

Supplementary Material

Manuscript Title: “A novel scaffold for EGFR inhibition: Introducing N-(3-(3-phenylureido)quinoxalin-6-yl) acrylamide derivatives.”

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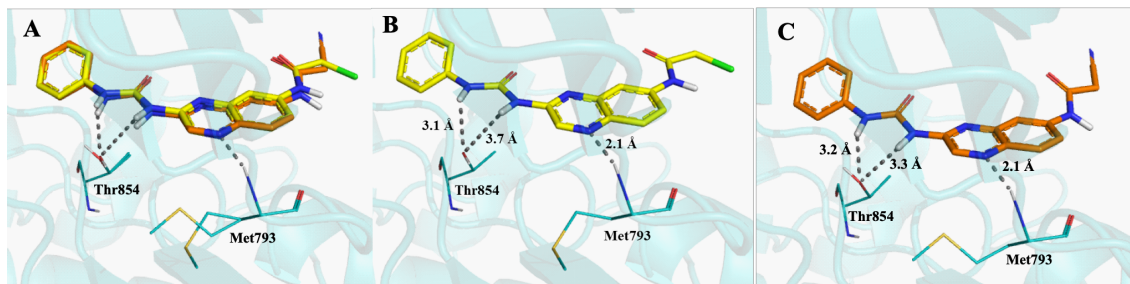


Figure S1: Simple docking best poses for compounds **7j** and **7k**, with electrophilic carbon of the α -carbon of carbonyl subunit, in the ATP binding site of EGFRwt. (A) Superposition of **7j** and **7k**; (B) Interaction profile of compound **7j** (carbon atoms in yellow); (C) Interaction profile of compound **7i** (carbon atoms in orange). Dashed gray lines: Hydrogen bonds.

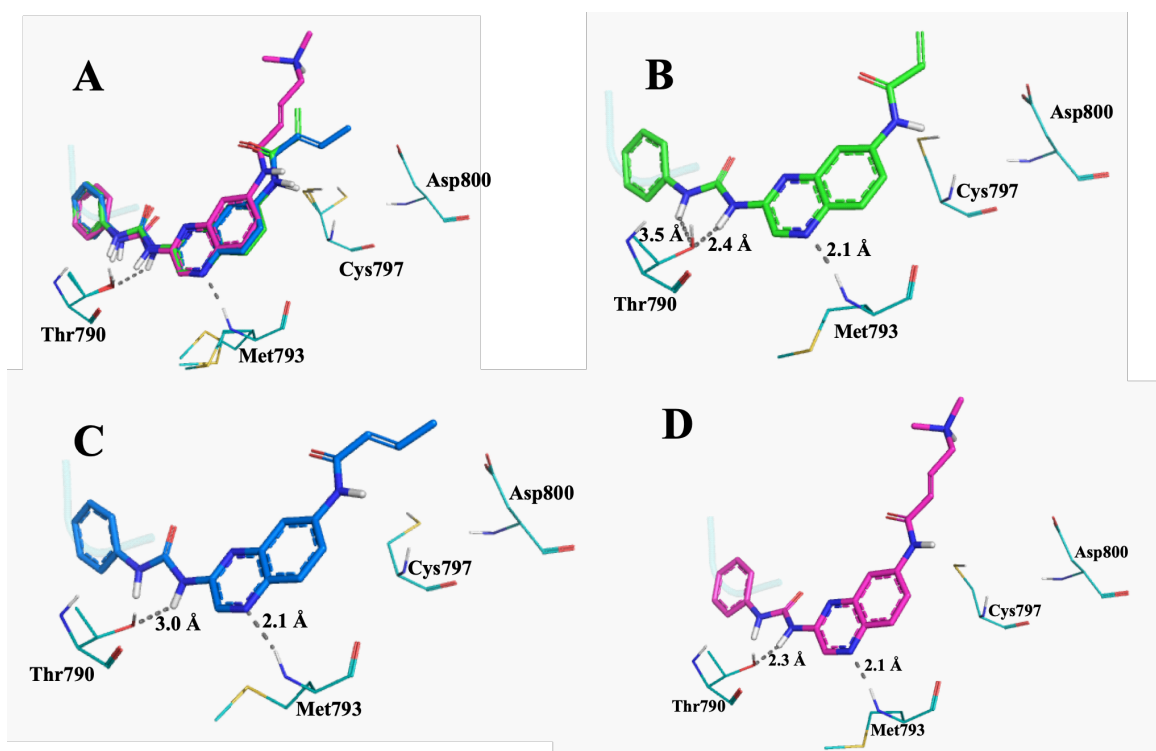


Figure S2: Simple docking best poses for compounds **7h**, **7i** and **7l**, with electrophilic carbon of the enone subunit, in the ATP binding site of EGFRwt. (A) Superposition of **7h**, **7i** and **7l**; (B) Interaction profile of compound **7h** (carbon atoms in green); (C) Interaction profile of compound **7i** (carbon atoms in blue); (D) Interaction profile of compound **7l** (carbon atoms in magenta). Dashed gray lines: Hydrogen bonds.

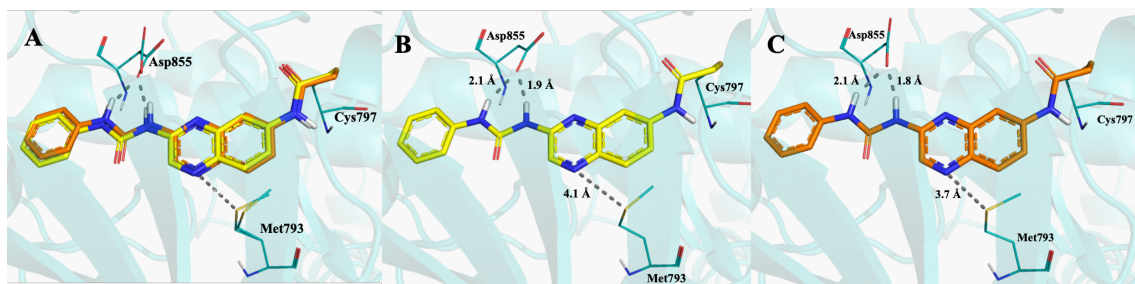


Figure S3: Covalent docking best poses for compounds **7j** and **7k**, with electrophilic carbon of the α -carbon of carbonyl subunit, in the ATP binding site of EGFR_{wt}. (A) Superposition of **7j** and **7k**; (B) Interaction profile of compound **7j** (carbon atoms in yellow); (C) Interaction profile of compound **7k** (carbon atoms in orange). Dashed gray lines: Hydrogen bonds.

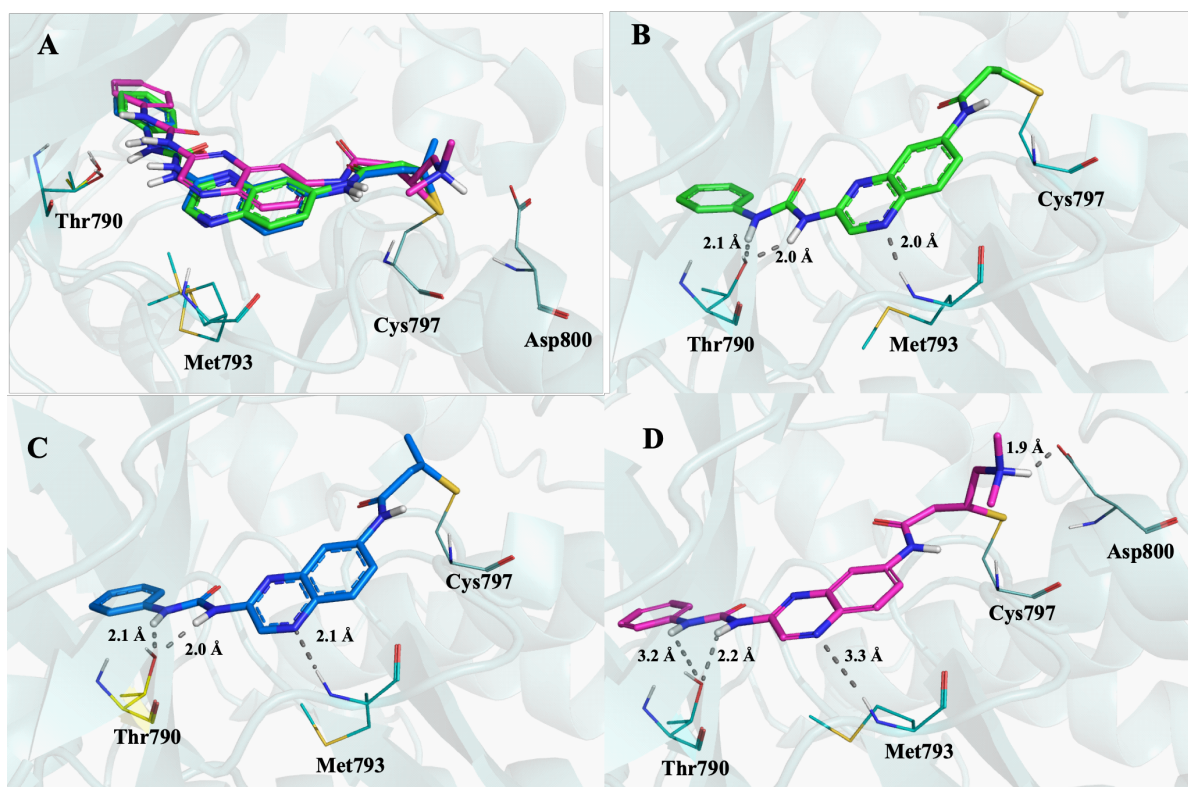


Figure S4: Covalent docking best poses for compounds **7h**, **7i** and **7l**, with electrophilic carbon of the enone subunit, in the ATP binding site of EGFR_{wt}. (A) Superposition of **7h**, **7i** and **7l**; (B) Interaction profile of compound **7h** (carbon atoms in green); (C) Interaction profile of compound **7i** (carbon atoms in blue); (D) Interaction profile of compound **7l** (carbon atoms in magenta). Dashed gray lines: Hydrogen bonds.

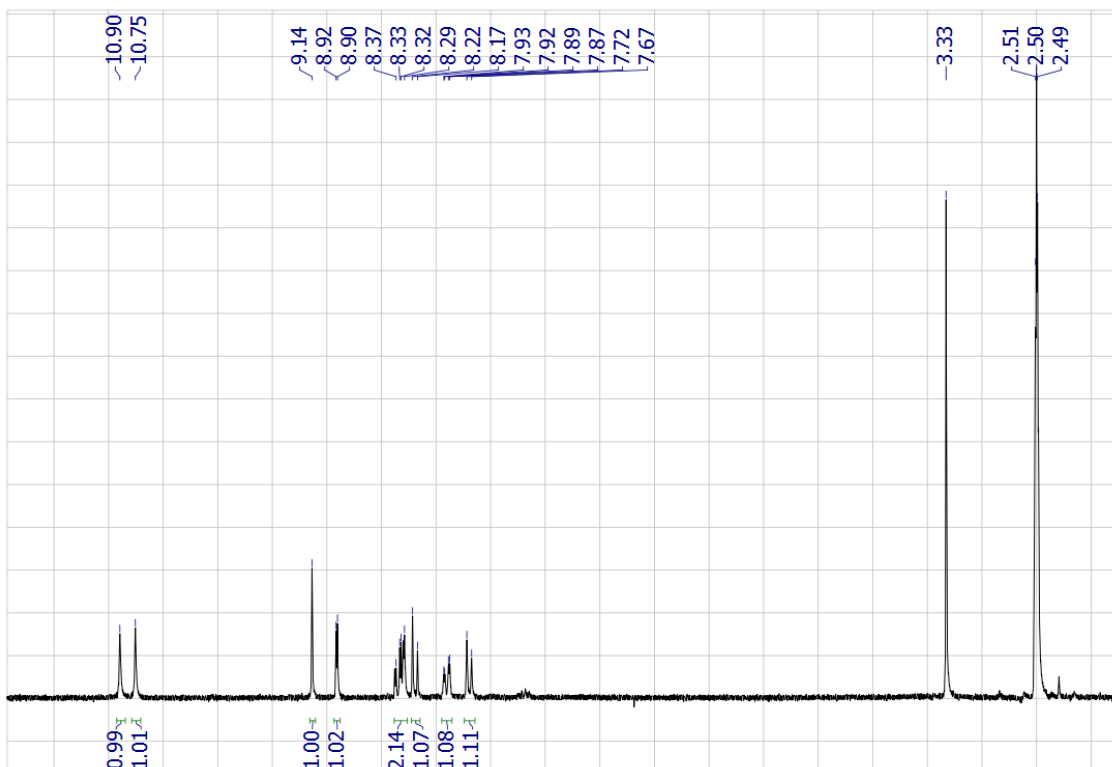


Figure S5. ^1H NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**9a**) (DMSO- d_6 /200MHz/TMS).

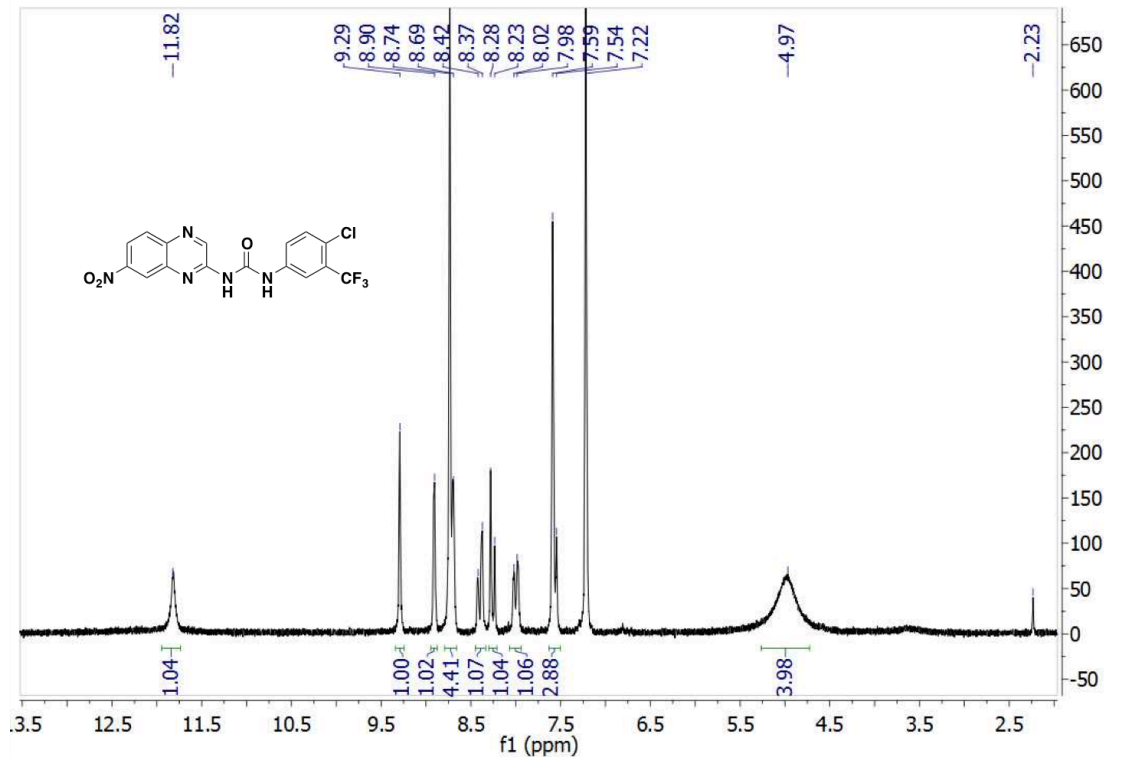


Figure S6. ^1H NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**9a**) (pyridine- d_5 /200MHz/TMS)

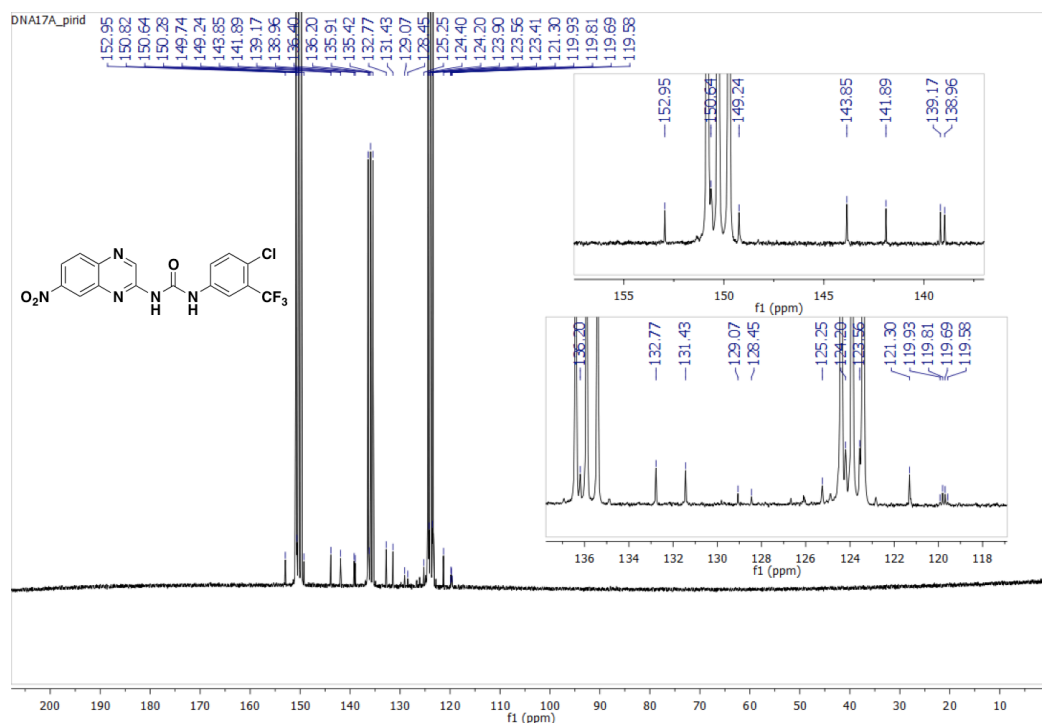


Figure S7. ¹³C NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**9a**) (pyridine-d₅/200MHz/TMS)

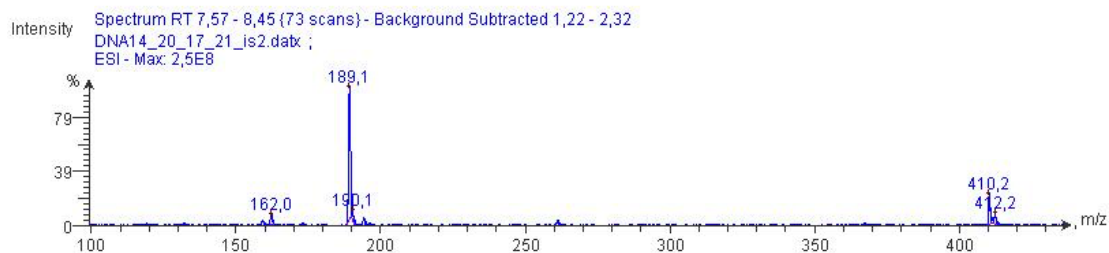


Figure S8. Mass spectrometry of compound 1-(7-nitroquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**9a**) in negative mode (ESI-).

