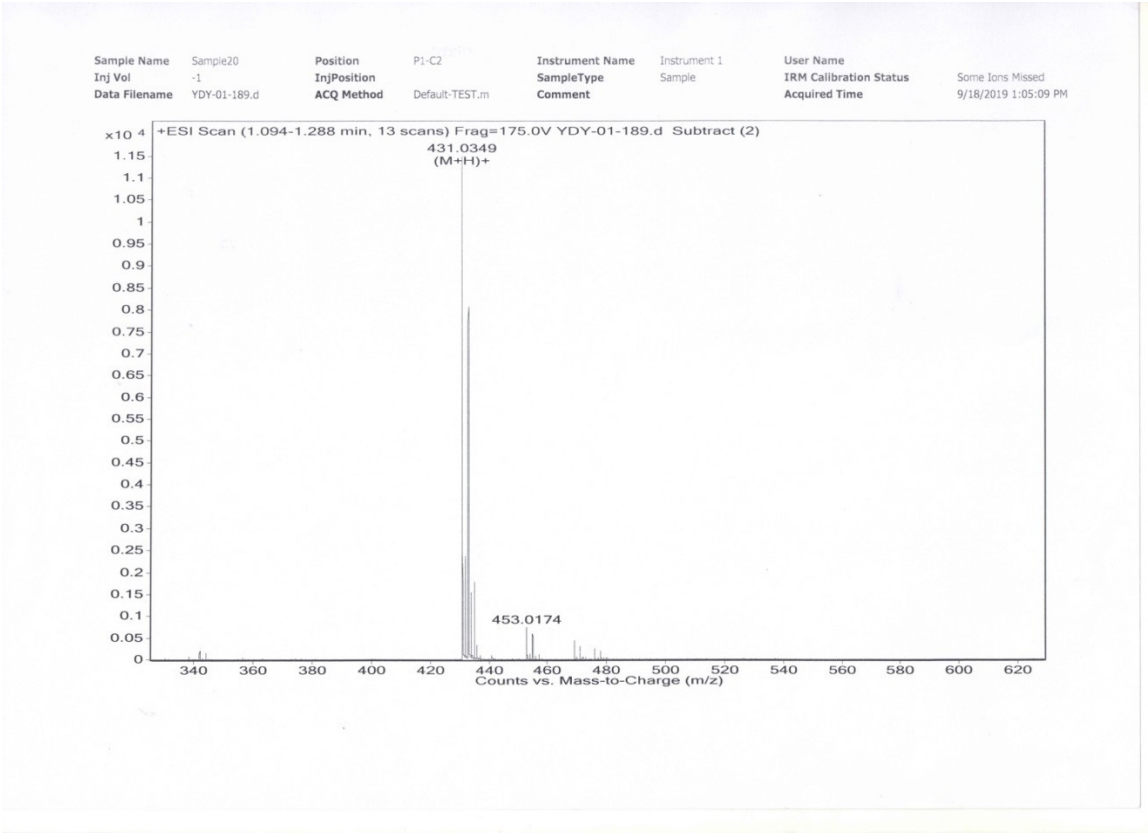


Figure S63. The HRMS spectra of **7a**

Data for 2-((E)-1-(methoxyimino)-2-(methylamino)-2-oxoethyl)benzyl (E)-3,4-dichloro-N-methoxyisothiazole-5-carbimidate (**7b**). Yield 68%; white solid; mp90-91 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 7.3, 1.6 Hz, 1H), 7.42 (dtd, *J* = 15.1, 7.4, 1.6 Hz, 2H), 7.23 – 7.18 (m, 1H), 6.79 (d, *J* = 5.7 Hz, 1H), 5.25 (s, 2H), 3.92 (s, 6H), 2.91 (d, *J* = 5.0 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.62, 151.83, 150.33, 149.22, 145.79, 134.33, 129.61, 129.05, 128.93, 128.36, 128.29, 120.65, 72.58, 63.33, 63.31, 26.28. HRMS (ESI) m/z calcd for $C_{16}H_{17}Cl_2N_4O_4S$ $(M+H)^+$431.0342, found 431.0345.

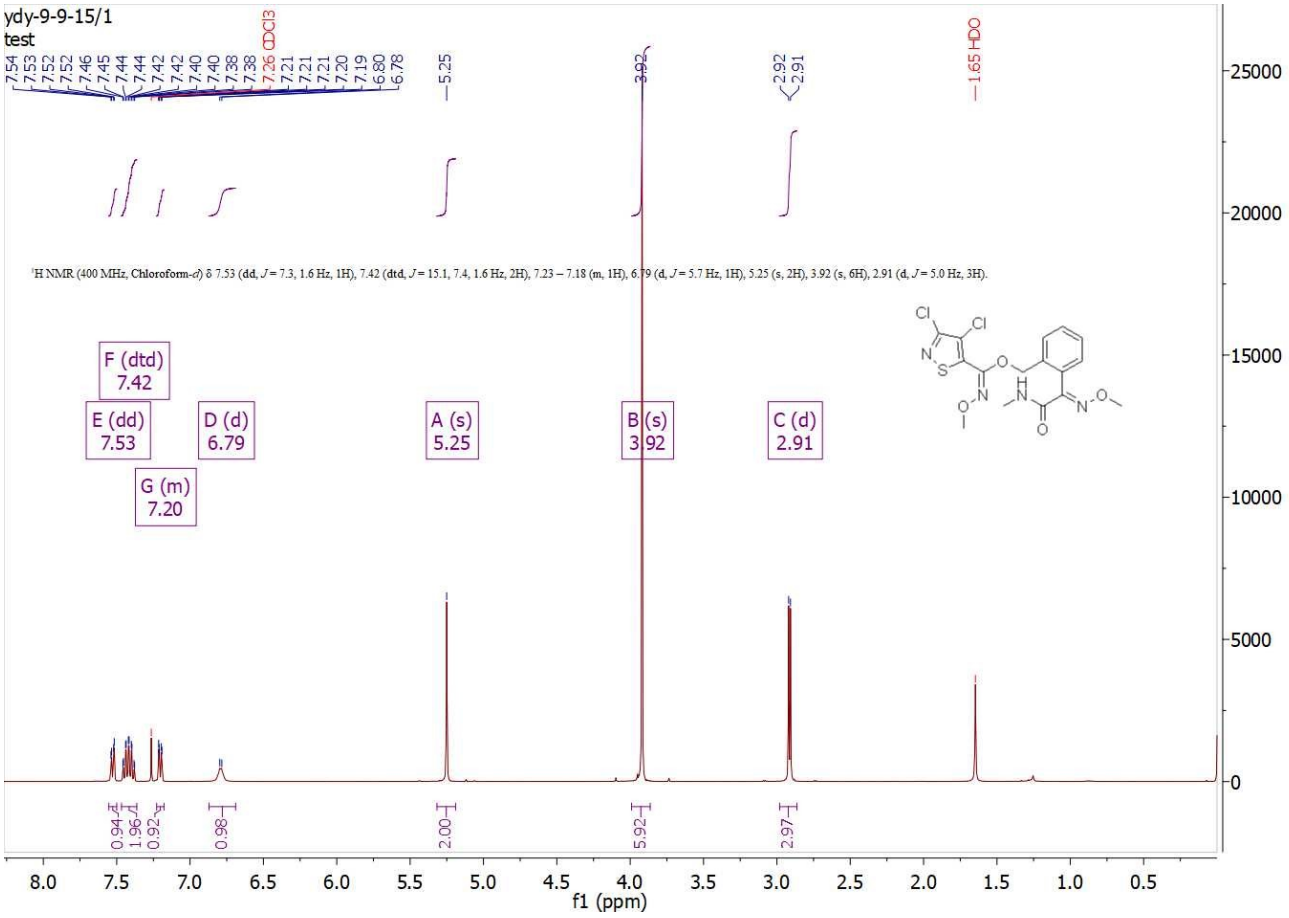


Figure S64. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **7b**

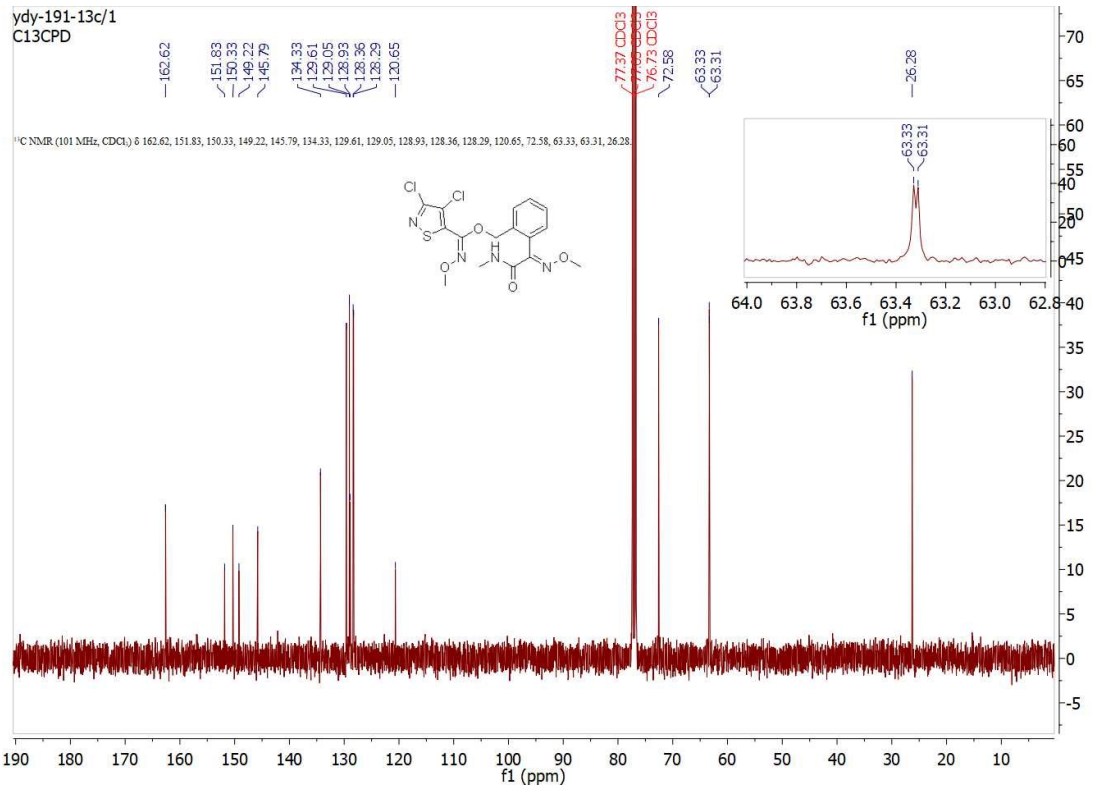


Figure S65. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **7b**

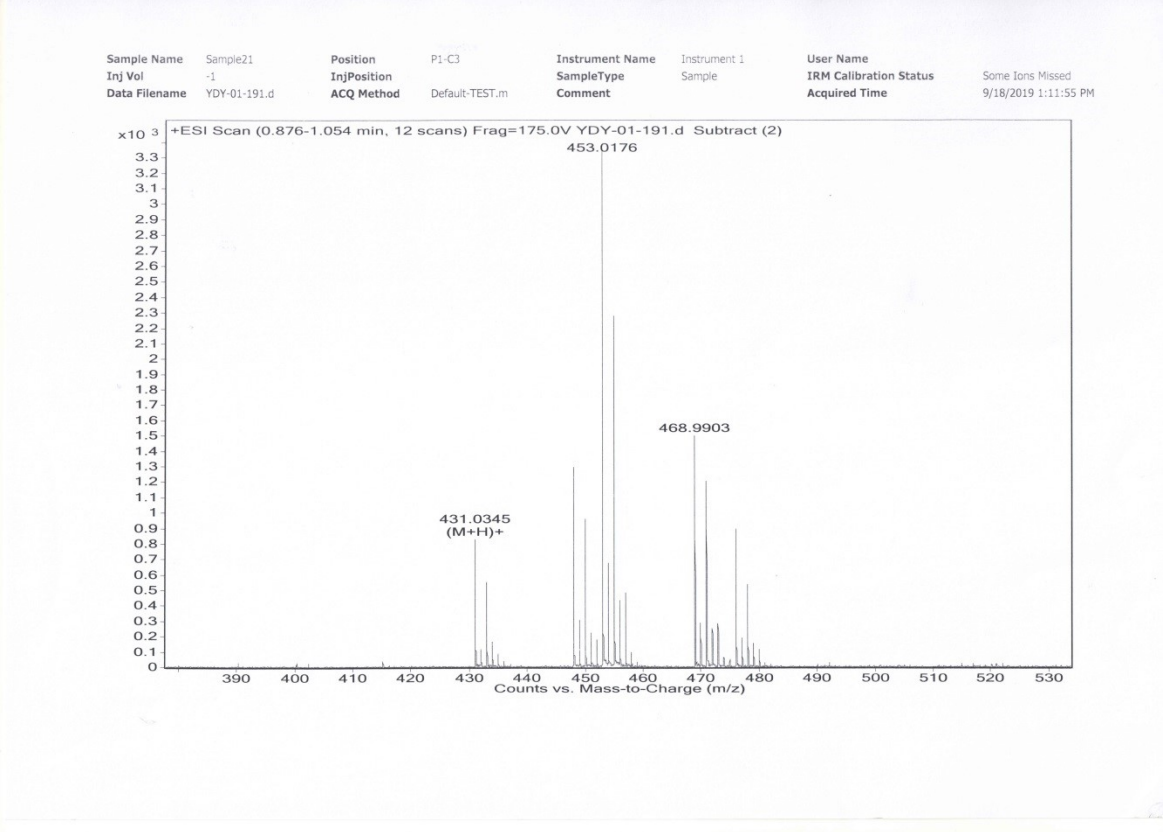


Figure S66. The HRMS spectra of **7b**

Data for 2-((E)-2-(cyclopropylamino)-1-(methoxyimino)-2-oxoethyl)benzyl (E)-3,4-dichloro-N-methoxyisothiazole-5-carbimidate (**7c**). Yield 59%; white solid; mp103-104 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.41 (dtd, *J* = 16.1, 7.4, 1.6 Hz, 2H), 7.20 (dd, *J* = 7.2, 1.7 Hz, 1H), 6.91 – 6.83 (m, 1H), 5.25 (s, 2H), 3.92 (s, 3H), 3.91 (s, 3H), 2.78 (tq, *J* = 7.3, 3.7 Hz, 1H), 0.82 (td, *J* = 7.1, 5.3 Hz, 2H), 0.66 – 0.51 (m, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.25, 151.85, 150.26, 149.23, 145.79, 134.37, 129.59, 129.19, 128.76, 128.34, 128.22, 120.64,72.68, 63.32, 63.31, 22.63, 6.64. HRMS (ESI) m/z calcd for $C_{18}H_{19}Cl_2N_4O_4S$ $(M+H)^+$457.0499, found 457.0506.