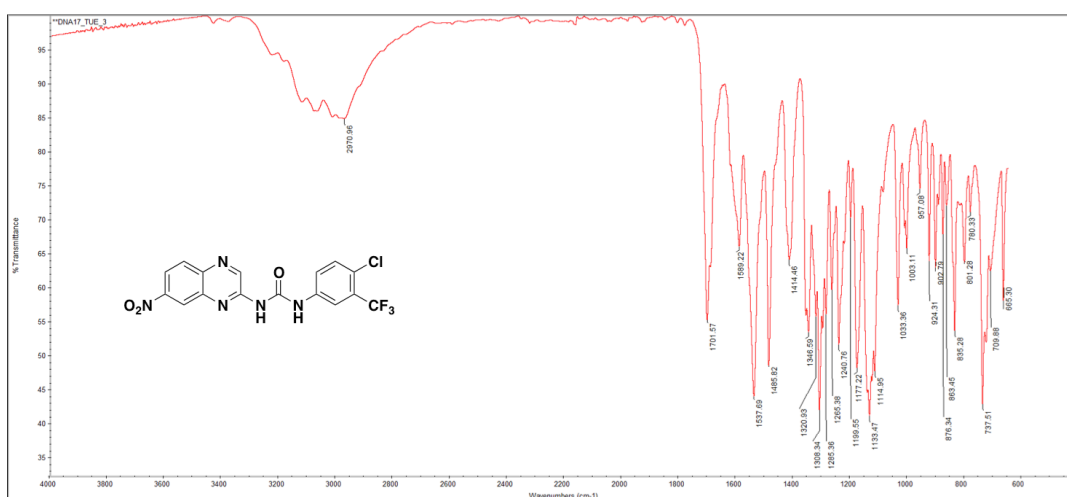


Figure S9. Infra red spectrum (ATR-FTIR) of compound 1-(7-nitroquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**9a**) (bands in cm⁻¹).

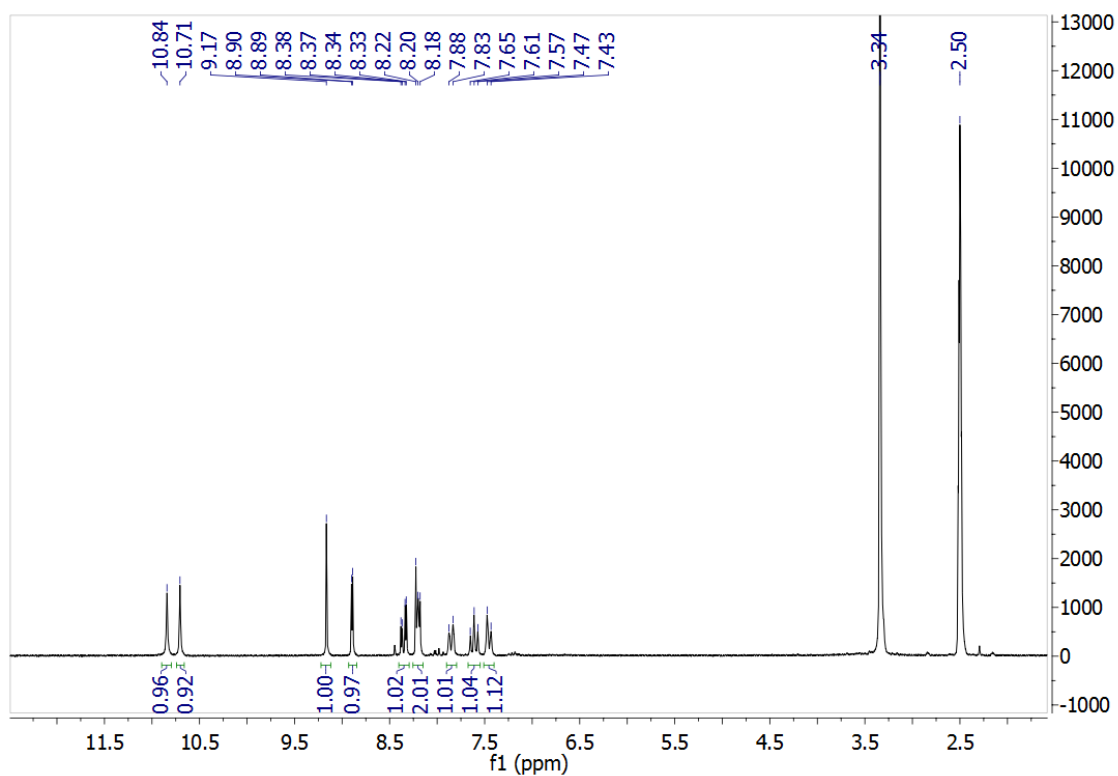


Figure S10. ^1H NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl)urea (**9b**) (DMSO- d_6 /200MHz/TMS)

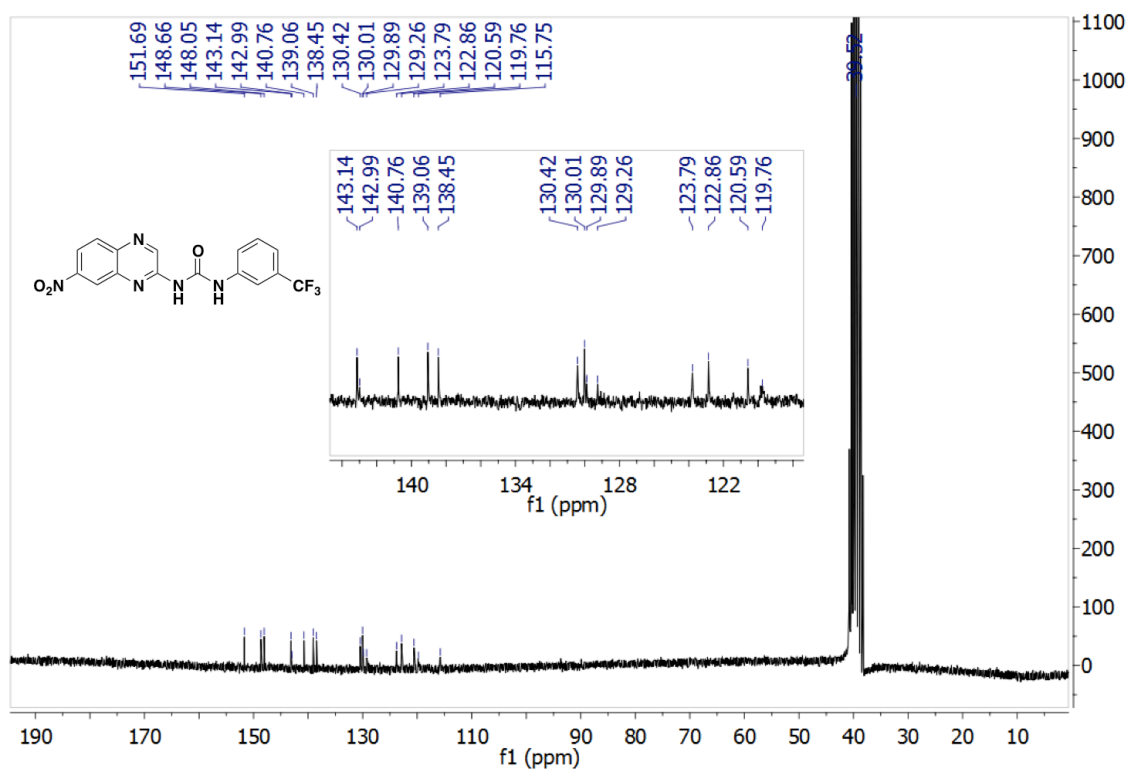


Figure S11. ^{13}C NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl)urea (**9b**) (DMSO- d_6 /50MHz/TMS)

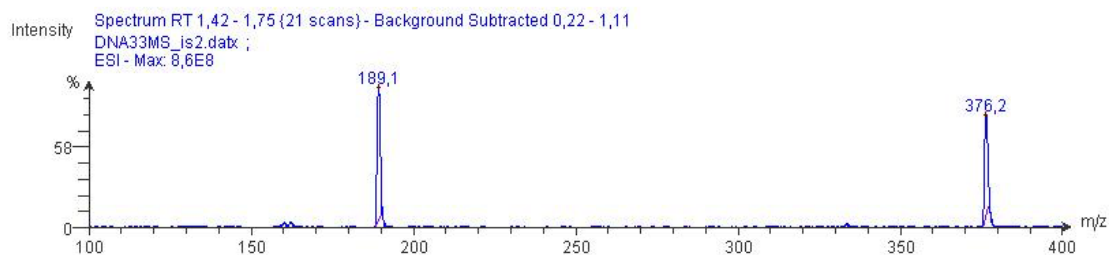


Figure S12. Mass spectrometry of compound 1-(7-nitroquinoxalin-2-yl)-3-(3-(trifluormethyl)phenyl) urea (**9b**) in negative mode (ESI-).

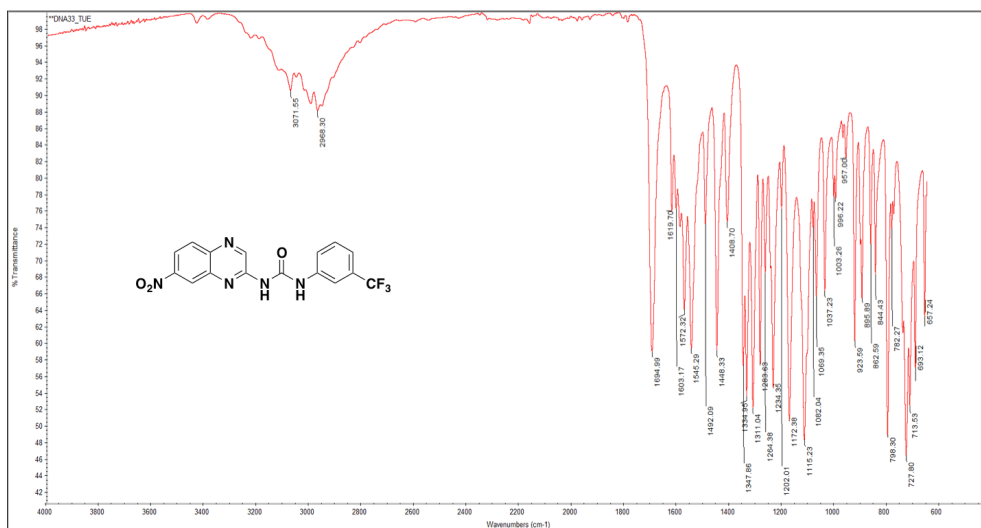


Figure S13. Infra red spectrum (ATR-FTIR) of compound 1-(7-nitroquinoxalin-2-yl)-3-(3-(trifluormethyl) phenyl) urea (**9b**) (bands in cm⁻¹).

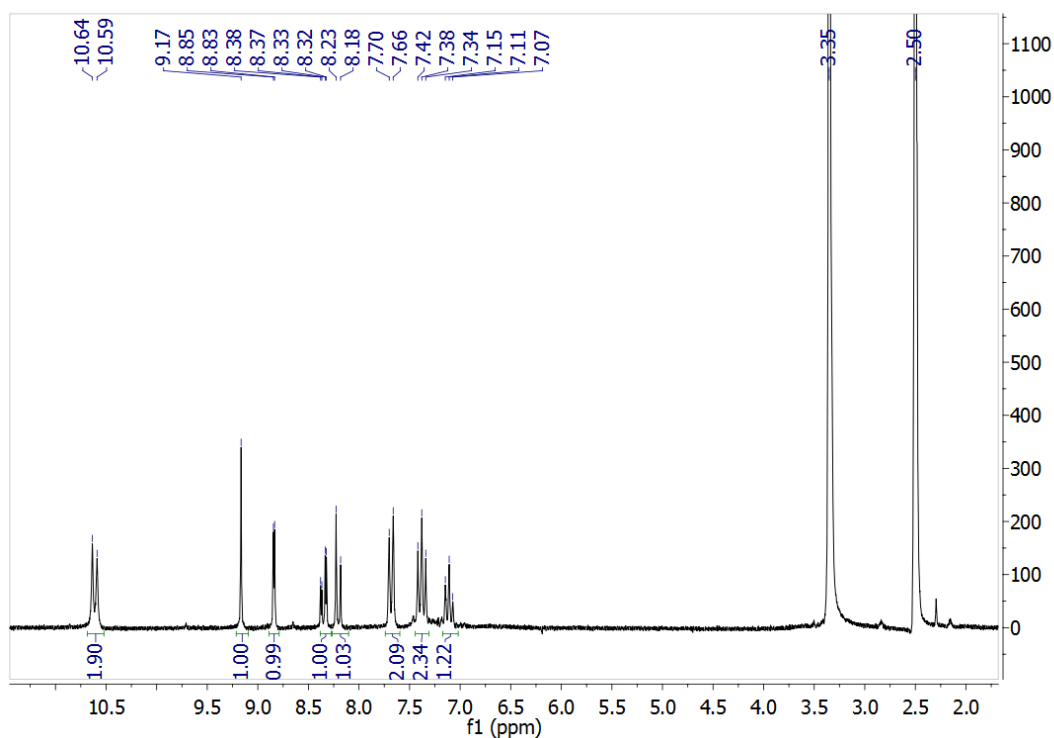


Figure S14. ¹H NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) (DMSO-d₆/200MHz/TMS)

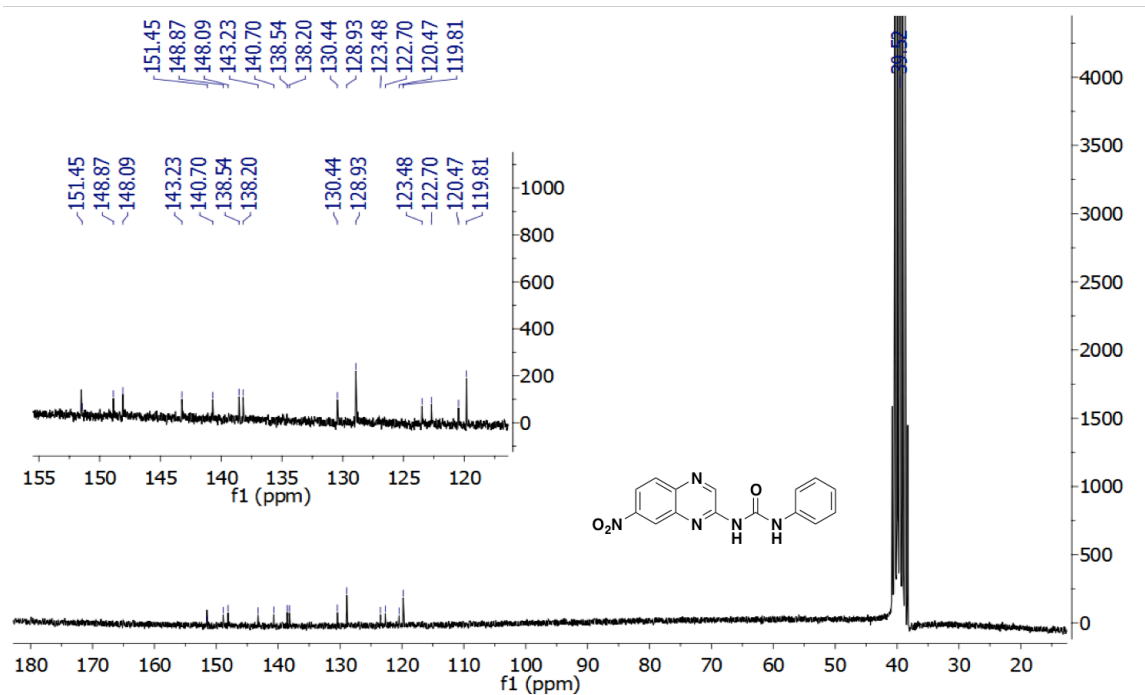


Figure S15. ^{13}C NMR spectrum of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) (DMSO- d_6 /50MHz/TMS)

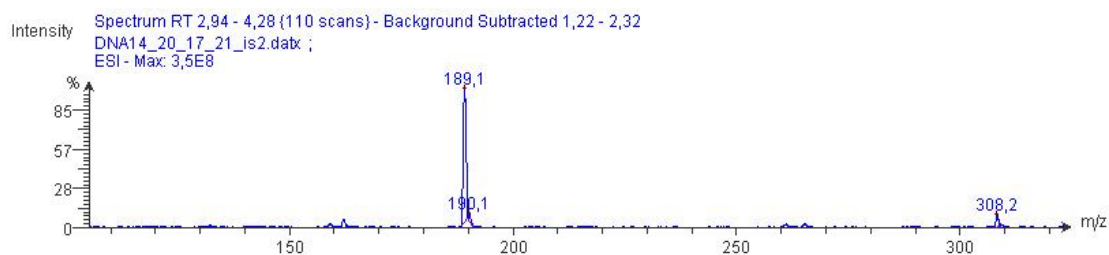


Figure S16. Mass spectrometry of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) in negative mode (ESI-).