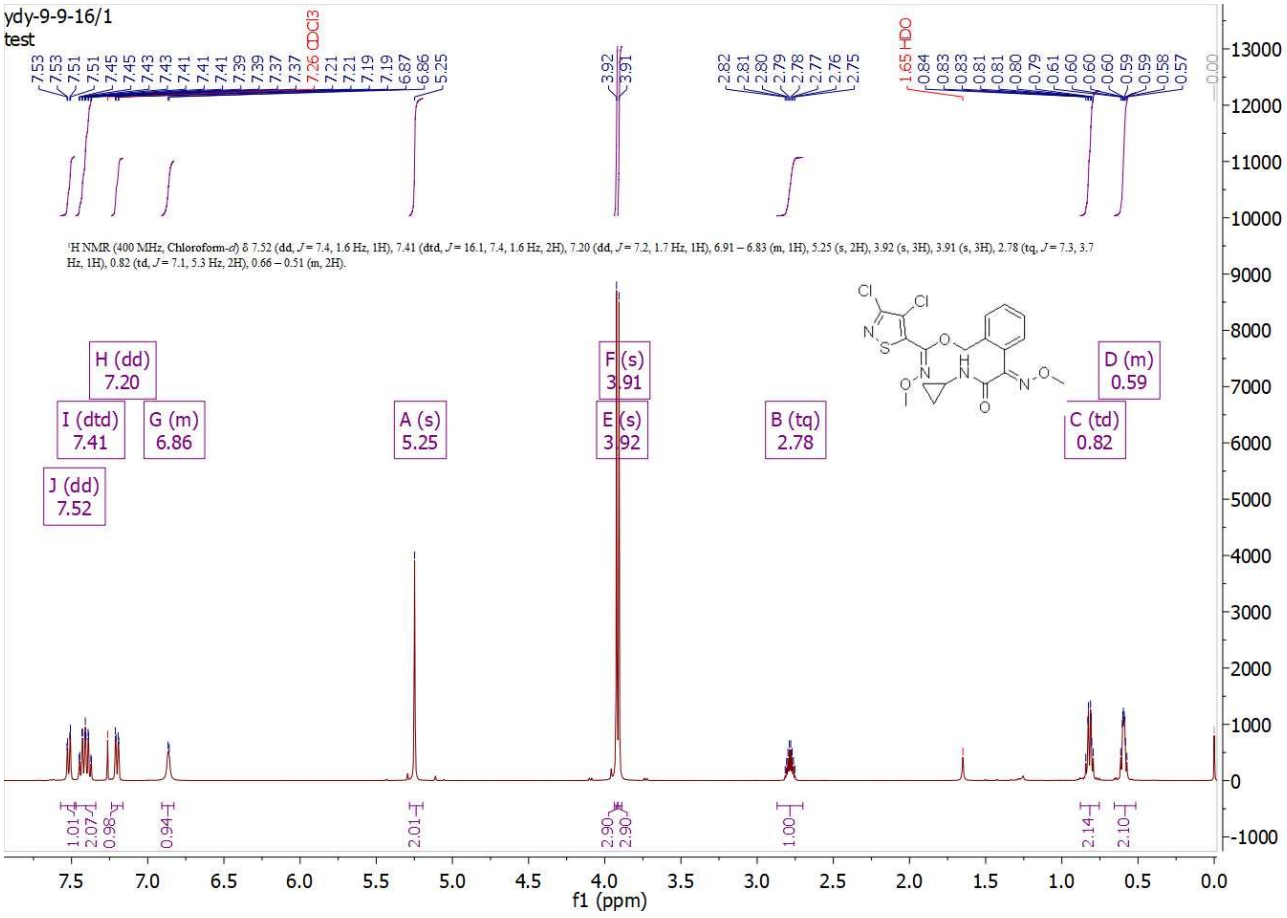


Figure S67. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **7c**

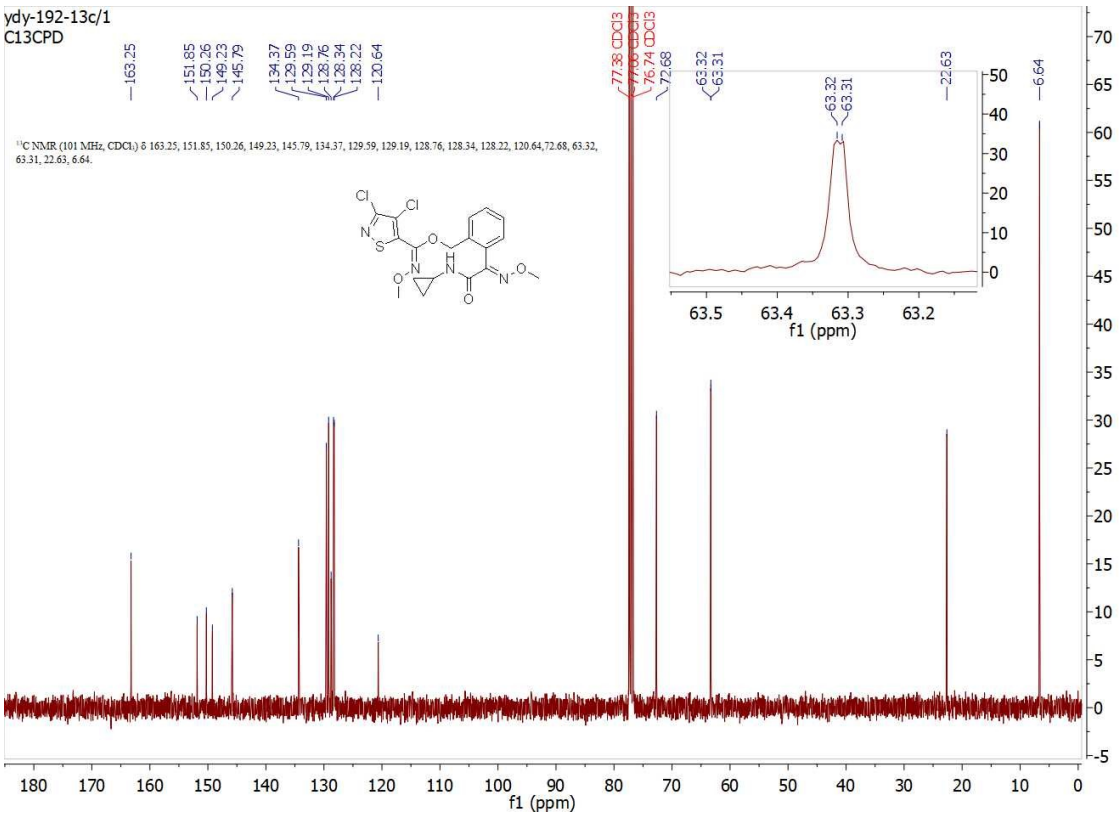


Figure S68. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **7c**

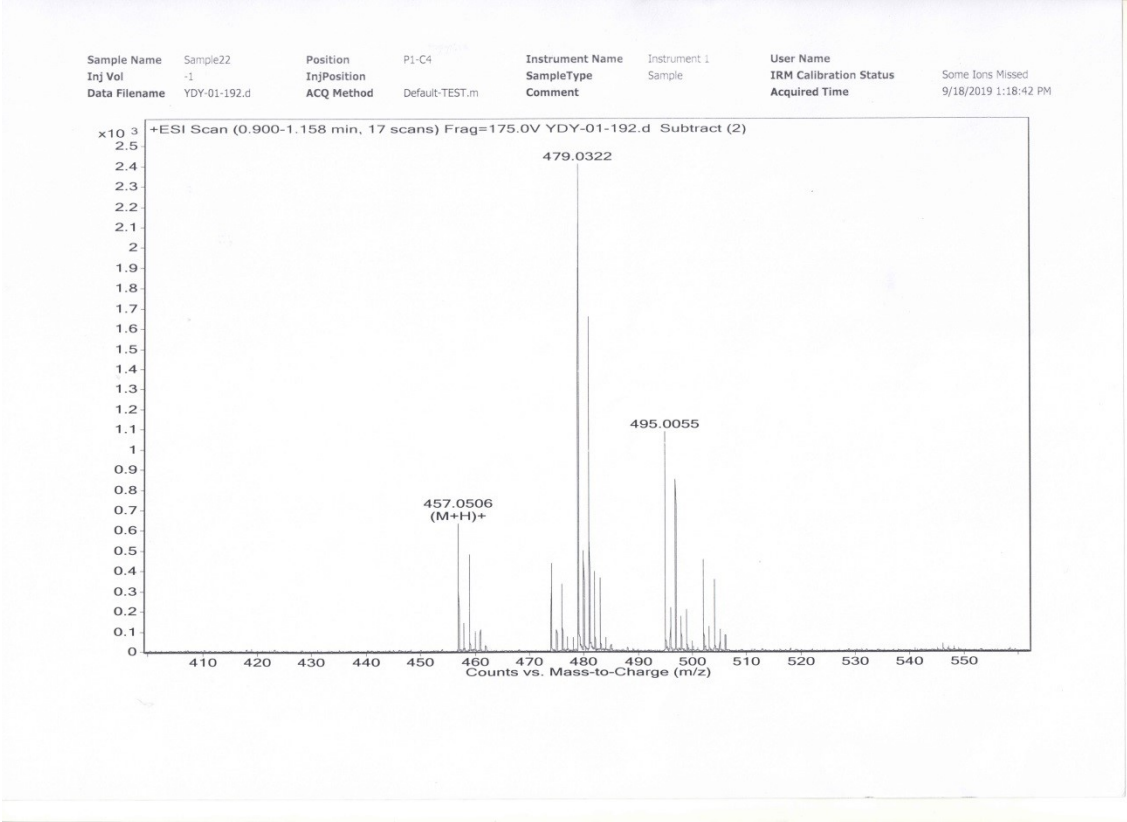


Figure S69. The HRMS spectra of **7c**

Data for (E)-3,4-dichloro-N-((2-(1-(methoxyimino)-2-(methylamino)-2-oxoethyl)benzyl)oxy)isothiazole-5-carboxamide (**7d**). Yield 57%; white solid; mp154-155 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 7.42 (dtd, *J* = 21.8, 7.4, 1.5 Hz, 2H), 7.33 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.16 (dd, *J* = 7.4, 1.5 Hz, 1H), 6.99 (d, *J* = 5.8 Hz, 1H), 5.00 (s, 2H), 3.96 (s, 3H), 2.92 (d, *J* = 5.1 Hz, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 164.33, 155.12, 154.31, 151.38, 149.18, 133.43, 131.30, 130.73, 129.37, 129.22, 128.24, 120.24, 76.76, 63.55, 26.37. HRMS (ESI) m/z calcd for $C_{15}H_{15}Cl_2N_4O_4S$ $(M+H)^+$417.0186, found 417.0191.

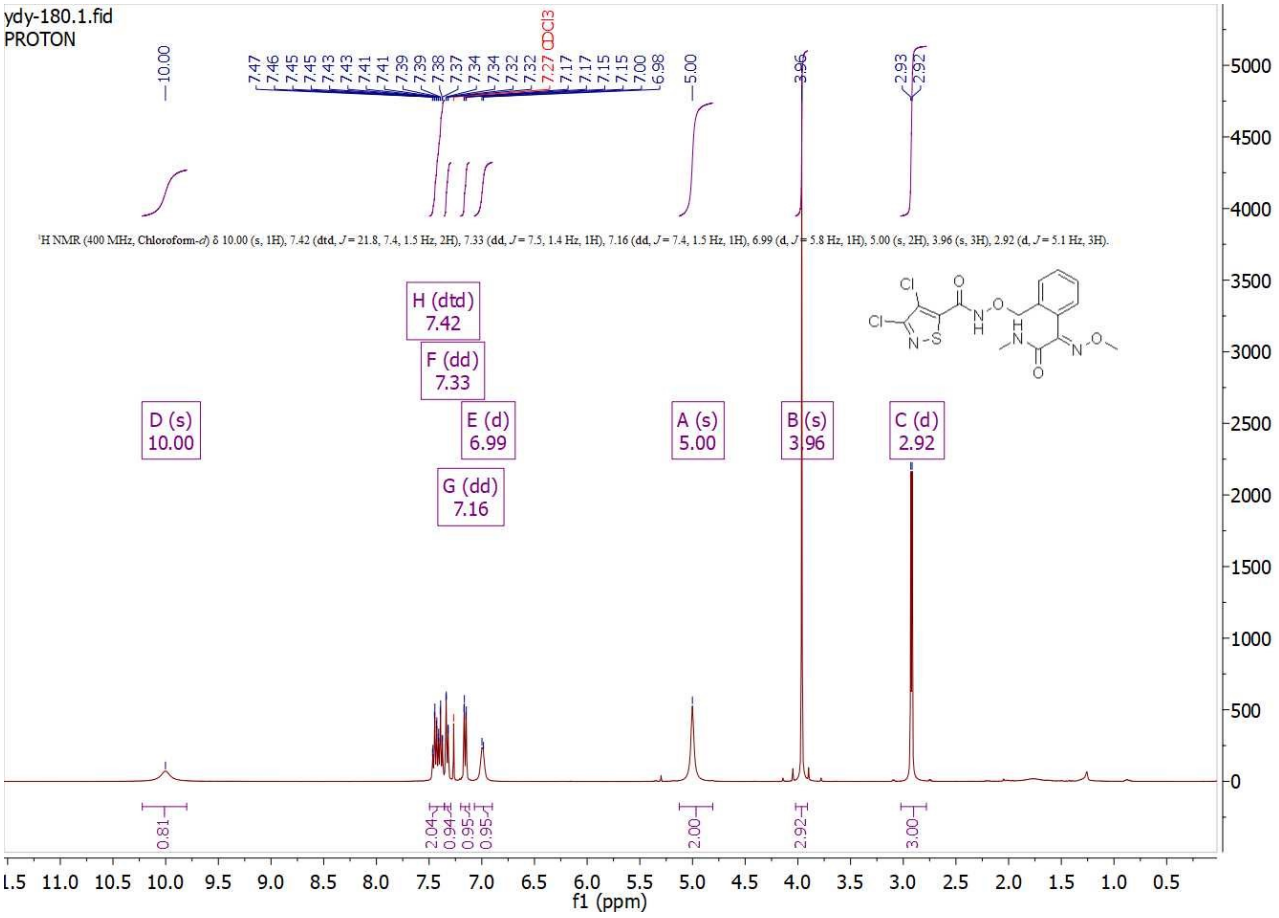


Figure S70. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **7d**

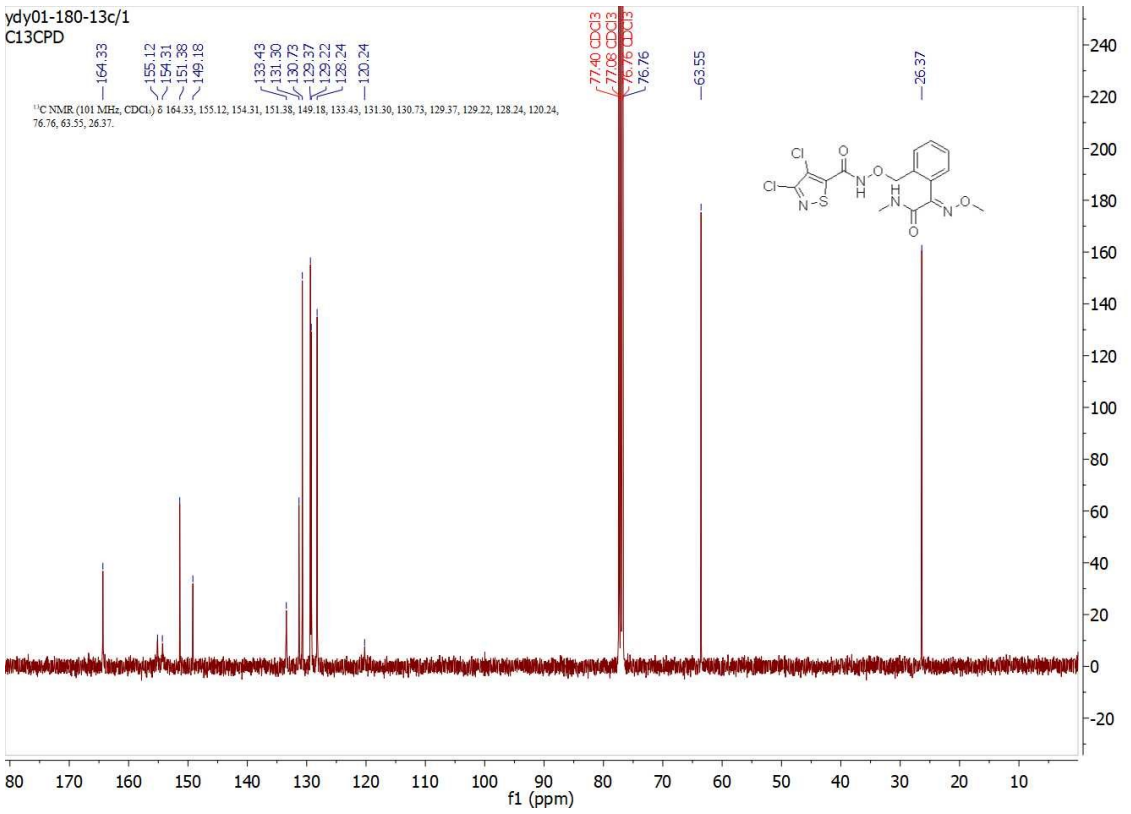


Figure S71. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **7d**

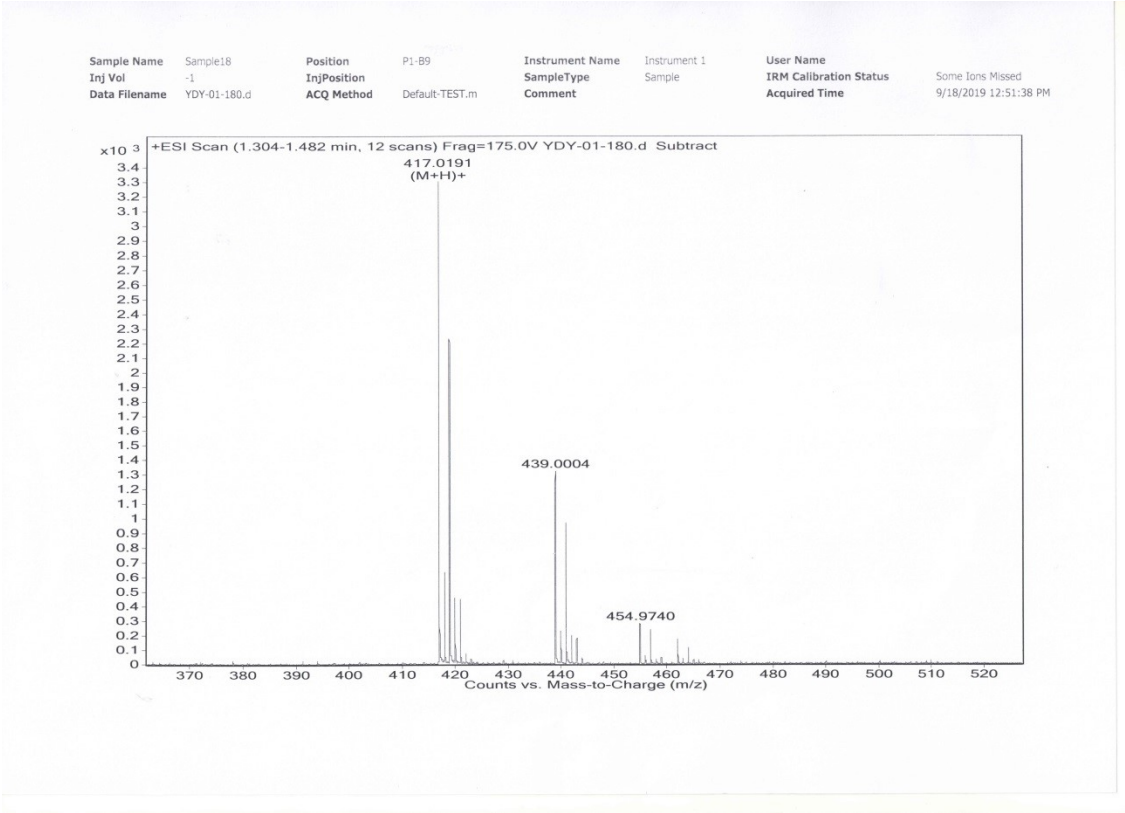


Figure S72. The HRMS spectra of **7d**

Data for (E)-3,4-dichloro-N-((2-(2-(cyclopropylamino)-1-(methoxyimino)-2-oxoethyl)benzyl)oxy)isothiazole-5-carboxamide (**7e**). Yield 61%; white solid; mp122-123 °C. $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 7.45 (dtd, *J* = 23.1, 7.5, 1.4 Hz, 2H), 7.35 (d, *J* = 7.4 Hz, 1H), 7.18 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.11 – 6.95 (m, 1H), 5.01 (s, 2H), 3.98 (s, 3H), 2.80 (tq, *J* = 7.3, 3.7 Hz, 1H), 0.92 – 0.76 (m, 2H), 0.66 (q, *J* = 3.9, 3.4 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 165.00, 155.22, 154.35, 151.32, 149.19, 133.32, 131.22, 130.75, 129.36, 129.24, 128.37, 120.30, 76.76, 63.56, 22.74, 6.68. HRMS (ESI) m/z calcd for $C_{17}H_{17}Cl_2N_4O_4S$ $(M+H)^+$443.0342, found 443.0351.