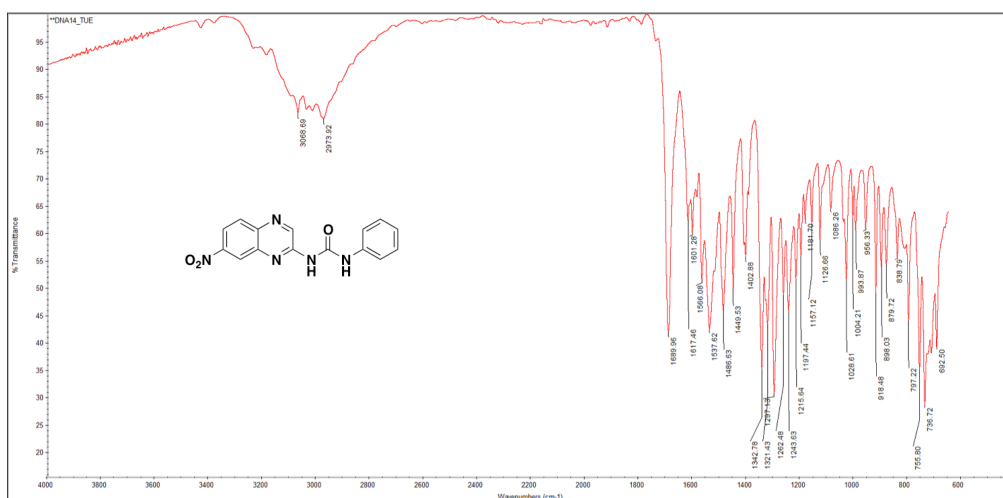


Figure S17. Infra red spectrum (ATR-FTIR) of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) (bands in cm^{-1}).

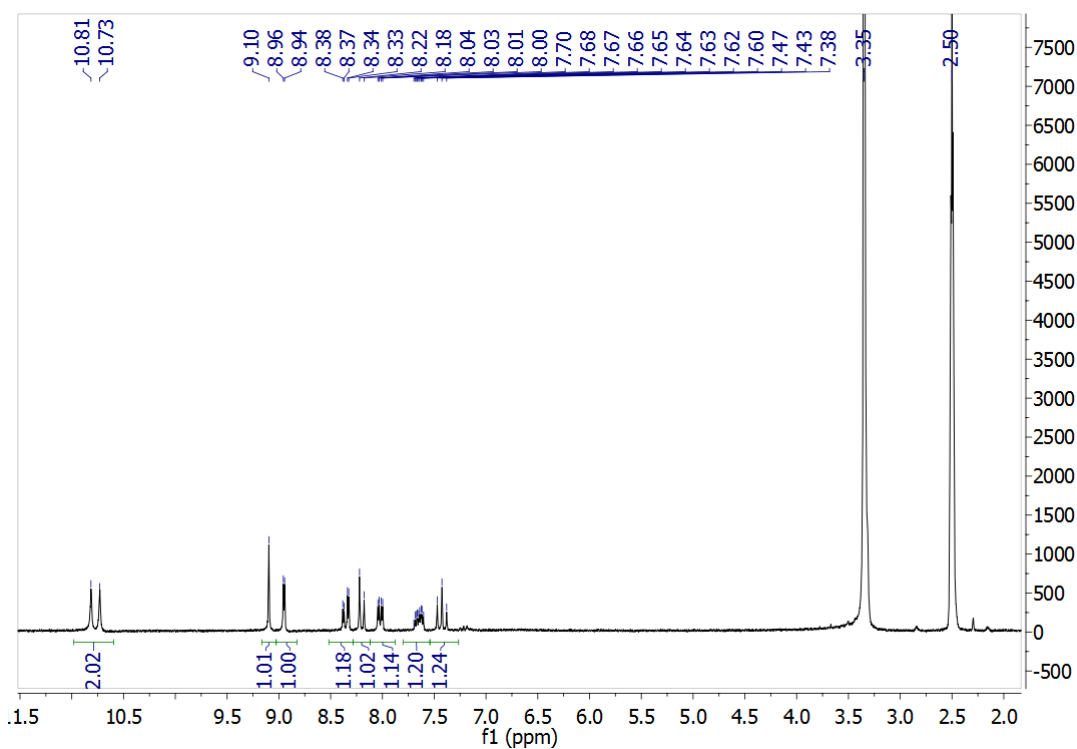


Figure S18. ^1H NMR spectrum of compound 1-(3-chloro-4-fluorophenyl)-3-(7-nitroquinoxalin-2-yl)urea (**9d**) (DMSO- d_6 /200MHz/TMS)

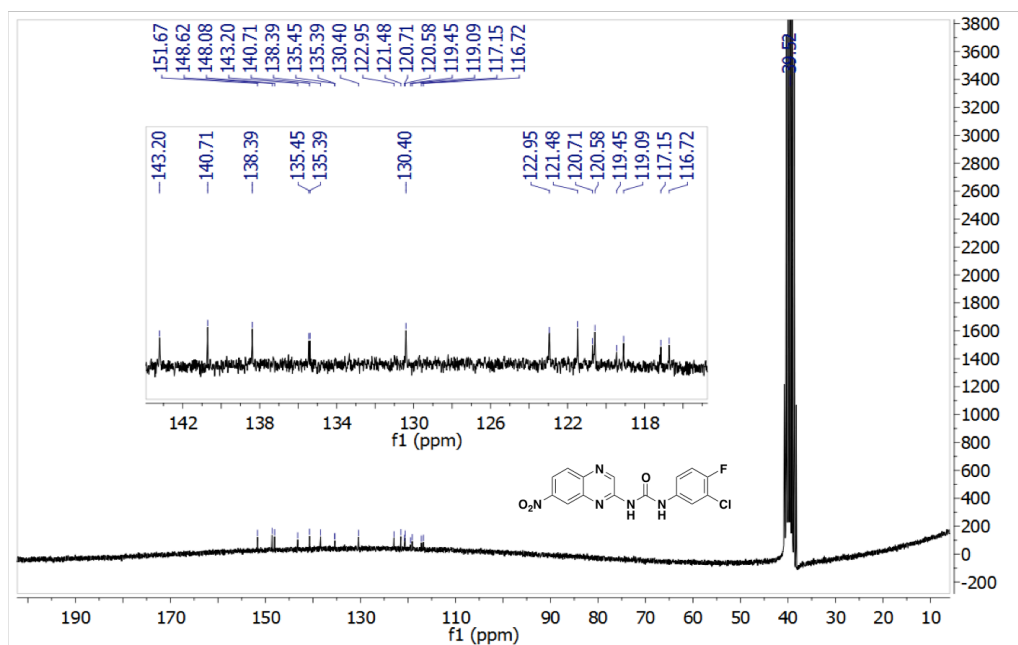


Figure S19. ^{13}C NMR spectrum of compound 1-(3-chloro-4-fluorophenyl)-3-(7-nitroquinoxalin-2-yl)urea (**9d**) (DMSO- d_6 /50MHz/TMS)

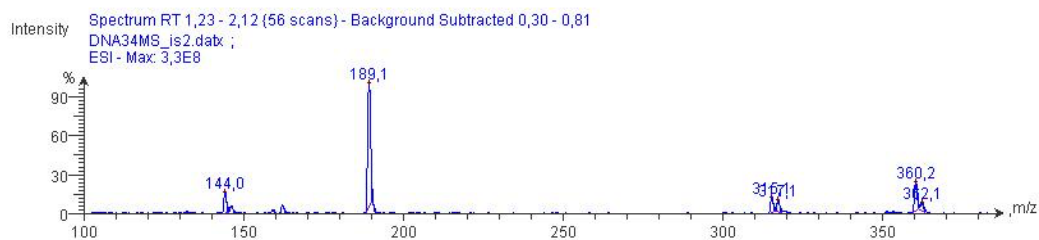


Figure S20. Mass spectrometry of compound 1-(3-chloro-4-fluorophenyl)-3-(7-nitroquinoxalin-2-yl)urea (**9d**) in negative mode (ESI-).

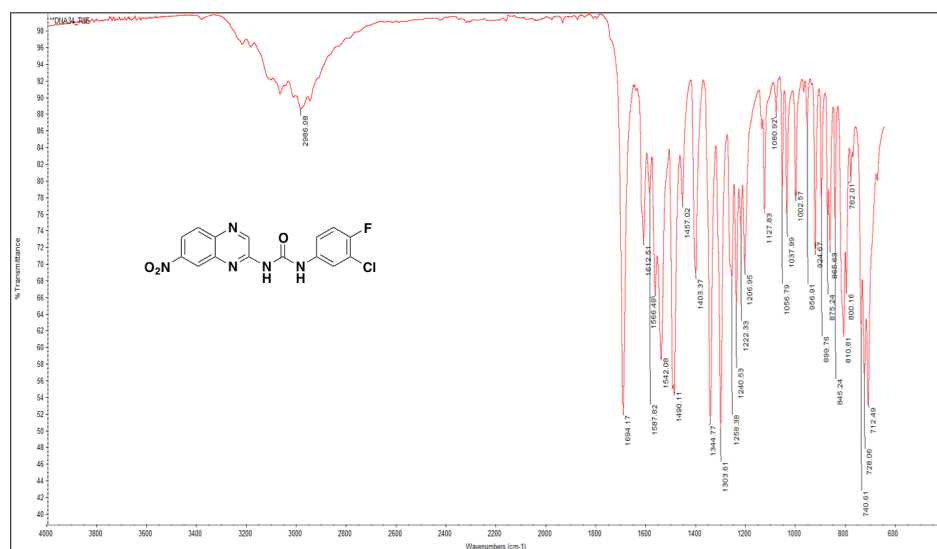


Figure S21. Infra red spectrum (ATR-FTIR) of compound 1-(3-chloro-4-fluorophenyl)-3-(7-nitroquinoxalin-2-yl)urea (**9d**) (bands in cm⁻¹).

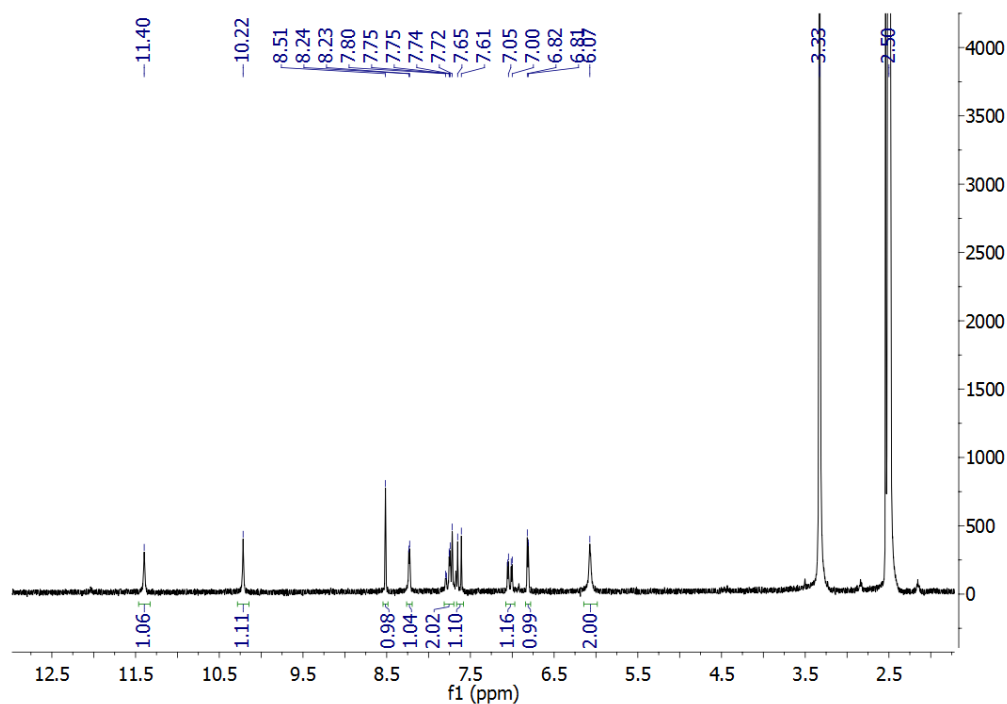


Figure S22. ¹H NMR spectrum of 1-(7-aminoquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl)phenyl)urea (**10a**) (DMSO-d₆/200MHz/TMS)

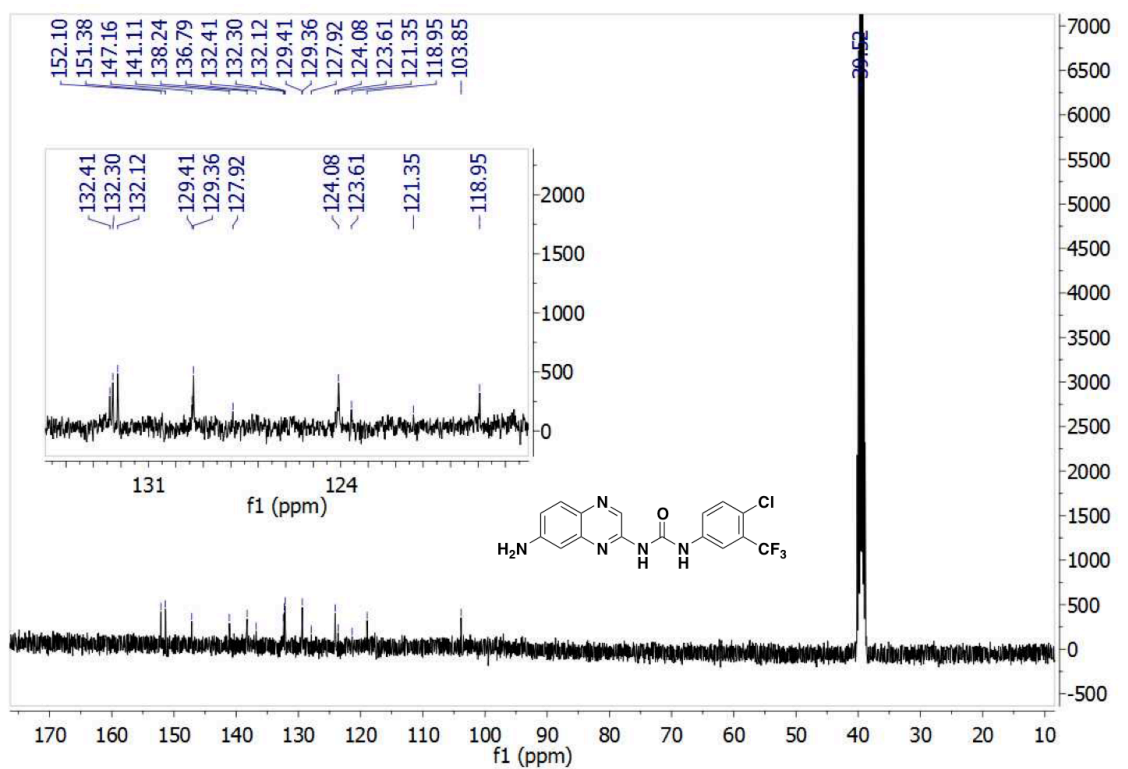


Figure S23. ^{13}C NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl) phenyl)urea (**10a**) (DMSO- d_6 /100MHz/TMS)

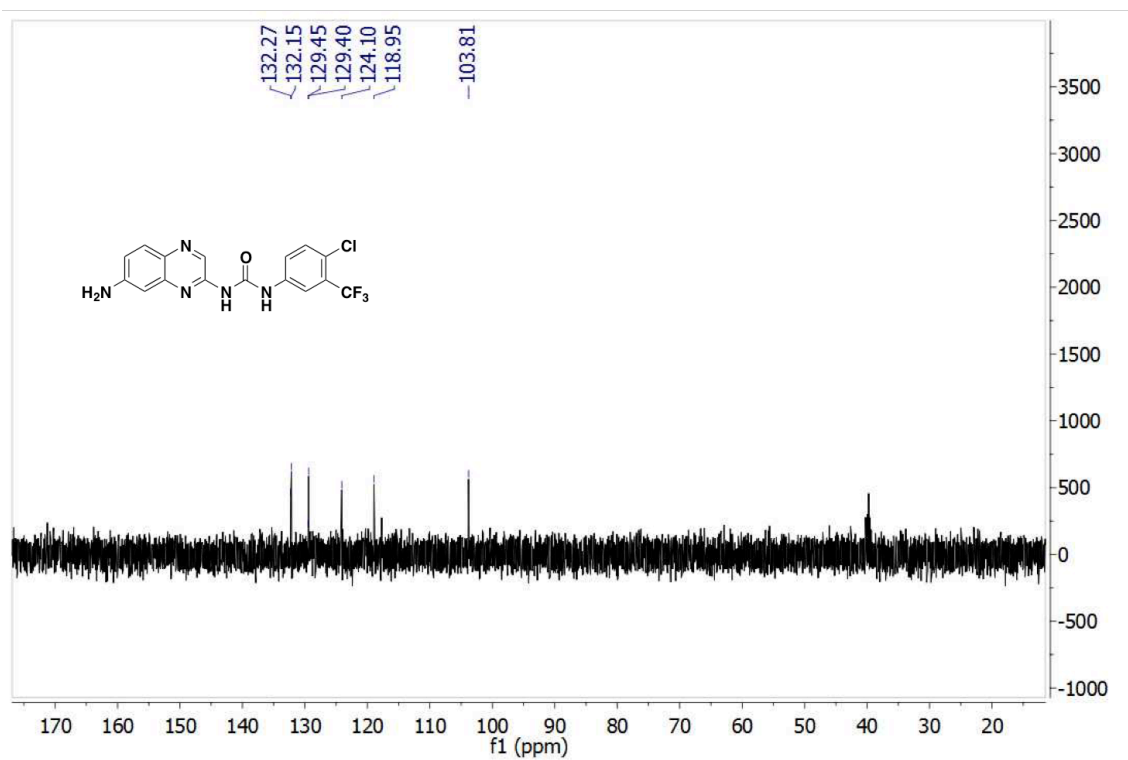


Figure S24. Espectro de DEPT 135 of compound 1-(7-aminoquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl) phenyl)urea (**10a**) (DMSO- d_6 /100MHz/TMS)

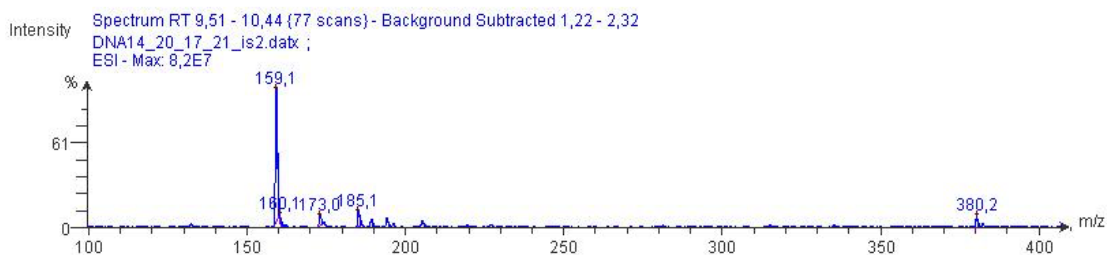


Figure S25. Mass spectrometry of compound 1-(7-aminoquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl) phenyl) urea (**10a**) in negative mode (ESI-).

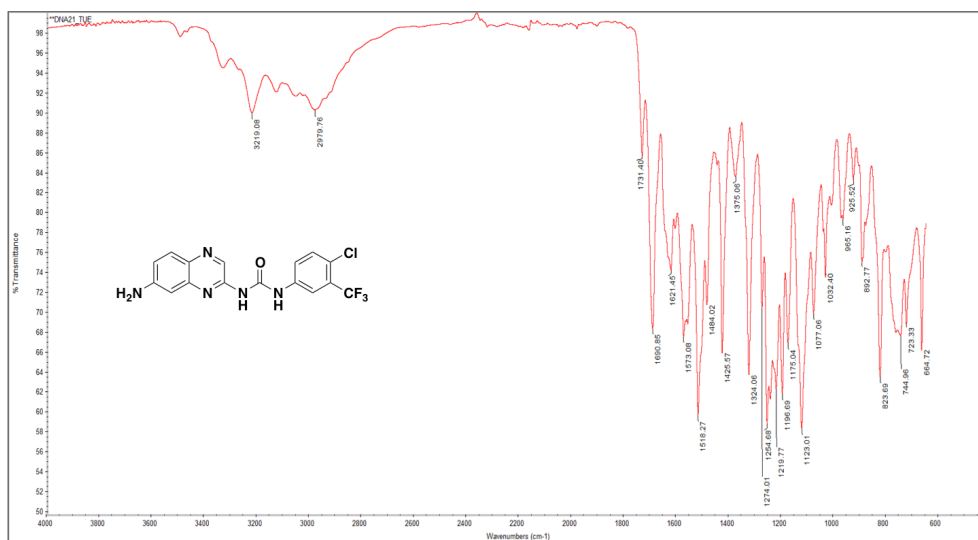


Figure S26. Infra red spectrum (ATR-FTIR) of compound 1-(7-aminoquinoxalin-2-yl)-3-(4-chloro-3-(trifluoromethyl) phenyl) urea (**10a**) (bands in cm⁻¹).

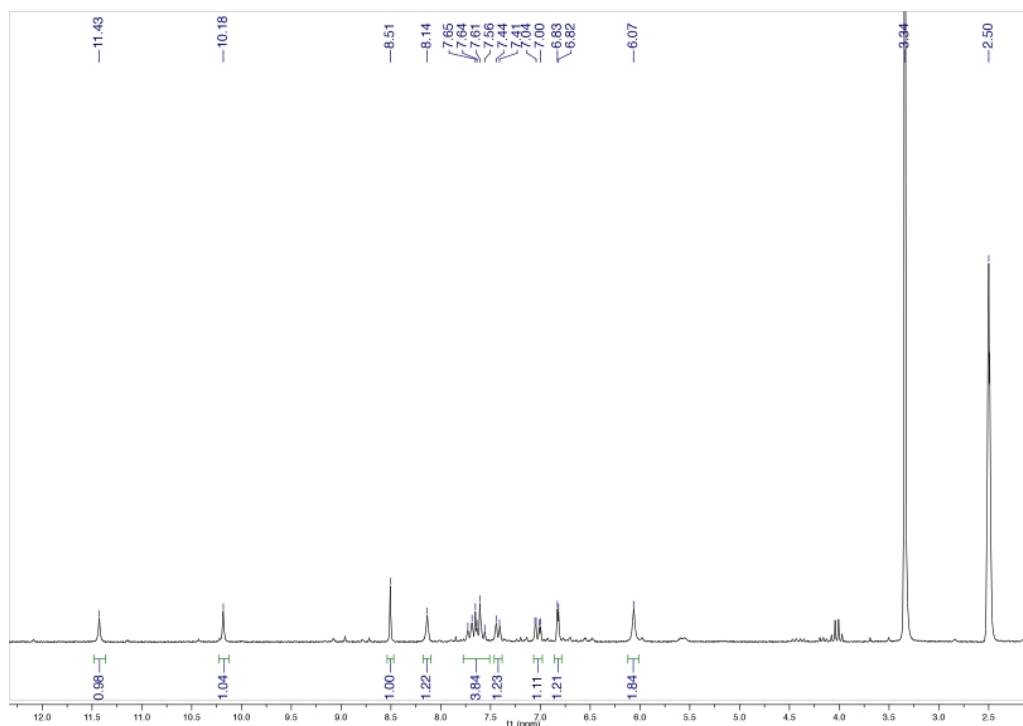


Figure S27. ¹H NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl) urea (**10b**) (DMSO-d₆/200MHz/TMS)

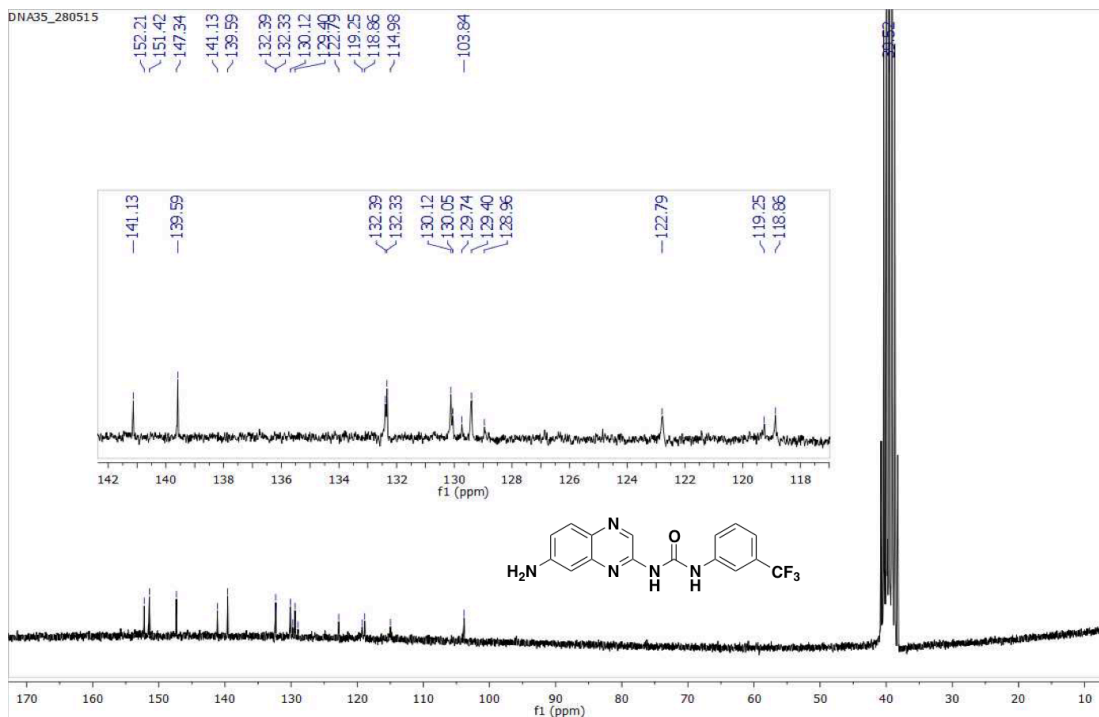


Figure S28. ¹³C NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl) urea (**10b**) (DMSO-d₆/50MHz/TMS)

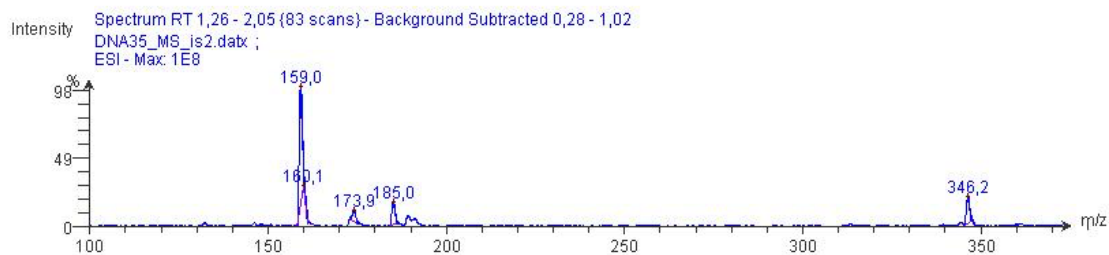


Figure S29. Mass spectrometry of compound 1-(7-aminoquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl) urea (**10b**) in negative mode (ESI-).

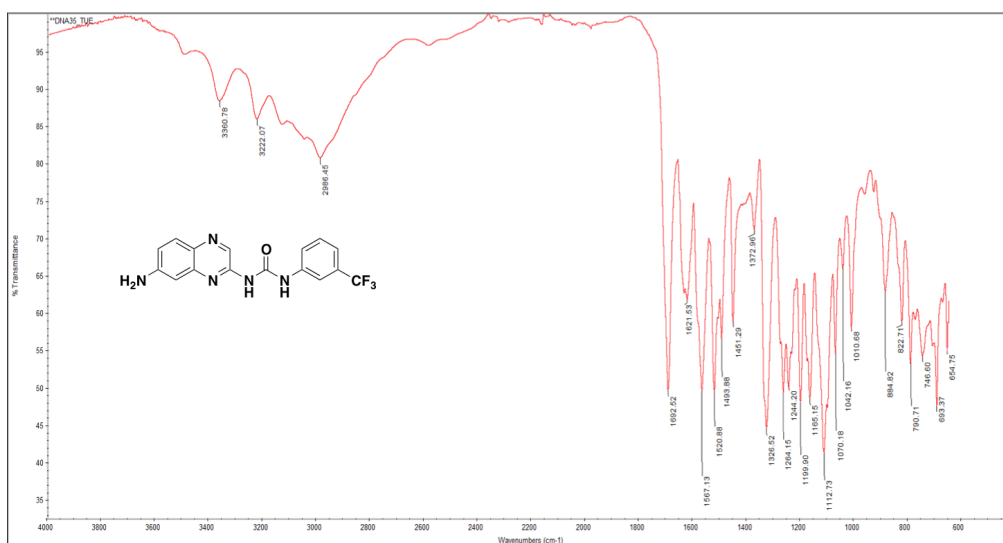


Figure S30. Infra red spectrum (ATR-FTIR) of compound 1-(7-aminoquinoxalin-2-yl)-3-(3-(trifluoromethyl)phenyl) urea (**10b**) (bands in cm⁻¹).

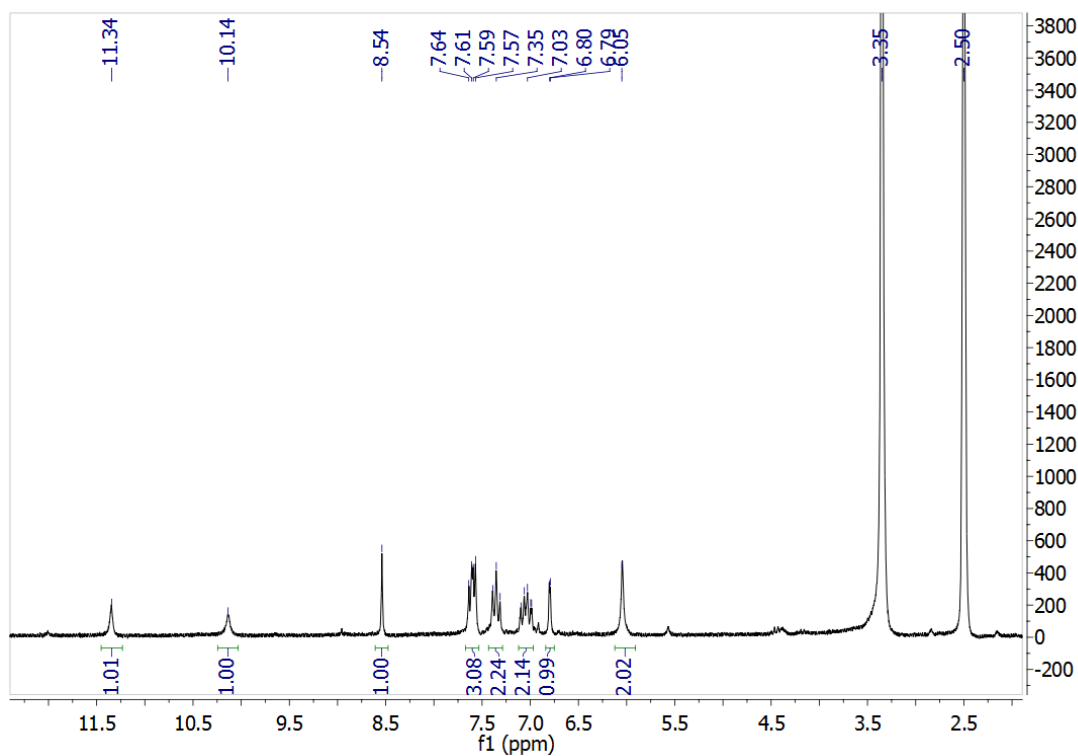


Figure S31. ^1H NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-phenylurea (**10c**) (DMSO- d_6 /200MHz/TMS)

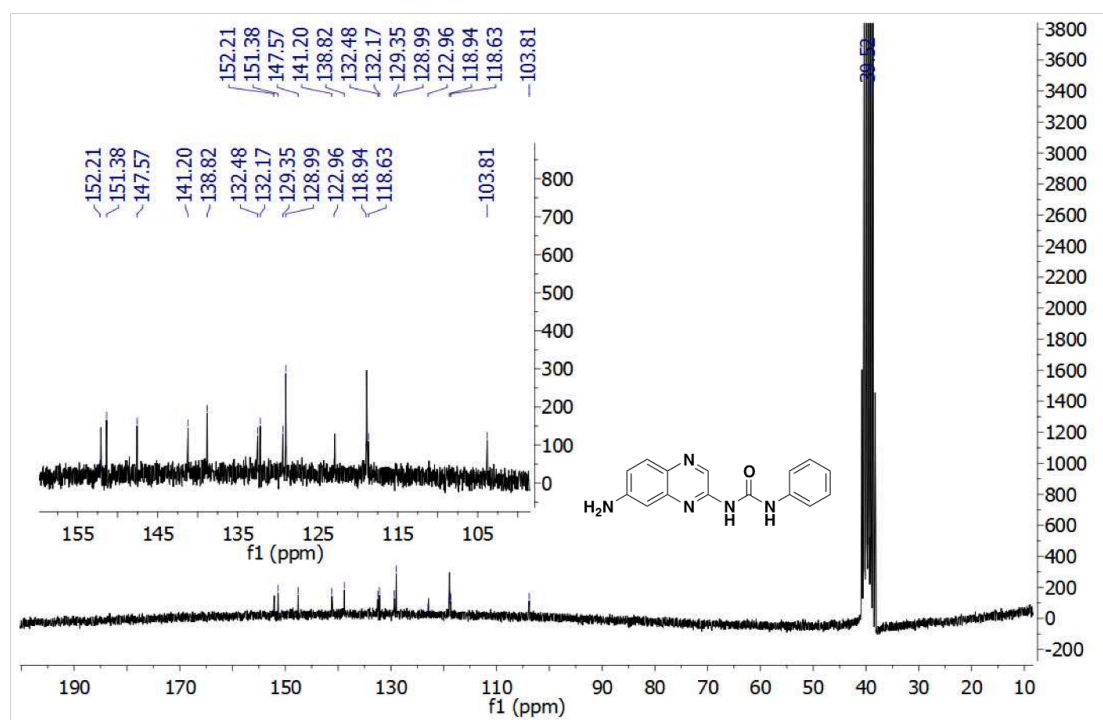


Figure S32. ^{13}C NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-phenylurea (**10c**) (DMSO- d_6 /50MHz/TMS)

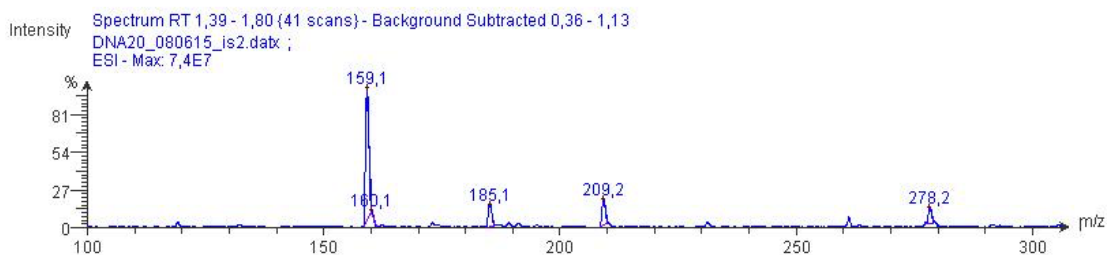


Figure S33. Mass spectrometry of compound 1-(7-aminoquinoxalin-2-yl)-3-phenylurea (**10c**) in negative mode (ESI-).