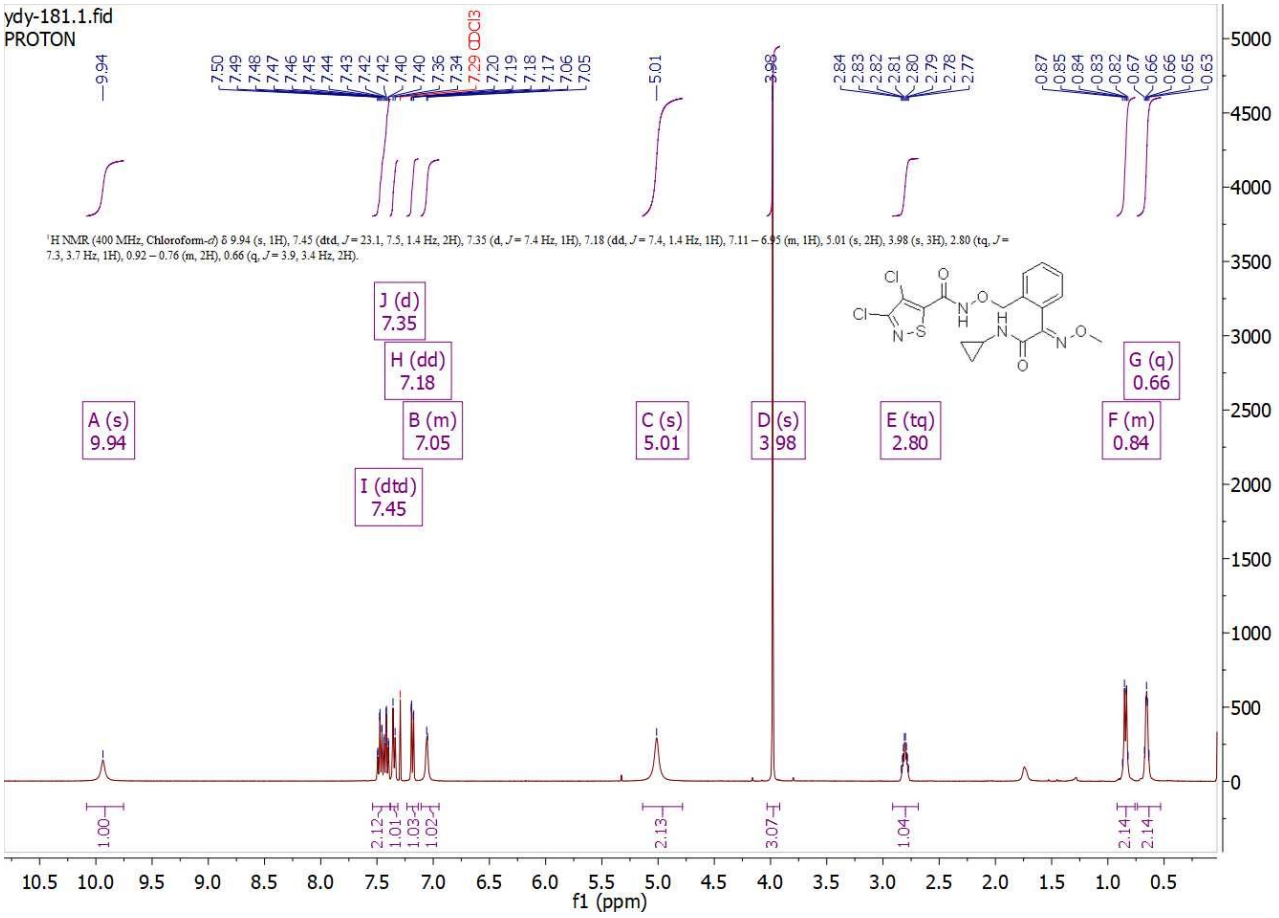


Figure S73. The $^{1}$H NMR (400 MHz, $CDCl_3$) of **7e**

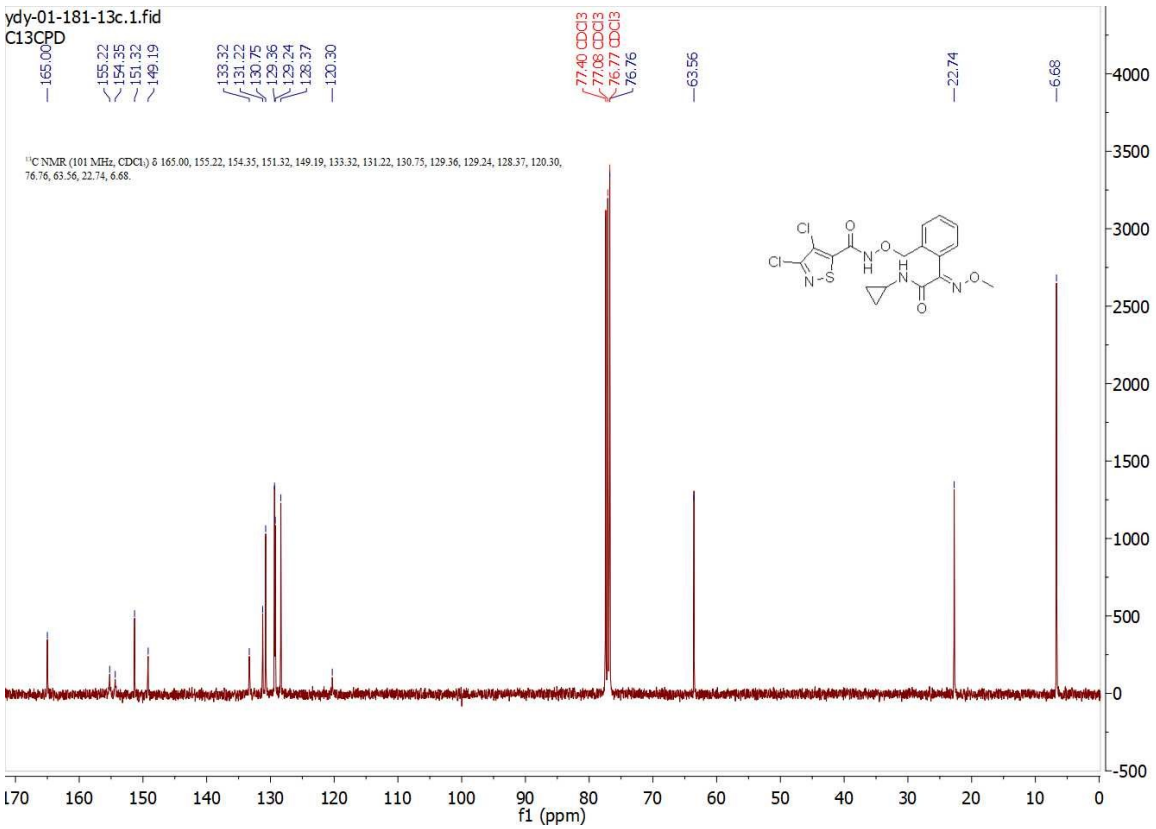


Figure S74. The $^{13}C$ NMR (400 MHz, $CDCl_3$) of **7e**

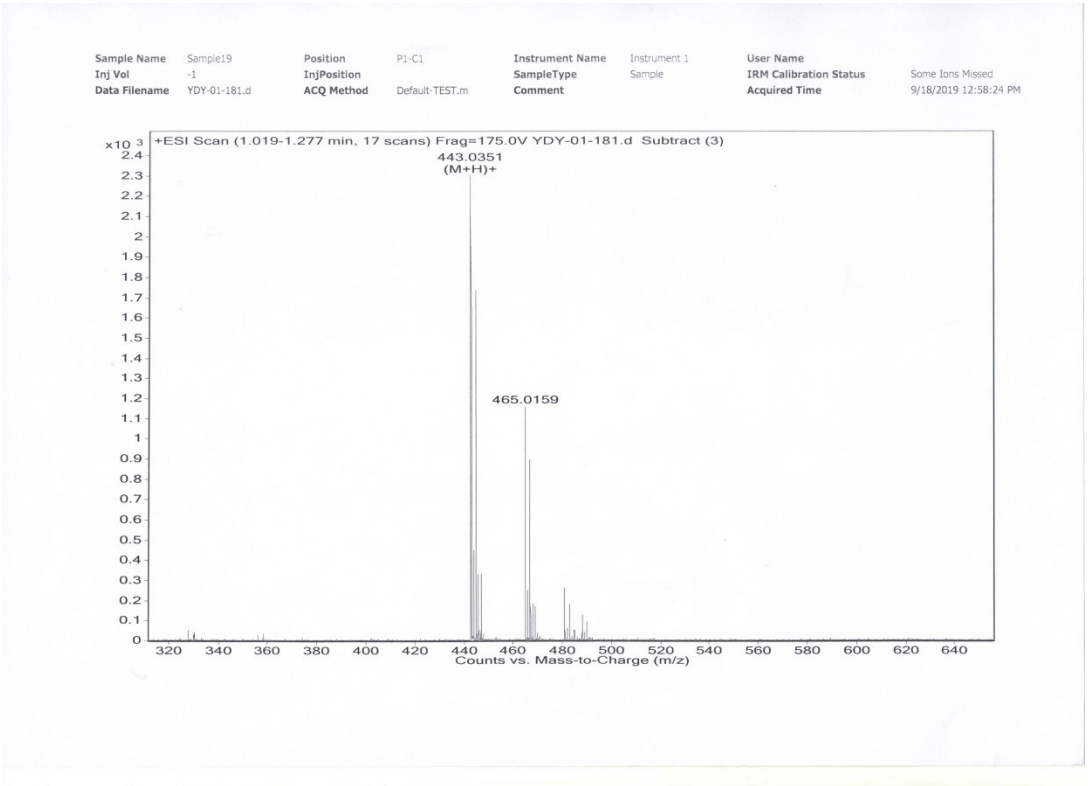


Figure S75. The HRMS spectra of **7e**

# Single crystal X-Ray data for compound 1e and 2e

Table S1. Crystal data and structure refinement for **1e**.

| ITEMS DATAS | |
|---|---|
| Identification code | **1e** |
| Empirical formula | $C_{19}H_{19}Cl_2N_3O_5S$ |
| Formula weight | 472.33 |
| Temperature/K | 113（2） |
| Wavelength | 0.71073 A |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a=8.6714(17)A alpha=85.84(3) deg. |
| | b=10.866(2)A beta =79.04(3)deg. |
| | c=11.901(2)A gamma=71.60(3) deg. |
| Volume | 1044.6(4)A^3 |
| Z, Calculated density | 2, 1.502 Mg/m^3 |
| Absorption coefficient | 0.448 mm^-1 |
| F(000) | 488 |
| Crystal size | 0.200 x 0.180 x 0.120 mm |
| Theta range for data collection | 1.743 to 25.019 deg. |
| Limiting indices | -10<=h<=10,-12<=k<=12,-14<=l<=14 |
| Reflections collected / unique | 9891 / 3664 [R(int) = 0.0656] |
| Completeness to theta = 25.019 | 99.5 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1 and 0.7273 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3664 / 0 / 273 |
| Goodness-of-fit on F^2 | 1.046 |
| Final R indices [I>2sigma(I)] | R1 = 0.0537, wR2 = 0.1332 |
| R indices (all data) | R1 = 0.0684, wR2 = 0.1399 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 1.068 and -0.460 e.A^-3 |

Table S2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1e**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| S(1) | 5316(1) | 1257(1) | 720(1) | 57(1) |
| Cl(1) | 4552(1) | 6133(1) | 6477(1) | 38(1) |
| Cl(2) | 1459(1) | 5700(1) | 5526(1) | 54(1) |
| O(1) | 6285(3) | 8145(2) | 5643(2) | 45(1) |
| O(2) | 6358(2) | 8610(2) | 2712(2) | 24(1) |
| O(3) | 2551(2) | 7273(2) | 1059(2) | 30(1) |
| O(4) | 3393(2) | 5232(2) | 1746(2) | 27(1) |
| O(5) | 8066(2) | 4979(2) | 728(2) | 24(1) |
| N(1) | 2240(3) | 7257(3) | 3888(2) | 35(1) |
| N(2) | 6954(3) | 8441(2) | 3752(2) | 29(1) |
| N(3) | 6415(3) | 5049(2) | 1083(2) | 20(1) |
| C(1) | 2598(4) | 6663(3) | 4831(3) | 32(1) |
| C(2) | 3955(3) | 6828(3) | 5241(2) | 27(1) |
| C(3) | 4643(3) | 7616(3) | 4499(2) | 24(1) |
| C(4) | 6015(3) | 8098(3) | 4686(3) | 29(1) |
| C(5) | 8170(4) | 9078(4) | 3849(3) | 47(1) |
| C(6) | 8069(5) | 10254(4) | 3179(3) | 50(1) |
| C(7) | 9123(5) | 10313(4) | 2045(3) | 60(1) |
| C(8) | 9482(4) | 10818(3) | 3076(3) | 40(1) |
| C(9) | 7337(3) | 7553(3) | 1928(2) | 24(1) |
| C(10) | 6826(3) | 7915(3) | 789(2) | 21(1) |
| C(11) | 7278(3) | 8919(3) | 159(2) | 25(1) |
| C(12) | 6879(3) | 9274(3) | -910(3) | 31(1) |
| C(13) | 6004(4) | 8640(3) | -1382(3) | 31(1) |
| C(14) | 5511(4) | 7653(3) | -762(2) | 26(1) |
| C(15) | 5924(3) | 7282(3) | 309(2) | 20(1) |
| C(16) | 5446(3) | 6165(3) | 892(2) | 21(1) |
| C(17) | 3618(3) | 6307(3) | 1231(2) | 22(1) |
| C(18) | 1685(3) | 5260(3) | 2138(3) | 34(1) |
| C(19) | 9078(3) | 3699(3) | 987(3) | 28(1) |

Table S3. Bond lengths [A] and angles [deg] for **1e**

| Bond | lengths [A] and angles [deg] | Bond | Lengths [A] and angles [deg] |
|---|---|---|---|
| S(1)-N(1) | 1.644(3) | O(1)-C(4)-N(2) | 121.8(3) |
| S(1)-C(3) | 1.707(3) | O(1)-C(4)-C(3) | 120.7(3) |
| Cl(1)-C(2) | 1.698(3) | N(2)-C(4)-C(3) | 117.5(3) |
| Cl(2)-C(1) | 1.723(3) | C(6)-C(5)-N(2) | 115.8(3) |
| O(1)-C(4) | 1.213(3) | C(6)-C(5)-H(5A) | 108.3 |
| O(2)-N(2) | 1.407(3) | N(2)-C(5)-H(5A) | 108.3 |
| O(2)-C(9) | 1.467(3) | C(6)-C(5)-H(5B) | 108.3 |
| O(3)-C(17) | 1.195(3) | N(2)-C(5)-H(5B) | 108.3 |
| O(4)-C(17) | 1.332(3) | H(5A)-C(5)-H(5B) | 107.4 |
| O(4)-C(18) | 1.457(3) | C(5)-C(6)-C(7) | 123.9(4) |
| O(5)-N(3) | 1.393(3) | C(5)-C(6)-C(8) | 117.8(3) |
| O(5)-C(19) | 1.438(3) | C(7)-C(6)-C(8) | 60.0(2) |
| N(1)-C(1) | 1.293(4) | C(5)-C(6)-H(6) | 114.7 |
| N(2)-C(4) | 1.351(4) | C(7)-C(6)-H(6) | 114.7 |
| N(2)-C(5) | 1.457(4) | C(8)-C(6)-H(6) | 114.7 |
| N(3)-C(16) | 1.272(3) | C(6)-C(7)-C(8) | 60.9(2) |
| C(1)-C(2) | 1.422(4) | C(6)-C(7)-H(7A) | 117.7 |
| C(2)-C(3) | 1.372(4) | C(8)-C(7)-H(7A) | 117.7 |
| C(3)-C(4) | 1.501(4) | C(6)-C(7)-H(7B) | 117.7 |
| C(5)-C(6) | 1.444(5) | C(8)-C(7)-H(7B) | 117.7 |
| C(5)-H(5A) | 0.9900 | H(7A)-C(7)-H(7B) | 114.8 |
| C(5)-H(5B) | 0.9900 | C(7)-C(8)-C(6) | 59.1(2) |
| C(6)-C(7) | 1.489(5) | C(7)-C(8)-H(8A) | 117.9 |
| C(6)-C(8) | 1.516(5) | C(6)-C(8)-H(8A) | 117.9 |
| C(6)-H(6) | 1.0000 | C(7)-C(8)-H(8B) | 117.9 |
| C(7)-C(8) | 1.502(5) | C(6)-C(8)-H(8B) | 117.9 |
| C(7)-H(7A) | 0.9900 | H(8A)-C(8)-H(8B) | 115.0 |
| C(7)-H(7B) | 0.9900 | O(2)-C(9)-C(10) | 107.3(2) |
| C(8)-H(8A) | 0.9900 | O(2)-C(9)-H(9A) | 110.3 |
| C(8)-H(8B) | 0.9900 | C(10)-C(9)-H(9A) | 110.3 |
| C(9)-C(10) | 1.492(4) | O(2)-C(9)-H(9B) | 110.3 |
| C(9)-H(9A) | 0.9900 | C(10)-C(9)-H(9B) | 110.3 |
| C(9)-H(9B) | 0.9900 | H(9A)-C(9)-H(9B) | 108.5 |
| C(10)-C(11) | 1.395(4) | C(11)-C(10)-C(15) | 118.0(3) |
| C(10)-C(15) | 1.407(4) | C(11)-C(10)-C(9) | 118.8(2) |