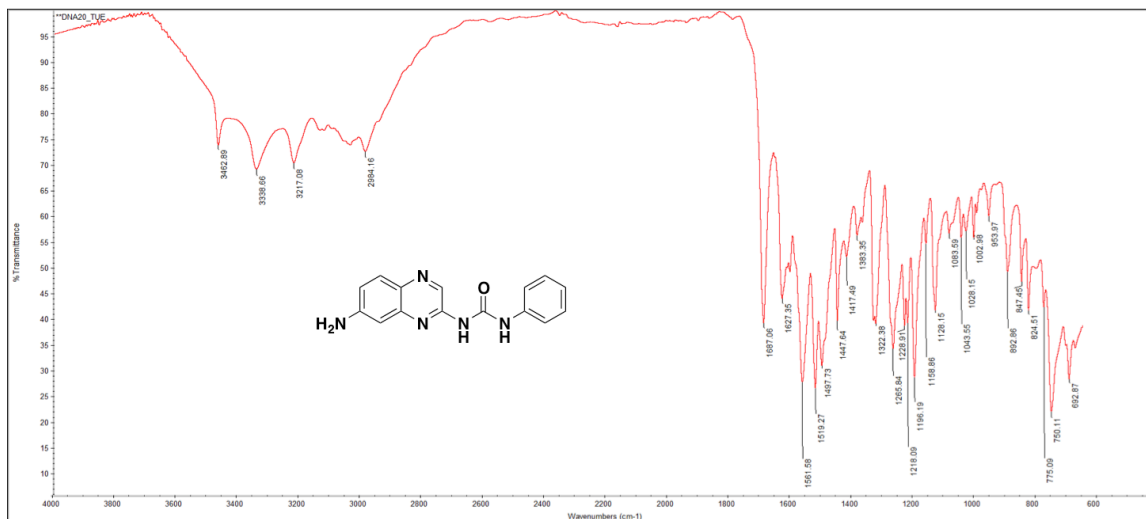


Figure S34. Infra red spectrum (ATR-FTIR) of compound 1-(7-aminoquinoxalin-2-yl)-3-phenylurea (**10c**) (bands in cm^{-1})

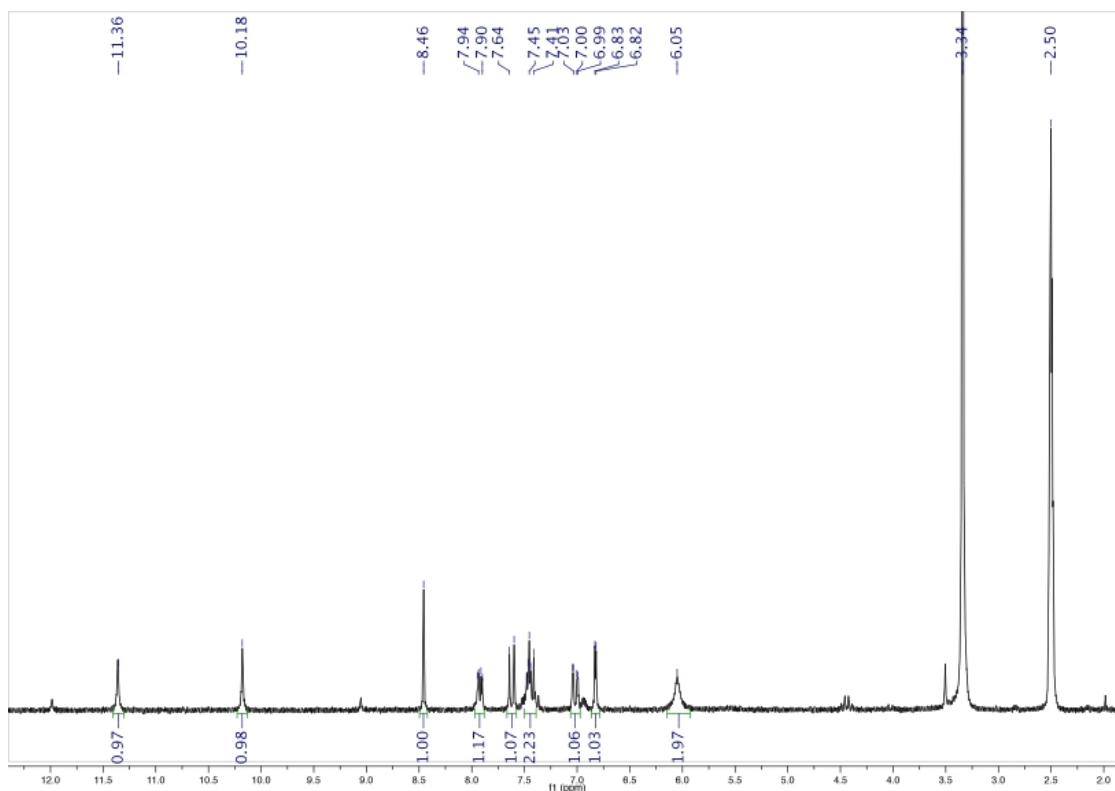


Figure S35. ^1H NMR spectrum of compound 1-(7-aminoquinoxalin-2-yl)-3-(3-chloro-4-fluorophenyl) urea (**10d**) ($\text{DMSO-d}_6/200\text{MHz/TMS}$)

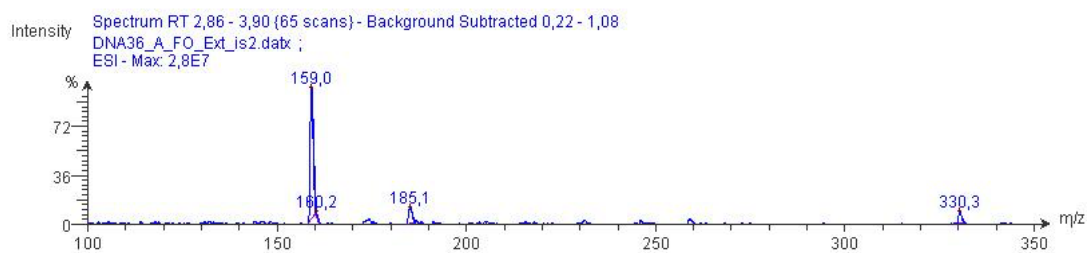


Figure S36. Mass spectrometry of compound 1 - (7-aminoquinoxalin-2-yl)-3-(3-chloro-4-fluorophenyl) urea (**10d**) in negative mode (ESI-).

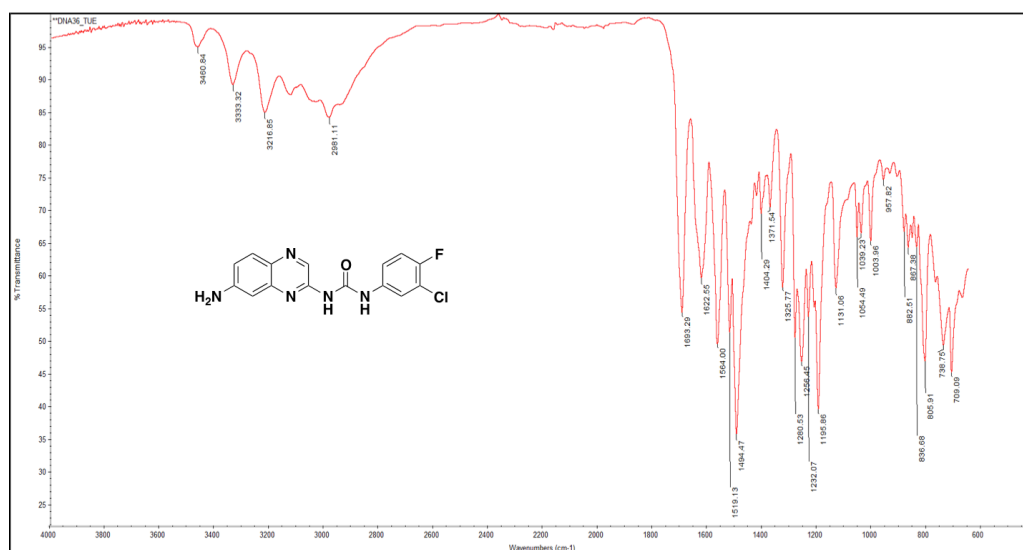


Figure S37. Infra red spectrum (ATR-FTIR) of compound 1 - (7-aminoquinoxalin-2-yl)-3-(3-chloro-4-fluorophenyl) urea (**10d**) (bands in cm⁻¹).

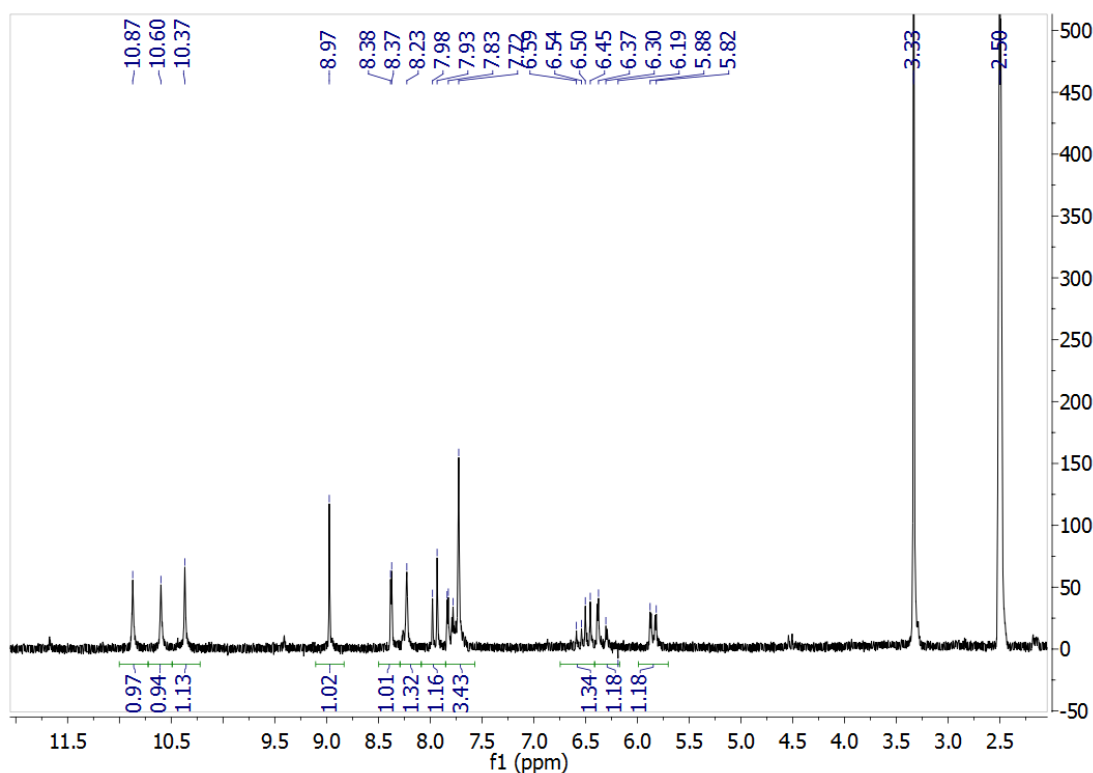


Figure S38. ^1H NMR spectrum of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acrylamide (**7a**) (DMSO- d_6 /200MHz/TMS)

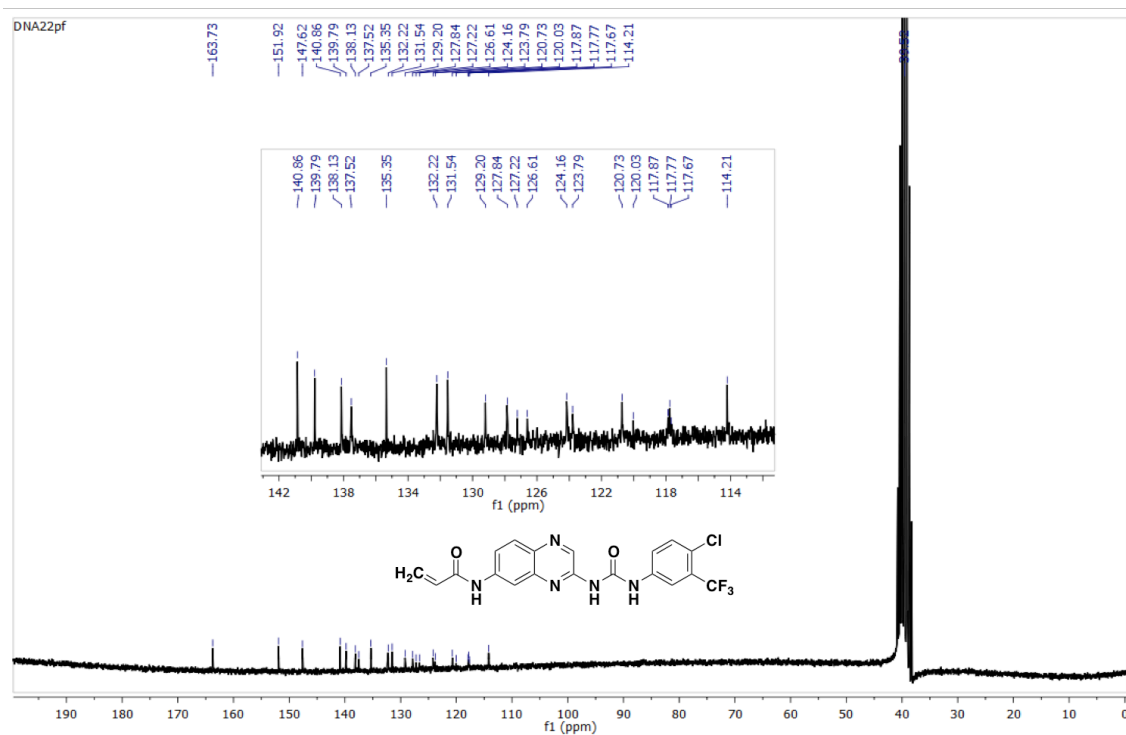


Figure S39. ^{13}C NMR spectrum of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acrylamide (**7a**) (DMSO- d_6 /50MHz/TMS)

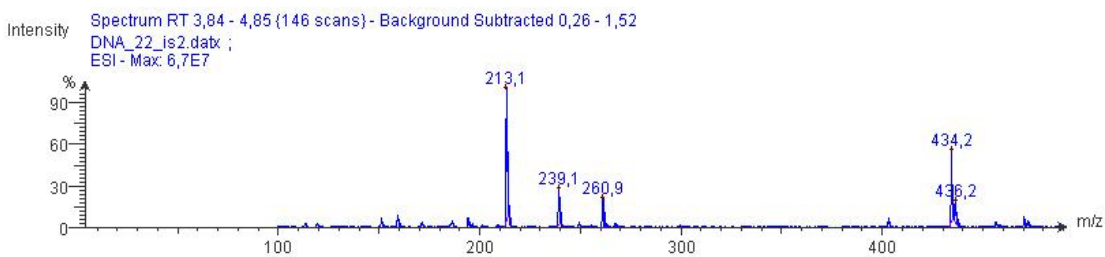


Figure S40. Mass spectrometry of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acrylamide (**7a**) in negative mode (ESI-).

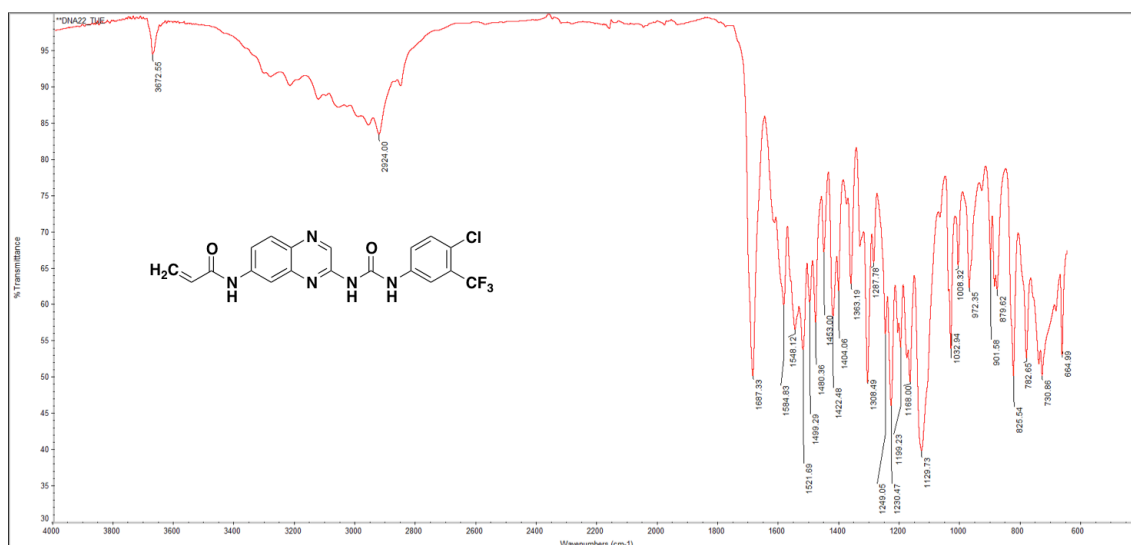


Figure S41. Infra red spectrum (ATR-FTIR) of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acrylamide (**7a**) (bands in cm^{-1}).

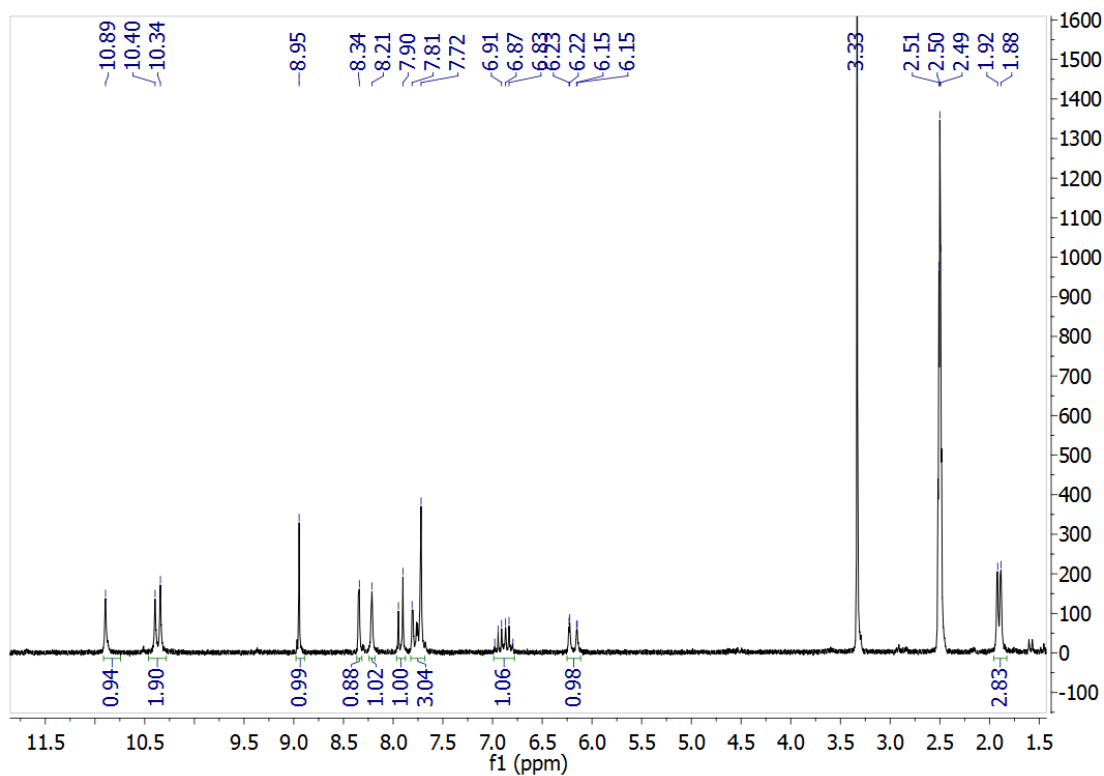


Figure S42. ^1H NMR spectrum of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)but-2-enamide (**7b**) ($\text{DMSO-d}_6/200\text{MHz/TMS}$)

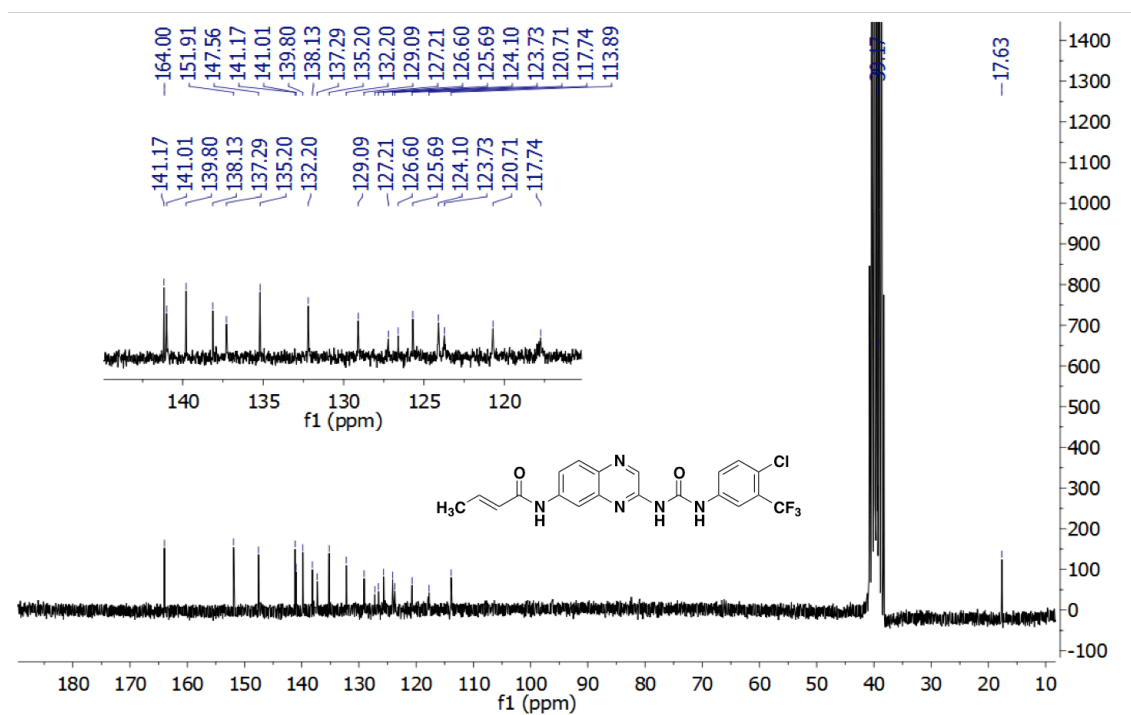


Figure S43. ^{13}C NMR spectrum of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)but-2-enamide (**7b**) ($\text{DMSO-d}_6/50\text{MHz/TMS}$).

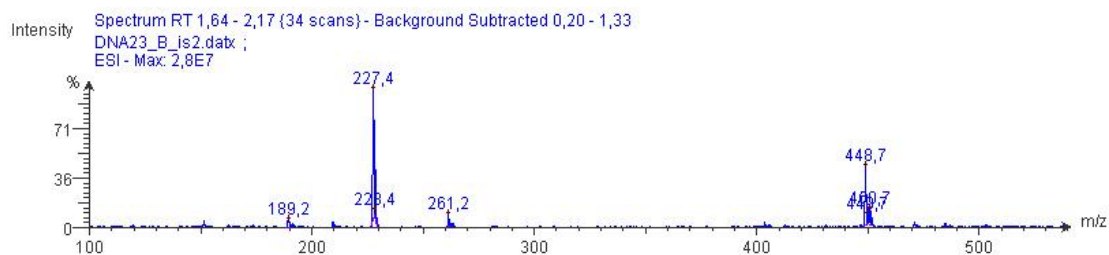


Figure S44. Mass spectrometry of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido) quinoxalin-6-yl)but-2-enamide (**7b**) in negative mode (ESI-).

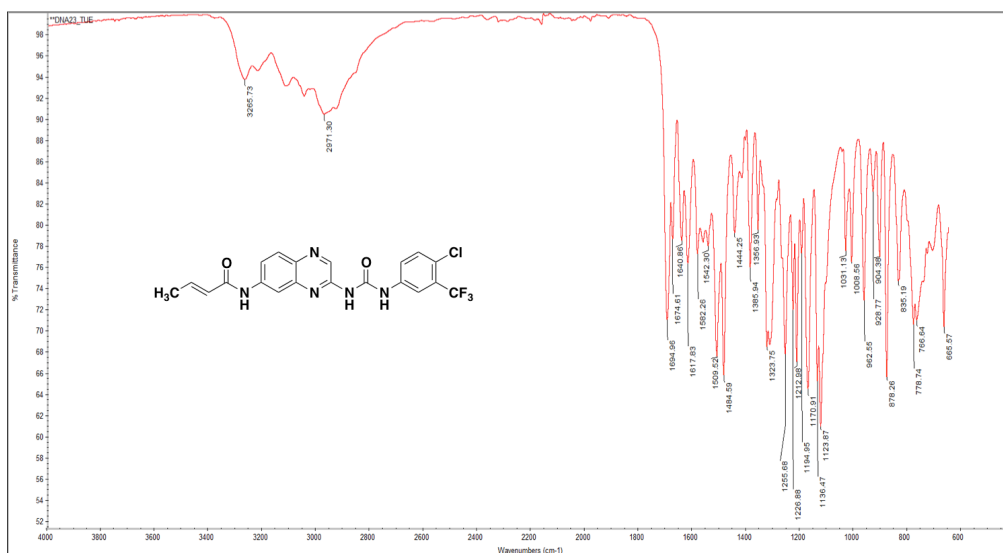


Figure S45. Infra red spectrum (ATR-FTIR) of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido) quinoxalin-6-yl)but-2-enamide (**7b**) (bands in cm⁻¹).

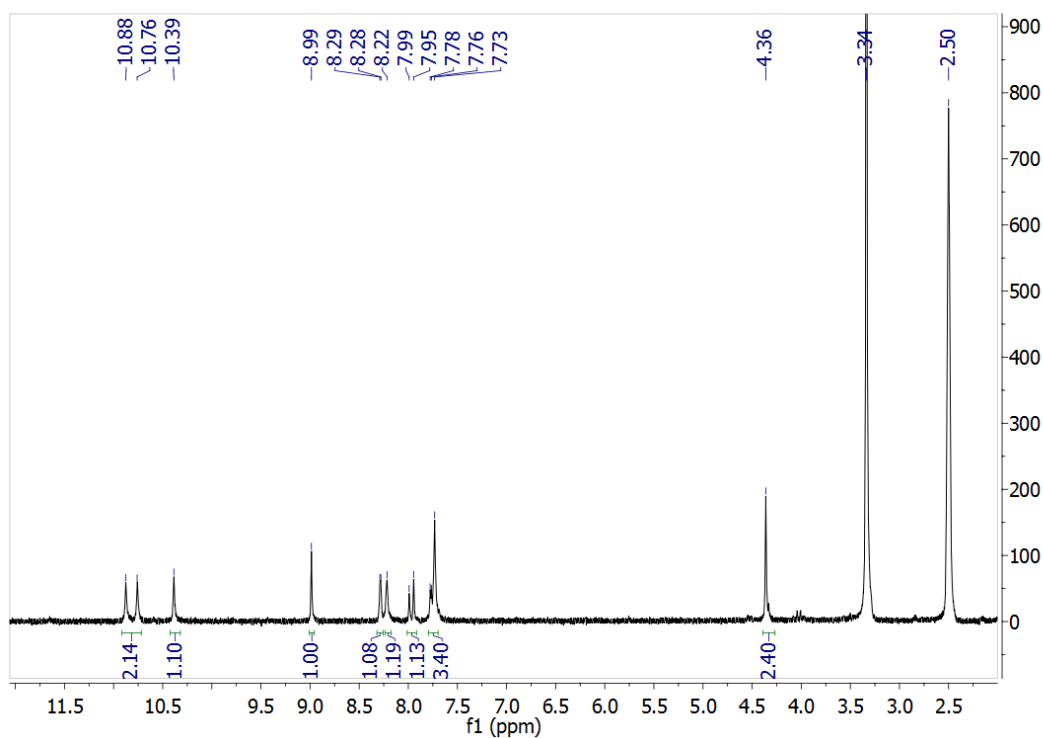


Figure S46. ¹H NMR spectrum of compound 2-chloro-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido) quinoxalin-6-yl)acetamide (**7c**) (DMSO-d₆/200MHz/TMS)

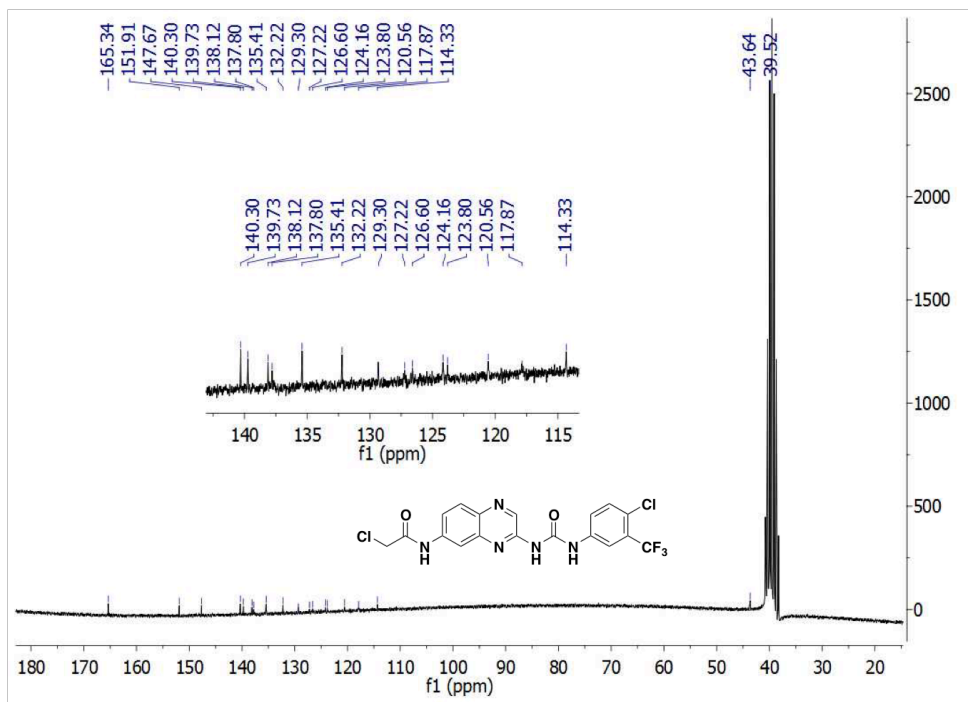


Figure S47. ¹³C NMR spectrum of compound 2-chloro-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acetamide (**7c**) (DMSO-*d*₆/50MHz/TMS)

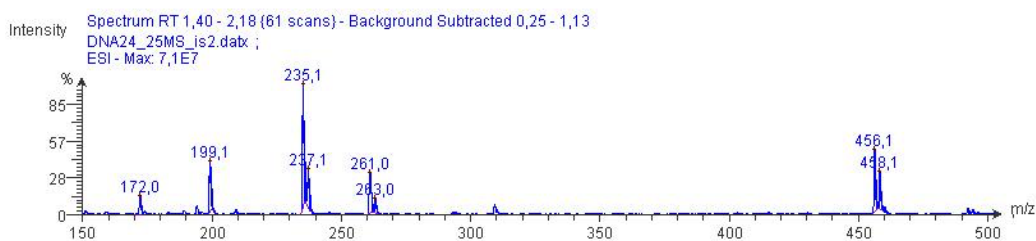


Figure S48. Mass spectrometry of compound 2-chloro-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acetamide (**7c**) in negative mode (ESI-).

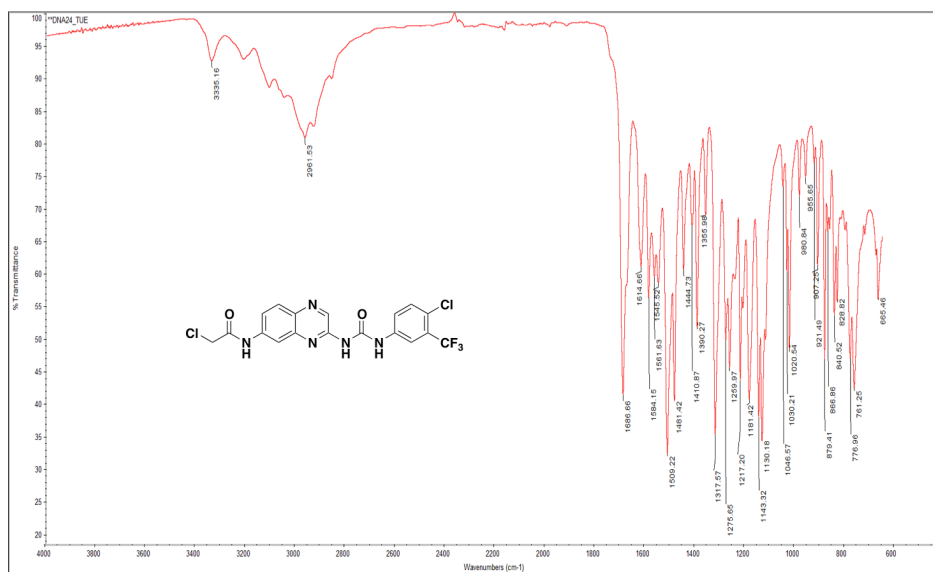


Figure S49. Infra red spectrum (ATR-FTIR) of compound 2-chloro-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)acetamide (**7c**) (bands in cm⁻¹).