| | | | |
|---|---|---|---|
| C(11)-C(12) | 1.377(4) | C(15)-C(10)-C(9) | 123.2(2) |
| C(11)-H(11) | 0.9500 | C(12)-C(11)-C(10) | 121.4(3) |
| C(12)-C(13) | 1.384(4) | C(12)-C(11)-H(11) | 119.3 |
| C(12)-H(12) | 0.9500 | C(10)-C(11)-H(11) | 119.3 |
| C(13)-C(14) | 1.390(4) | C(11)-C(12)-C(13) | 120.4(3) |
| C(13)-H(13) | 0.9500 | C(11)-C(12)-H(12) | 119.8 |
| C(14)-C(15) | 1.386(4) | C(13)-C(12)-H(12) | 119.8 |
| C(14)-H(14) | 0.9500 | C(12)-C(13)-C(14) | 119.4(3) |
| C(15)-C(16) | 1.488(4) | C(12)-C(13)-H(13) | 120.3 |
| C(16)-C(17) | 1.520(4) | C(14)-C(13)-H(13) | 120.3 |
| C(18)-H(18A) | 0.9800 | C(15)-C(14)-C(13) | 120.5(3) |
| C(18)-H(18B) | 0.9800 | C(15)-C(14)-H(14) | 119.7 |
| C(18)-H(18C) | 0.9800 | C(13)-C(14)-H(14) | 119.7 |
| C(19)-H(19A) | 0.9800 | C(14)-C(15)-C(10) | 120.3(3) |
| C(19)-H(19B) | 0.9800 | C(14)-C(15)-C(16) | 117.6(3) |
| C(19)-H(19C) | 0.9800 | C(10)-C(15)-C(16) | 122.0(2) |
| N(1)-S(1)-C(3) | 95.46(14) | N(3)-C(16)-C(15) | 126.7(2) |
| N(2)-O(2)-C(9) | 110.59(19) | N(3)-C(16)-C(17) | 115.0(2) |
| C(17)-O(4)-C(18) | 116.1(2) | C(15)-C(16)-C(17) | 118.2(2) |
| N(3)-O(5)-C(19) | 108.53(18) | O(3)-C(17)-O(4) | 125.8(3) |
| C(1)-N(1)-S(1) | 109.2(2) | O(3)-C(17)-C(16) | 123.2(3) |
| C(4)-N(2)-O(2) | 117.6(2) | O(4)-C(17)-C(16) | 111.0(2) |
| C(4)-N(2)-C(5) | 121.6(3) | O(4)-C(18)-H(18A) | 109.5 |
| O(2)-N(2)-C(5) | 117.0(2) | O(4)-C(18)-H(18B) | 109.5 |
| C(16)-N(3)-O(5) | 111.9(2) | H(18A)-C(18)-H(18B) | 109.5 |
| N(1)-C(1)-C(2) | 117.4(3) | O(4)-C(18)-H(18C) | 109.5 |
| N(1)-C(1)-Cl(2) | 119.9(2) | H(18A)-C(18)-H(18C) | 109.5 |
| C(2)-C(1)-Cl(2) | 122.7(2) | H(18B)-C(18)-H(18C) | 109.5 |
| C(3)-C(2)-C(1) | 109.6(3) | O(5)-C(19)-H(19A) | 109.5 |
| C(3)-C(2)-Cl(1) | 127.6(2) | O(5)-C(19)-H(19B) | 109.5 |
| C(1)-C(2)-Cl(1) | 122.8(2) | H(19A)-C(19)-H(19B) | 109.5 |
| C(2)-C(3)-C(4) | 125.2(3) | O(5)-C(19)-H(19C) | 109.5 |
| C(2)-C(3)-S(1) | 108.4(2) | H(19A)-C(19)-H(19C) | 109.5 |
| C(4)-C(3)-S(1) | 126.2(2) | H(19B)-C(19)-H(19C) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **1e**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| S(1) | 28(1) | 43(1) | 25(1) | 4(1) | -8(1) | -15(1) |
| Cl(1) | 50(1) | 40(1) | 25(1) | 9(1) | -6(1) | -17(1) |
| Cl(2) | 57(1) | 73(1) | 44(1) | -7(1) | 10(1) | -49(1) |
| O(1) | 46(1) | 83(2) | 20(1) | 1(1) | -9(1) | -38(1) |
| O(2) | 27(1) | 28(1) | 18(1) | 3(1) | -5(1) | -10(1) |
| O(3) | 22(1) | 28(1) | 36(1) | 0(1) | -7(1) | -3(1) |
| O(4) | 18(1) | 29(1) | 35(1) | 4(1) | -1(1) | -10(1) |
| O(5) | 16(1) | 21(1) | 31(1) | 6(1) | 1(1) | -6(1) |
| N(1) | 26(1) | 54(2) | 32(2) | -4(1) | 0(1) | -22(1) |
| N(2) | 36(2) | 40(2) | 20(1) | 6(1) | -11(1) | -24(1) |
| N(3) | 13(1) | 23(1) | 22(1) | 1(1) | -1(1) | -4(1) |
| C(1) | 30(2) | 42(2) | 28(2) | -7(1) | 6(1) | -21(2) |
| C(2) | 27(2) | 30(2) | 21(2) | -3(1) | -2(1) | -7(1) |
| C(3) | 23(2) | 31(2) | 19(2) | -1(1) | -3(1) | -10(1) |
| C(4) | 27(2) | 37(2) | 23(2) | 0(1) | -3(1) | -12(2) |
| C(5) | 52(2) | 63(3) | 45(2) | 10(2) | -18(2) | -41(2) |
| C(6) | 50(2) | 52(2) | 61(3) | -6(2) | -10(2) | -32(2) |
| C(7) | 69(3) | 72(3) | 56(3) | -7(2) | 3(2) | -53(2) |
| C(8) | 35(2) | 32(2) | 60(2) | -7(2) | -2(2) | -21(2) |
| C(9) | 21(2) | 24(2) | 24(2) | -2(1) | 0(1) | -6(1) |
| C(10) | 16(1) | 19(2) | 24(2) | 0(1) | 2(1) | -3(1) |
| C(11) | 20(2) | 24(2) | 29(2) | 2(1) | 2(1) | -8(1) |
| C(12) | 29(2) | 28(2) | 30(2) | 7(1) | 6(1) | -8(2) |
| C(13) | 35(2) | 28(2) | 22(2) | 6(1) | -3(1) | -2(2) |
| C(14) | 29(2) | 24(2) | 22(2) | 0(1) | -4(1) | -2(1) |
| C(15) | 19(1) | 18(2) | 19(2) | 1(1) | 1(1) | -1(1) |
| C(16) | 21(2) | 23(2) | 20(2) | -1(1) | -2(1) | -8(1) |
| C(17) | 22(2) | 23(2) | 21(2) | -5(1) | -4(1) | -7(1) |
| C(18) | 21(2) | 46(2) | 38(2) | -3(2) | 2(1) | -20(2) |
| C(19) | 22(2) | 24(2) | 35(2) | 5(1) | -6(1) | -4(1) |

Table S5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1e**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(5A) | 8053 | 9283 | 4664 | 56 |
| H(5B) | 9285 | 8456 | 3619 | 56 |
| H(6) | 6947 | 10910 | 3282 | 60 |
| H(7A) | 8634 | 10955 | 1475 | 72 |
| H(7B) | 9902 | 9488 | 1718 | 72 |
| H(8A) | 9206 | 11768 | 3144 | 49 |
| H(8B) | 10475 | 10299 | 3387 | 49 |
| H(9A) | 7129 | 6731 | 2212 | 28 |
| H(9B) | 8529 | 7436 | 1865 | 28 |
| H(11) | 7874 | 9367 | 473 | 30 |
| H(12) | 7206 | 9958 | -1324 | 38 |
| H(13) | 5742 | 8878 | -2123 | 37 |
| H(14) | 4887 | 7229 | -1075 | 31 |
| H(18A) | 1134 | 5964 | 2686 | 51 |
| H(18B) | 1660 | 4431 | 2511 | 51 |
| H(18C) | 1113 | 5406 | 1483 | 51 |
| H(19A) | 8989 | 3583 | 1819 | 42 |
| H(19B) | 10231 | 3591 | 639 | 42 |
| H(19C) | 8703 | 3052 | 681 | 42 |

Table S6. Torsion angles [deg] for **1e**.

| | Torsion angles [deg] | | Torsion angles [deg] |
|---|---|---|---|
| C(3)-S(1)-N(1)-C(1) | -1.3(3) | C(5)-C(6)-C(7)-C(8) | -105.0(4) |
| C(9)-O(2)-N(2)-C(4) | -108.7(3) | C(5)-C(6)-C(8)-C(7) | 115.1(4) |
| C(9)-O(2)-N(2)-C(5) | 92.9(3) | N(2)-O(2)-C(9)-C(10) | -170.5(2) |
| C(19)-O(5)-N(3)-C(16) | 179.2(2) | O(2)-C(9)-C(10)-C(11) | 70.8(3) |
| S(1)-N(1)-C(1)-C(2) | 1.4(4) | O(2)-C(9)-C(10)-C(15) | -110.0(3) |
| S(1)-N(1)-C(1)-Cl(2) | -177.79(17) | C(15)-C(10)-C(11)-C(12) | -0.9(4) |
| N(1)-C(1)-C(2)-C(3) | -0.7(4) | C(9)-C(10)-C(11)-C(12) | 178.3(3) |
| Cl(2)-C(1)-C(2)-C(3) | 178.5(2) | C(10)-C(11)-C(12)-C(13) | 0.3(4) |
| N(1)-C(1)-C(2)-Cl(1) | 178.9(2) | C(11)-C(12)-C(13)-C(14) | 0.9(4) |
| Cl(2)-C(1)-C(2)-Cl(1) | -2.0(4) | C(12)-C(13)-C(14)-C(15) | -1.5(4) |
| C(1)-C(2)-C(3)-C(4) | 175.0(3) | C(13)-C(14)-C(15)-C(10) | 1.0(4) |
| Cl(1)-C(2)-C(3)-C(4) | -4.5(5) | C(13)-C(14)-C(15)-C(16) | -176.3(3) |
| C(1)-C(2)-C(3)-S(1) | -0.3(3) | C(11)-C(10)-C(15)-C(14) | 0.2(4) |
| Cl(1)-C(2)-C(3)-S(1) | -179.85(18) | C(9)-C(10)-C(15)-C(14) | -178.9(2) |
| N(1)-S(1)-C(3)-C(2) | 0.9(2) | C(11)-C(10)-C(15)-C(16) | 177.4(2) |
| N(1)-S(1)-C(3)-C(4) | -174.3(3) | C(9)-C(10)-C(15)-C(16) | -1.8(4) |
| O(2)-N(2)-C(4)-O(1) | -167.3(3) | O(5)-N(3)-C(16)-C(15) | 3.0(4) |
| C(5)-N(2)-C(4)-O(1) | -9.9(5) | O(5)-N(3)-C(16)-C(17) | 178.6(2) |
| O(2)-N(2)-C(4)-C(3) | 14.4(4) | C(14)-C(15)-C(16)-N(3) | 111.0(3) |
| C(5)-N(2)-C(4)-C(3) | 171.8(3) | C(10)-C(15)-C(16)-N(3) | -66.2(4) |
| C(2)-C(3)-C(4)-O(1) | -22.2(5) | C(14)-C(15)-C(16)-C(17) | -64.5(3) |
| S(1)-C(3)-C(4)-O(1) | 152.3(3) | C(10)-C(15)-C(16)-C(17) | 118.4(3) |
| C(2)-C(3)-C(4)-N(2) | 156.1(3) | C(18)-O(4)-C(17)-O(3) | -0.7(4) |
| S(1)-C(3)-C(4)-N(2) | -29.5(4) | C(18)-O(4)-C(17)-C(16) | 178.5(2) |
| C(4)-N(2)-C(5)-C(6) | -128.7(3) | N(3)-C(16)-C(17)-O(3) | -176.5(3) |
| O(2)-N(2)-C(5)-C(6) | 28.8(4) | C(15)-C(16)-C(17)-O(3) | -0.5(4) |
| N(2)-C(5)-C(6)-C(7) | -98.1(4) | N(3)-C(16)-C(17)-O(4) | 4.3(3) |
| N(2)-C(5)-C(6)-C(8) | -169.0(3) | C(15)-C(16)-C(17)-O(4) | -179.8(2) |