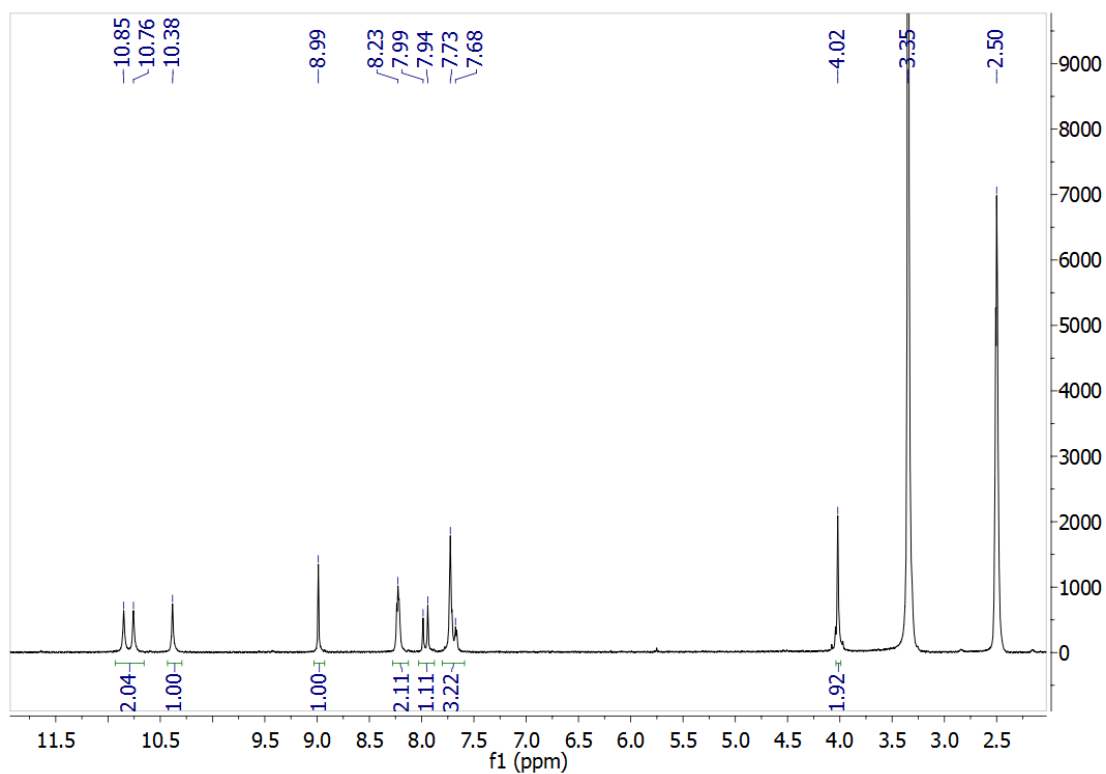


Figure S50. ^1H NMR spectrum of compound 2-chloro- *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-2-cianoacetamide (**7d**) (DMSO- d_6 /200MHz/TMS)

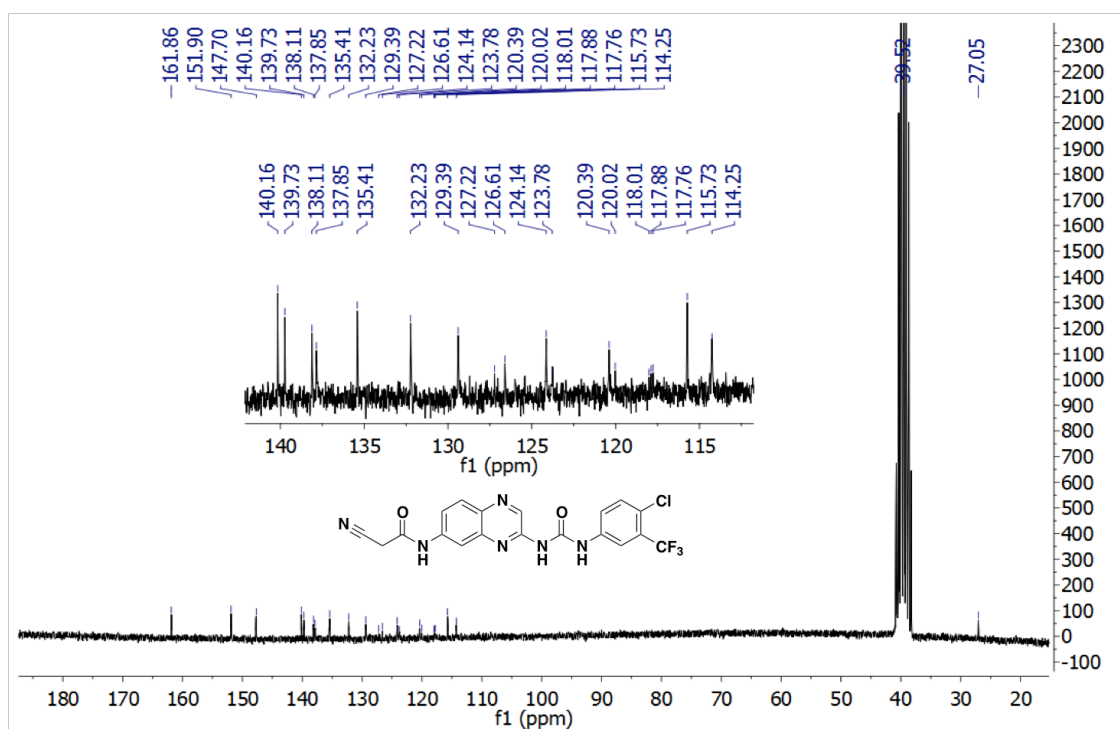


Figure S51. ^{13}C NMR spectrum of compound 2-chloro- *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-2-cianoacetamide (**7d**) (DMSO- d_6 /50MHz/TMS)

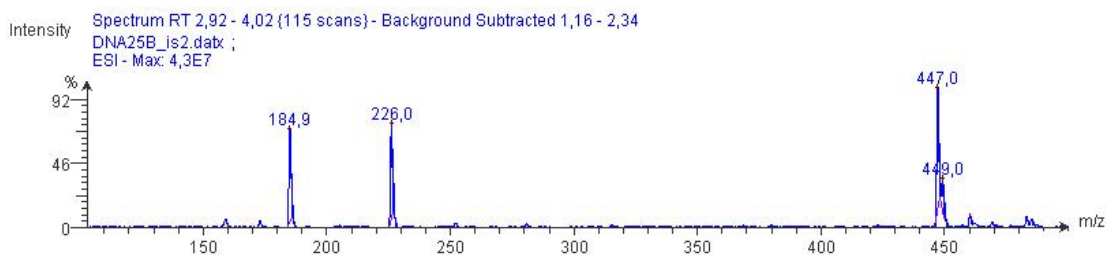


Figure S52. Mass spectrometry of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-2-cianoacetamide (**7d**) in negative mode (ESI-).

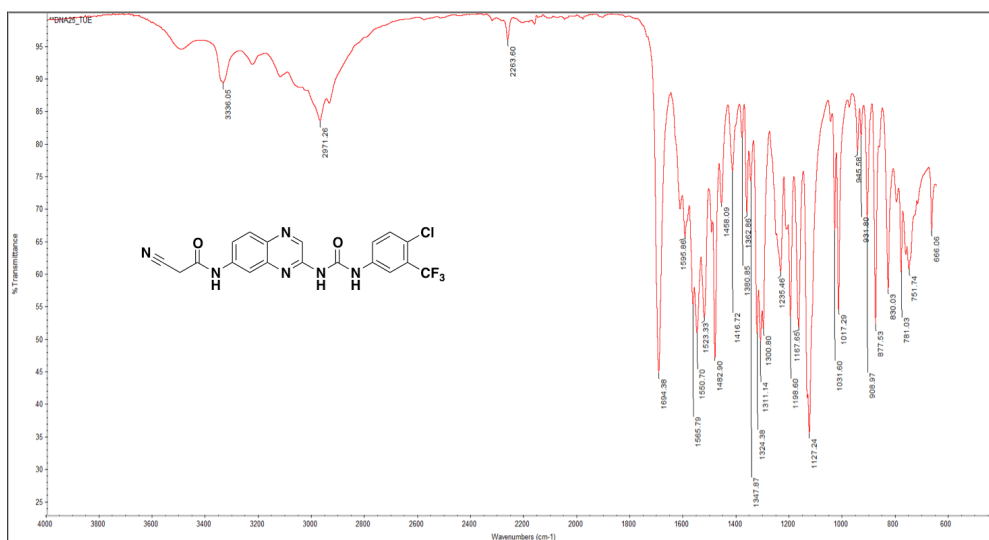


Figure S53. Infra red spectrum (ATR-FTIR) of compound *N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-2-cianoacetamide (**7d**) (bands in cm^{-1}).

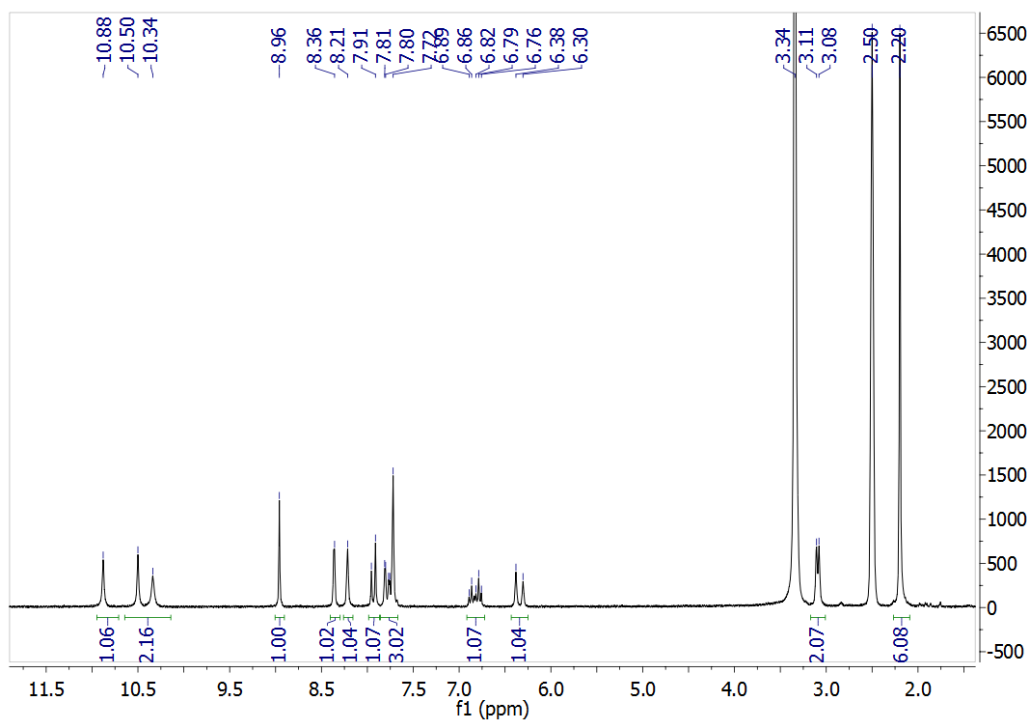


Figure S54. ^1H NMR spectrum of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-4-(dimethylamino)but-2-enamide (**7e**) ($\text{DMSO}-d_6/200\text{MHz/TMS}$)

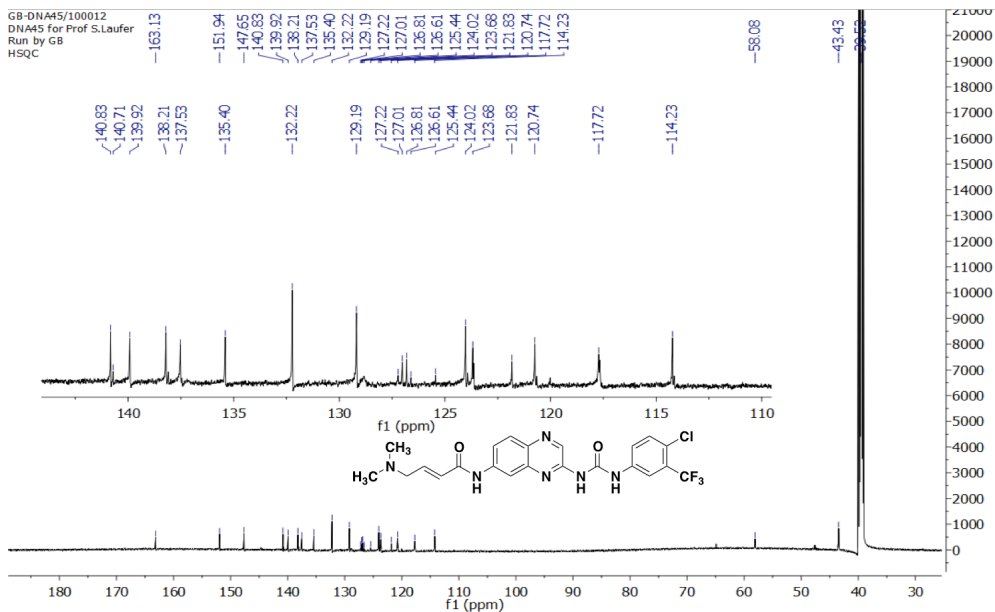


Figure S55. ^{13}C NMR spectrum of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-4-(dimethylamino)but-2-enamide (**7e**) (DMSO- d_6 /150MHz/TMS)

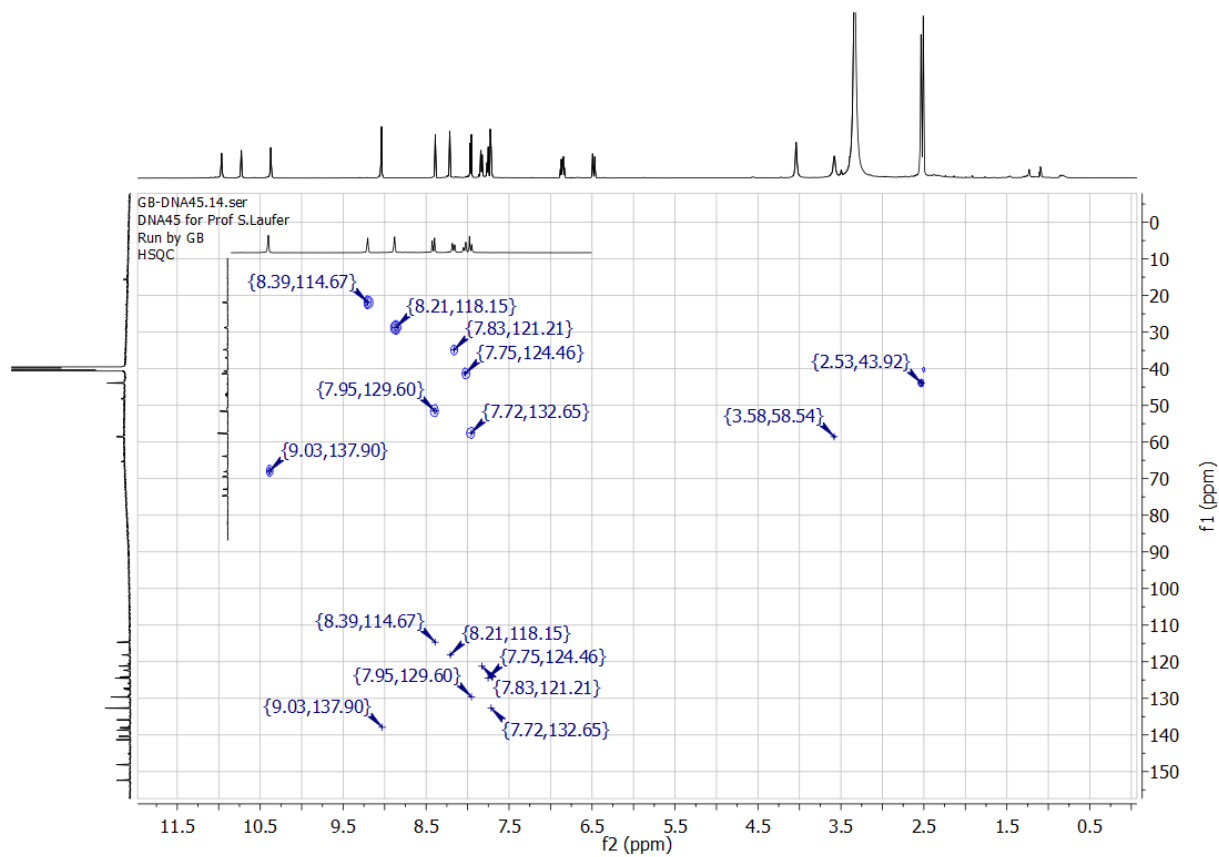


Figure S56. HSQC spectrum of compound (*E*)-*N*-(3-(3-(4-chloro-3-(trifluoromethyl)phenyl)ureido)quinoxalin-6-yl)-4-(dimethylamino)but-2-enamide (**7e**) (DMSO- d_6 /150MHz/TMS)

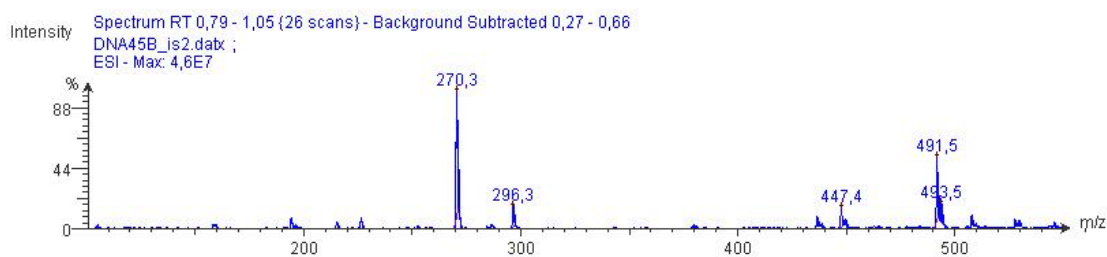


Figure S57. Mass spectrometry of compound *E*-*N*-(3-(3-(4-chloro-3-(trifluoromethyl) phenyl)ureido) quinoxalin-6-yl)-4-(dimethylamino)but-2-enamide (**7e**) in negative mode (ESI).