Symmetry transformations used to generate equivalent atoms:

Table S7. Crystal data and structure refinement for **2e**

| ITEMS | DATAS |
|---|---|
| Identification code | **2e** |
| Empirical formula | $C_{19}H_{19}Cl_2N_3O_5S$ |
| Formula weight | 472.33 |
| Temperature/K | 113（2） |
| Wavelength | 0.71073 A |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a=7.9695(16)A alpha= 83.69(3) deg.<br>b = 8.2413(16)A beta= 88.28(3) deg<br>c=16.800(3)A gamma= 77.67(3) deg |
| Volume | 1071.4(4) A^3 |
| Z, Calculated density | 2, 1.464 Mg/m^3 |
| Absorption coefficient | 0.437 mm^-1 |
| F(000) | 488 |
| Crystal size | 0.200 x 0.180 x 0.120 mm |
| Theta range for data collection | 2.440 to 27.855deg. |
| Limiting indices | -10<=h<=10,-10<=k<=10,-20<=l<=20 |
| Reflections collected / unique | 11105 /5030[R(int) = 0.0386] |
| Completeness to theta = 25.242 | 99.4 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1 and 0.8259 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 5030 / 0 / 273 |
| Goodness-of-fit on F^2 | 1.040 |
| Final R indices [I>2sigma(I)] | R1 = 0.0553, wR2 = 0.1497 |
| R indices (all data) | R1 = 0.0765, wR2 = 0.1676 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.978 and -0.586 e.A^-3 |

Table S8. Atomic coordinates ( x 10^4) and equivalent isotropic

displacement parameters (A^2 x 10^3) for **2e**.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| S(1) | 5316(1) | 1257(1) | 720(1) | 57(1) |
| Cl(1) | 9386(1) | 2089(1) | -653(1) | 63(1) |
| Cl(2) | 7870(1) | 5223(1) | 410(1) | 40(1) |
| O(1) | 3560(2) | 3095(2) | 1897(1) | 45(1) |
| O(2) | 3631(2) | 6214(2) | 2198(1) | 39(1) |
| O(3) | 5723(2) | 2976(2) | 3637(1) | 38(1) |
| O(4) | 3013(2) | 3462(2) | 4106(1) | 44(1) |
| O(5) | 3485(2) | 8237(2) | 4292(1) | 38(1) |
| N(1) | 6892(4) | 881(3) | 60(2) | 64(1) |
| N(2) | 4701(2) | 5543(3) | 1585(1) | 37(1) |
| N(3) | 3290(2) | 6590(2) | 4281(1) | 33(1) |
| C(1) | 7668(4) | 2147(3) | -19(2) | 48(1) |
| C(2) | 7022(3) | 3487(3) | 443(1) | 37(1) |
| C(3) | 5663(3) | 3156(3) | 908(2) | 36(1) |
| C(4) | 4563(3) | 4056(3) | 1495(2) | 37(1) |
| C(5) | 1710(3) | 3791(4) | 1962(2) | 54(1) |
| C(6) | 813(4) | 2339(4) | 2000(2) | 62(1) |
| C(7) | -918(3) | 2581(3) | 2349(2) | 44(1) |
| C(8) | 563(4) | 1509(4) | 2791(2) | 69(1) |
| C(9) | 4213(3) | 7682(3) | 2375(2) | 40(1) |
| C(10) | 5909(3) | 7230(3) | 2798(1) | 31(1) |
| C(11) | 7356(3) | 7703(3) | 2454(2) | 38(1) |
| C(12) | 8931(3) | 7272(3) | 2842(2) | 42(1) |
| C(13) | 9061(3) | 6369(3) | 3584(2) | 42(1) |
| C(14) | 7635(3) | 5854(3) | 3943(2) | 36(1) |
| C(15) | 6063(3) | 6281(3) | 3552(1) | 30(1) |
| C(16) | 4533(3) | 5700(3) | 3926(1) | 28(1) |
| C(17) | 4305(3) | 3943(3) | 3905(1) | 32(1) |
| C(18) | 5611(4) | 1259(3) | 3581(2) | 46(1) |
| C(19) | 1985(3) | 9139(3) | 4665(2) | 47(1) |

Table S9. Bond lengths [A] and angles [deg] for **2e**.

| Bond | Bond lengths [A] and angles [deg] | Bond | Bond lengths [A] and angles [deg] |
|---|---|---|---|
| S(1)-N(1) | 1.651(3) | N(2)-C(4)-C(3) | 118.7(2) |
| S(1)-C(3) | 1.710(3) | O(1)-C(4)-C(3) | 111.6(2) |
| Cl(1)-C(1) | 1.705(3) | O(1)-C(5)-C(6) | 106.9(2) |
| Cl(2)-C(2) | 1.703(2) | O(1)-C(5)-H(5A) | 110.3 |
| O(1)-C(4) | 1.357(3) | C(6)-C(5)-H(5A) | 110.3 |
| O(1)-C(5) | 1.468(3) | O(1)-C(5)-H(5B) | 110.3 |
| O(2)-N(2) | 1.402(3) | C(6)-C(5)-H(5B) | 110.3 |
| O(2)-C(9) | 1.447(3) | H(5A)-C(5)-H(5B) | 108.6 |
| O(3)-C(17) | 1.333(3) | C(8)-C(6)-C(7) | 60.9(2) |
| O(3)-C(18) | 1.451(3) | C(8)-C(6)-C(5) | 116.8(3) |
| O(4)-C(17) | 1.206(3) | C(7)-C(6)-C(5) | 117.3(3) |
| O(5)-N(3) | 1.401(2) | C(8)-C(6)-H(6) | 116.7 |
| O(5)-C(19) | 1.432(3) | C(7)-C(6)-H(6) | 116.7 |
| N(1)-C(1) | 1.315(4) | C(5)-C(6)-H(6) | 116.7 |
| N(2)-C(4) | 1.279(3) | C(6)-C(7)-C(8) | 59.2(2) |
| N(3)-C(16) | 1.275(3) | C(6)-C(7)-H(7A) | 117.9 |
| C(1)-C(2) | 1.417(4) | C(8)-C(7)-H(7A) | 117.9 |
| C(2)-C(3) | 1.374(4) | C(6)-C(7)-H(7B) | 117.9 |
| C(3)-C(4) | 1.457(4) | C(8)-C(7)-H(7B) | 117.9 |
| C(5)-C(6) | 1.514(4) | H(7A)-C(7)-H(7B) | 115.0 |
| C(5)-H(5A) | 0.9900 | C(6)-C(8)-C(7) | 59.9(2) |
| C(5)-H(5B) | 0.9900 | C(6)-C(8)-H(8A) | 117.8 |
| C(6)-C(8) | 1.455(5) | C(7)-C(8)-H(8A) | 117.8 |
| C(6)-C(7) | 1.465(4) | C(6)-C(8)-H(8B) | 117.8 |
| C(6)-H(6) | 1.0000 | C(7)-C(8)-H(8B) | 117.8 |
| C(7)-C(8) | 1.479(4) | H(8A)-C(8)-H(8B) | 114.9 |
| C(7)-H(7A) | 0.9900 | O(2)-C(9)-C(10) | 111.71(19) |
| C(7)-H(7B) | 0.9900 | O(2)-C(9)-H(9A) | 109.3 |
| C(8)-H(8A) | 0.9900 | C(10)-C(9)-H(9A) | 109.3 |
| C(8)-H(8B) | 0.9900 | O(2)-C(9)-H(9B) | 109.3 |
| C(9)-C(10) | 1.502(3) | C(10)-C(9)-H(9B) | 109.3 |
| C(9)-H(9A) | 0.9900 | H(9A)-C(9)-H(9B) | 107.9 |
| C(9)-H(9B) | 0.9900 | C(11)-C(10)-C(15) | 118.5(2) |
| C(10)-C(11) | 1.386(3) | C(11)-C(10)-C(9) | 121.2(2) |
| C(10)-C(15) | 1.407(3) | C(15)-C(10)-C(9) | 120.2(2) |
| C(11)-C(12) | 1.391(4) | C(10)-C(11)-C(12) | 121.3(2) |
| C(11)-H(11) | 0.9500 | C(10)-C(11)-H(11) | 119.4 |
| C(12)-C(13) | 1.374(4) | C(12)-C(11)-H(11) | 119.4 |
| C(12)-H(12) | 0.9500 | C(13)-C(12)-C(11) | 119.7(2) |
| C(13)-C(14) | 1.394(3) | C(13)-C(12)-H(12) | 120.1 |
| C(13)-H(13) | 0.9500 | C(11)-C(12)-H(12) | 120.1 |
| C(14)-C(15) | 1.391(3) | C(12)-C(13)-C(14) | 120.5(2) |
| C(14)-H(14) | 0.9500 | C(12)-C(13)-H(13) | 119.7 |
| C(15)-C(16) | 1.499(3) | C(14)-C(13)-H(13) | 119.7 |
| C(16)-C(17) | 1.502(3) | C(15)-C(14)-C(13) | 119.7(2) |
| C(18)-H(18A) | 0.9800 | C(15)-C(14)-H(14) | 120.2 |
| C(18)-H(18B) | 0.9800 | C(13)-C(14)-H(14) | 120.2 |