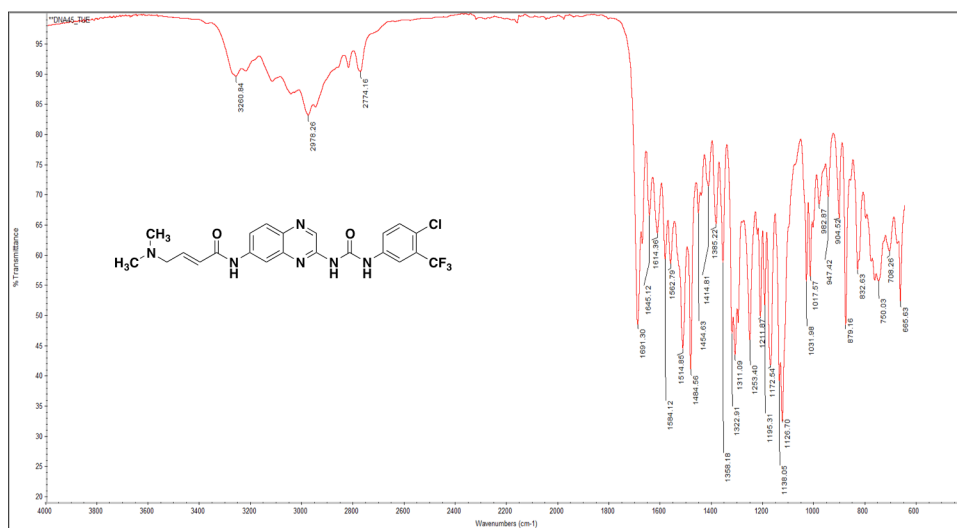


Figure S58. Infra red spectrum (ATR-FTIR) of compound *E*-*N*-(3-(3-(4-chloro-3-(trifluoromethyl) phenyl)ureido) quinoxalin-6-yl)-4-(dimethylamino)but-2-enamide (**7e**) (bands in cm⁻¹).

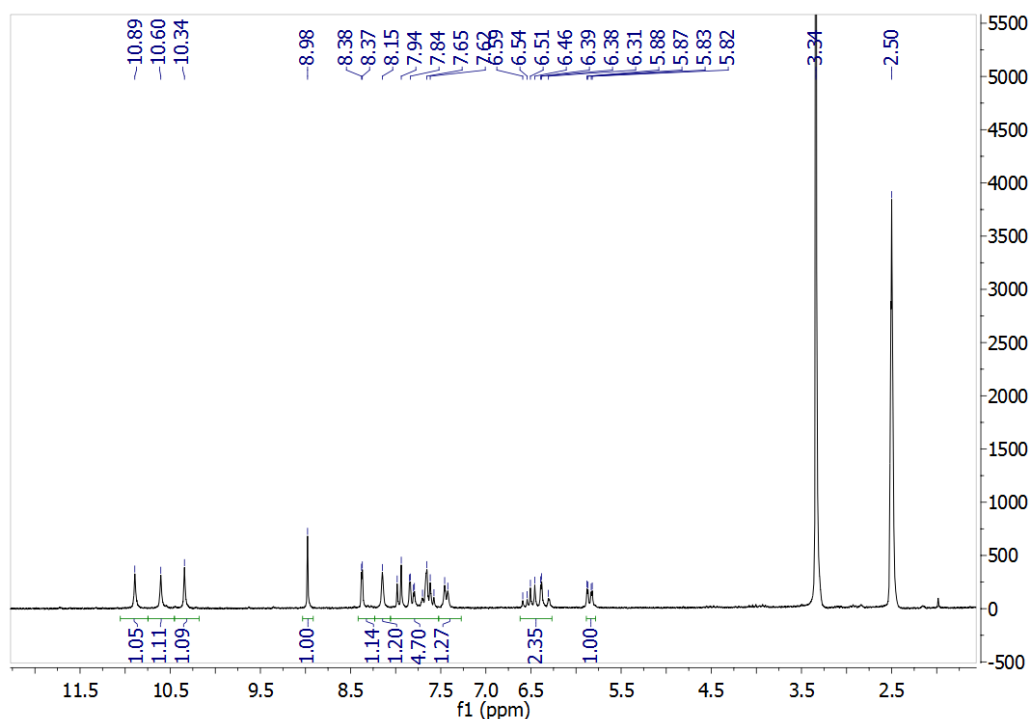
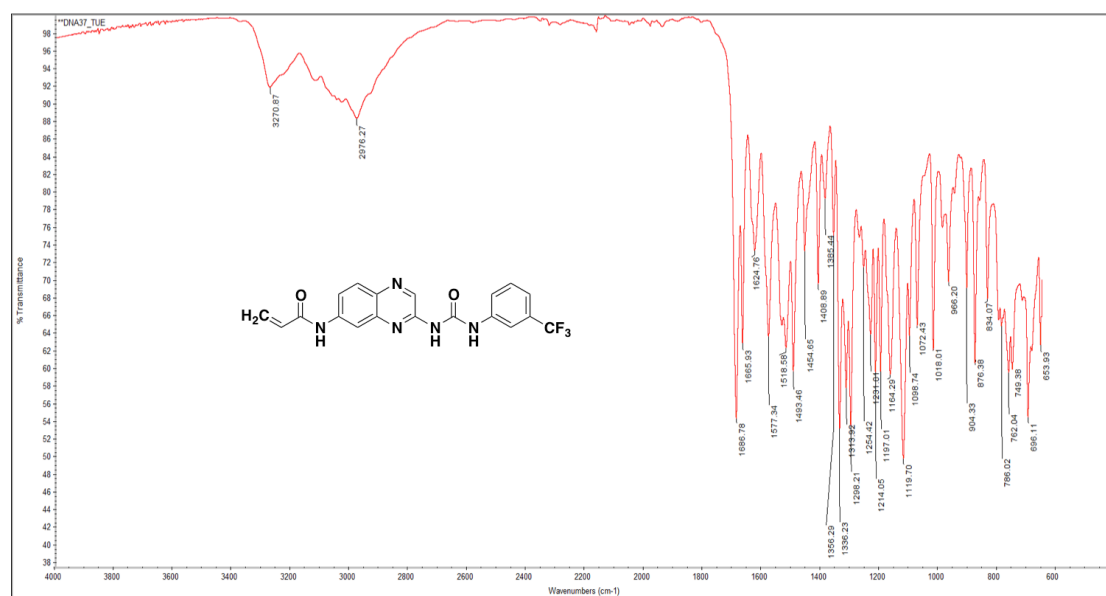
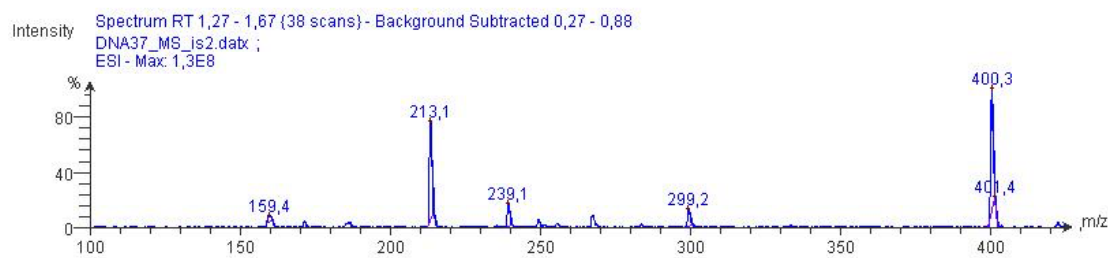
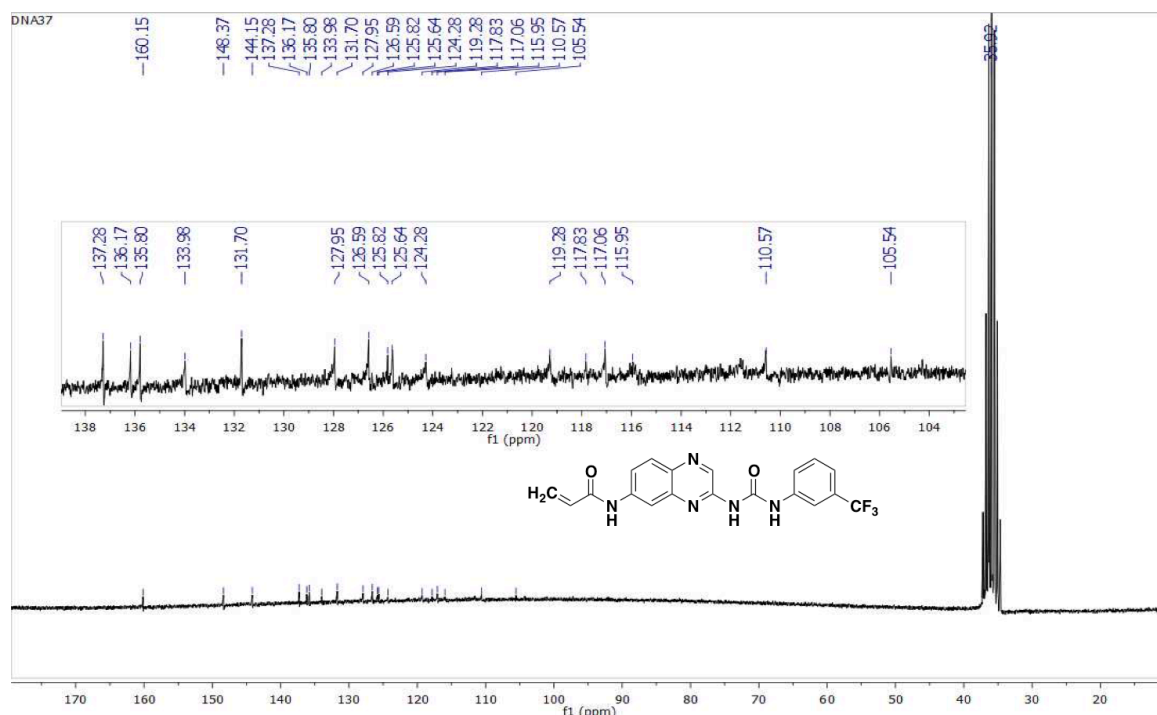


Figure S59. ¹H NMR spectrum of compound *N*-(3-(3-(3-(trifluoromethyl)phenyl)ureido) quinoxalin-6-yl)acrylamide (**7f**) (DMSO-d₆/200MHz/TMS)



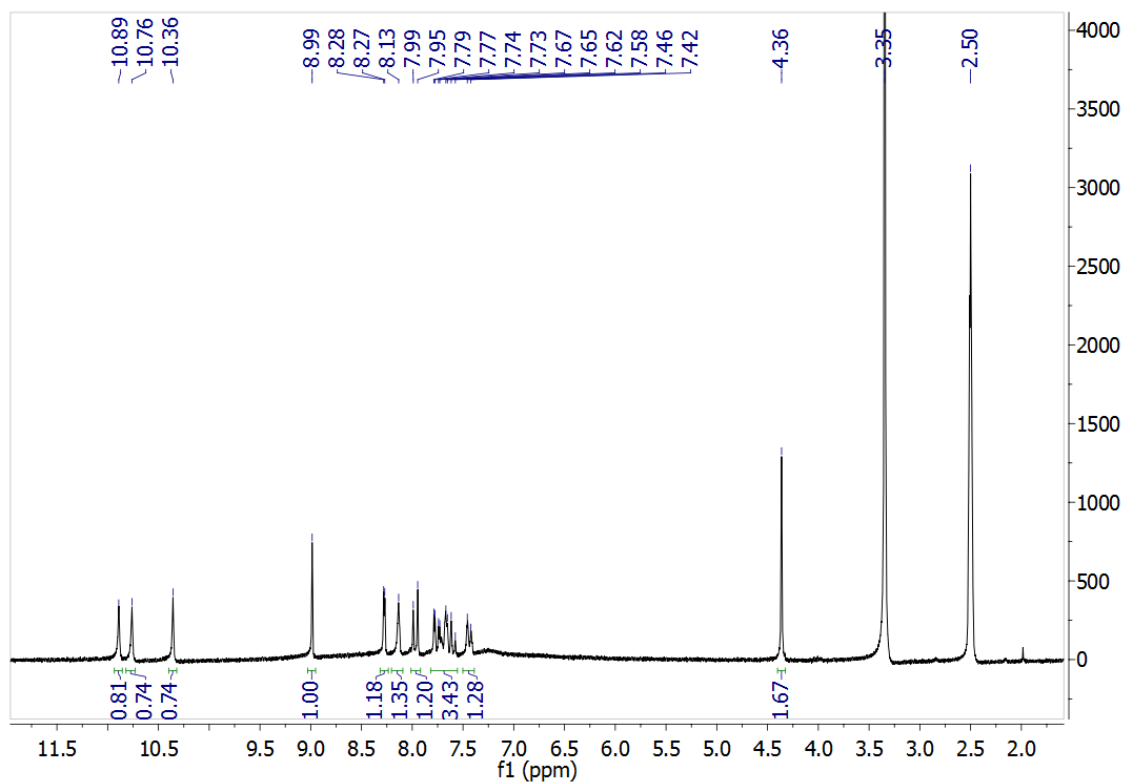


Figure S63. ^1H NMR spectrum of compound 2-chloro-*N*-(3-(3-(3-(trifluoromethyl) phenyl)ureido) quinoxalin-6-yl) acetamide (**7g**) (DMSO- d_6 /200MHz/TMS)

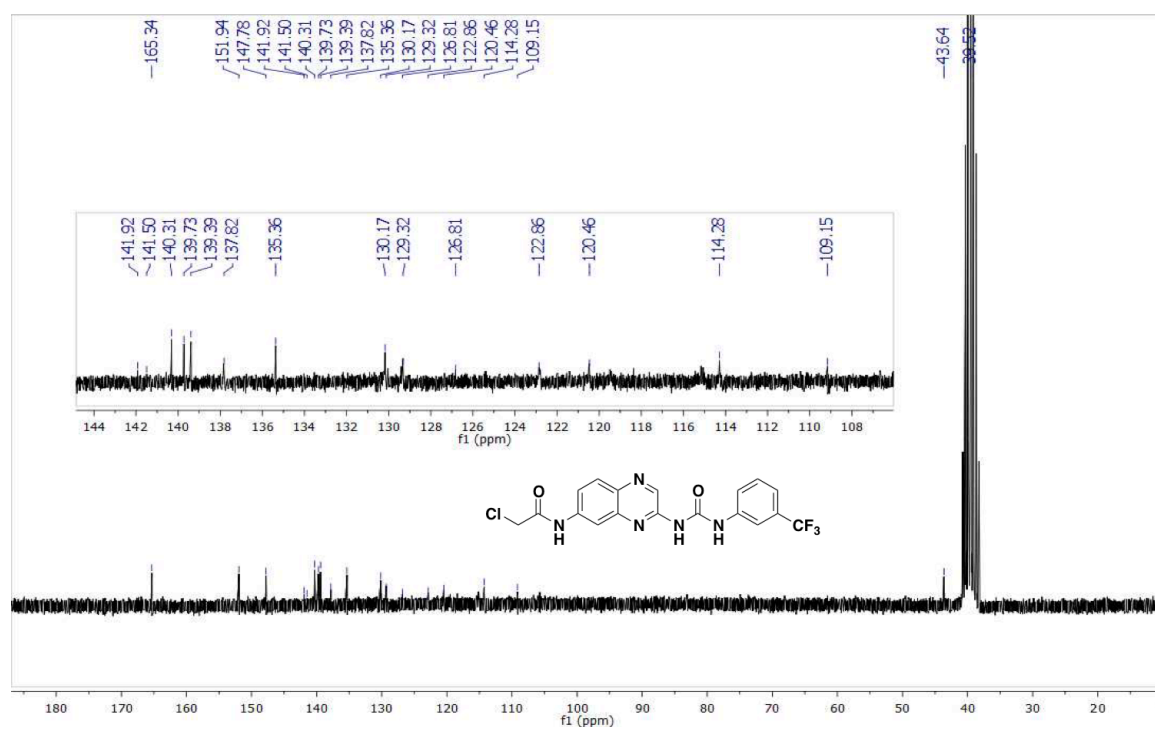


Figure S64. ^{13}C NMR spectrum of compound 2-chloro-*N*-(3-(3-(3-