| | | | |
|---|---|---|---|
| C(18)-H(18C) | 0.9800 | C(14)-C(15)-C(10) | 120.3(2) |
| C(19)-H(19A) | 0.9800 | C(14)-C(15)-C(16) | 120.0(2) |
| C(19)-H(19B) | 0.9800 | C(10)-C(15)-C(16) | 119.7(2) |
| C(19)-H(19C) | 0.9800 | N(3)-C(16)-C(15) | 125.9(2) |
| N(1)-S(1)-C(3) | 95.82(13) | N(3)-C(16)-C(17) | 112.25(19) |
| C(4)-O(1)-C(5) | 118.46(19) | C(15)-C(16)-C(17) | 121.82(18) |
| N(2)-O(2)-C(9) | 106.49(17) | O(4)-C(17)-O(3) | 124.2(2) |
| C(17)-O(3)-C(18) | 115.06(18) | O(4)-C(17)-C(16) | 124.6(2) |
| N(3)-O(5)-C(19) | 107.70(18) | O(3)-C(17)-C(16) | 111.14(18) |
| C(1)-N(1)-S(1) | 108.6(2) | O(3)-C(18)-H(18A) | 109.5 |
| C(4)-N(2)-O(2) | 112.1(2) | O(3)-C(18)-H(18B) | 109.5 |
| C(16)-N(3)-O(5) | 112.44(18) | H(18A)-C(18)-H(18B) | 109.5 |
| N(1)-C(1)-C(2) | 117.2(3) | O(3)-C(18)-H(18C) | 109.5 |
| N(1)-C(1)-Cl(1) | 119.1(2) | H(18A)-C(18)-H(18C) | 109.5 |
| C(2)-C(1)-Cl(1) | 123.7(2) | H(18B)-C(18)-H(18C) | 109.5 |
| C(3)-C(2)-C(1) | 110.2(2) | O(5)-C(19)-H(19A) | 109.5 |
| C(3)-C(2)-Cl(2) | 126.6(2) | O(5)-C(19)-H(19B) | 109.5 |
| C(1)-C(2)-Cl(2) | 123.3(2) | H(19A)-C(19)-H(19B) | 109.5 |
| C(2)-C(3)-C(4) | 133.5(2) | O(5)-C(19)-H(19C) | 109.5 |
| C(2)-C(3)-S(1) | 108.3(2) | H(19A)-C(19)-H(19C) | 109.5 |
| C(4)-C(3)-S(1) | 118.22(19) | H(19B)-C(19)-H(19C) | 109.5 |
| N(2)-C(4)-O(1) | 129.7(3) | | |

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for **2e**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| S(1) | 72(1) | 39(1) | 66(1) | 3(1) | -5(1) | -27(1) |
| Cl(1) | 78(1) | 48(1) | 57(1) | -7(1) | 16(1) | 0(1) |
| Cl(2) | 38(1) | 42(1) | 44(1) | -5(1) | 4(1) | -16(1) |
| O(1) | 28(1) | 45(1) | 58(1) | 14(1) | 0(1) | -11(1) |
| O(2) | 31(1) | 47(1) | 42(1) | -2(1) | 5(1) | -14(1) |
| O(3) | 36(1) | 27(1) | 51(1) | -8(1) | 9(1) | -8(1) |
| O(4) | 37(1) | 41(1) | 58(1) | -7(1) | 10(1) | -19(1) |
| O(5) | 31(1) | 31(1) | 52(1) | -13(1) | 13(1) | -6(1) |
| N(1) | 88(2) | 40(1) | 65(2) | -8(1) | 3(2) | -20(1) |
| N(2) | 31(1) | 46(1) | 34(1) | 2(1) | 0(1) | -13(1) |
| N(3) | 28(1) | 30(1) | 41(1) | -4(1) | 4(1) | -9(1) |
| C(1) | 60(2) | 37(1) | 44(2) | 0(1) | -4(1) | -8(1) |
| C(2) | 40(1) | 34(1) | 36(1) | 2(1) | -8(1) | -10(1) |
| C(3) | 34(1) | 36(1) | 39(1) | 6(1) | -10(1) | -11(1) |
| C(4) | 29(1) | 44(1) | 38(1) | 8(1) | -7(1) | -14(1) |
| C(5) | 30(1) | 48(2) | 80(2) | 12(1) | 6(1) | -11(1) |
| C(6) | 40(2) | 59(2) | 89(2) | -4(2) | 15(2) | -15(1) |
| C(7) | 34(1) | 48(2) | 51(2) | 6(1) | -5(1) | -16(1) |
| C(8) | 57(2) | 61(2) | 87(3) | 15(2) | -13(2) | -22(2) |
| C(9) | 33(1) | 32(1) | 50(2) | 3(1) | 4(1) | -4(1) |
| C(10) | 29(1) | 21(1) | 44(1) | -5(1) | 6(1) | -5(1) |
| C(11) | 36(1) | 28(1) | 51(2) | -5(1) | 13(1) | -10(1) |
| C(12) | 33(1) | 37(1) | 62(2) | -13(1) | 15(1) | -18(1) |
| C(13) | 27(1) | 47(2) | 54(2) | -16(1) | 4(1) | -14(1) |
| C(14) | 29(1) | 41(1) | 39(1) | -9(1) | 2(1) | -9(1) |
| C(15) | 24(1) | 28(1) | 39(1) | -9(1) | 8(1) | -8(1) |
| C(16) | 23(1) | 29(1) | 33(1) | -4(1) | 1(1) | -6(1) |
| C(17) | 30(1) | 31(1) | 35(1) | -5(1) | 3(1) | -10(1) |
| C(18) | 51(2) | 28(1) | 62(2) | -6(1) | 6(1) | -12(1) |
| C(19) | 35(1) | 45(2) | 58(2) | -16(1) | 12(1) | 2(1) |

Table S11. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2e**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(5A) | 1315 | 4602 | 1491 | 65 |
| H(5B) | 1459 | 4371 | 2451 | 65 |
| H(6) | 1050 | 1619 | 1550 | 75 |
| H(7A) | -1754 | 2028 | 2123 | 53 |
| H(7B) | -1417 | 3678 | 2539 | 53 |
| H(8A) | 987 | 1935 | 3258 | 82 |
| H(8B) | 650 | 285 | 2842 | 82 |
| H(9A) | 3346 | 8337 | 2715 | 48 |
| H(9B) | 4325 | 8392 | 1869 | 48 |
| H(11) | 7272 | 8334 | 1943 | 46 |
| H(12) | 9912 | 7600 | 2596 | 51 |
| H(13) | 10130 | 6094 | 3854 | 50 |
| H(14) | 7737 | 5215 | 4452 | 43 |
| H(18A) | 5321 | 750 | 4108 | 70 |
| H(18B) | 6718 | 633 | 3401 | 70 |
| H(18C) | 4718 | 1233 | 3197 | 70 |
| H(19A) | 975 | 9174 | 4340 | 70 |
| H(19B) | 2118 | 10280 | 4710 | 70 |
| H(19C) | 1837 | 8580 | 5200 | 70 |

Table S12. Torsion angles [deg] for **2e**.

| | Torsion angles [deg] | | Torsion angles [deg] |
|---|---|---|---|
| C(3)-S(1)-N(1)-C(1) | 0.1(2) | C(5)-C(6)-C(8)-C(7) | 107.8(3) |
| C(9)-O(2)-N(2)-C(4) | 165.76(19) | N(2)-O(2)-C(9)-C(10) | -71.5(2) |
| C(19)-O(5)-N(3)-C(16) | 177.0(2) | O(2)-C(9)-C(10)-C(11) | 117.1(2) |
| S(1)-N(1)-C(1)-C(2) | -0.5(3) | O(2)-C(9)-C(10)-C(15) | -61.7(3) |
| S(1)-N(1)-C(1)-Cl(1) | 178.82(15) | C(15)-C(10)-C(11)-C(12) | -0.6(3) |
| N(1)-C(1)-C(2)-C(3) | 0.8(3) | C(9)-C(10)-C(11)-C(12) | -179.4(2) |
| Cl(1)-C(1)-C(2)-C(3) | -178.49(19) | C(10)-C(11)-C(12)-C(13) | -0.4(4) |
| N(1)-C(1)-C(2)-Cl(2) | -179.8(2) | C(11)-C(12)-C(13)-C(14) | 1.3(4) |
| Cl(1)-C(1)-C(2)-Cl(2) | 0.9(3) | C(12)-C(13)-C(14)-C(15) | -1.0(4) |
| C(1)-C(2)-C(3)-C(4) | 178.6(2) | C(13)-C(14)-C(15)-C(10) | -0.1(3) |
| Cl(2)-C(2)-C(3)-C(4) | -0.8(4) | C(13)-C(14)-C(15)-C(16) | 178.7(2) |
| C(1)-C(2)-C(3)-S(1) | -0.7(3) | C(11)-C(10)-C(15)-C(14) | 0.9(3) |
| Cl(2)-C(2)-C(3)-S(1) | 179.94(14) | C(9)-C(10)-C(15)-C(14) | 179.7(2) |
| N(1)-S(1)-C(3)-C(2) | 0.4(2) | C(11)-C(10)-C(15)-C(16) | -177.89(19) |
| N(1)-S(1)-C(3)-C(4) | -179.00(19) | C(9)-C(10)-C(15)-C(16) | 0.9(3) |
| O(2)-N(2)-C(4)-O(1) | 0.2(3) | O(5)-N(3)-C(16)-C(15) | 0.0(3) |
| O(2)-N(2)-C(4)-C(3) | -176.79(19) | O(5)-N(3)-C(16)-C(17) | -179.15(17) |
| C(5)-O(1)-C(4)-N(2) | 52.5(4) | C(14)-C(15)-C(16)-N(3) | 103.2(3) |
| C(5)-O(1)-C(4)-C(3) | -130.4(3) | C(10)-C(15)-C(16)-N(3) | -78.0(3) |
| C(2)-C(3)-C(4)-N(2) | 7.5(4) | C(14)-C(15)-C(16)-C(17) | -77.7(3) |
| S(1)-C(3)-C(4)-N(2) | -173.36(17) | C(10)-C(15)-C(16)-C(17) | 101.1(2) |
| C(2)-C(3)-C(4)-O(1) | -170.0(2) | C(18)-O(3)-C(17)-O(4) | 1.3(3) |
| S(1)-C(3)-C(4)-O(1) | 9.2(3) | C(18)-O(3)-C(17)-C(16) | -178.83(19) |
| C(4)-O(1)-C(5)-C(6) | 149.7(3) | N(3)-C(16)-C(17)-O(4) | 8.8(3) |
| O(1)-C(5)-C(6)-C(8) | 89.1(3) | C(15)-C(16)-C(17)-O(4) | -170.4(2) |
| O(1)-C(5)-C(6)-C(7) | 158.4(3) | N(3)-C(16)-C(17)-O(3) | -170.99(19) |
| C(5)-C(6)-C(7)-C(8) | -107.0(4) | C(15)-C(16)-C(17)-O(3) | 9.8(3) |

Symmetry transformations used to generate equivalent atoms: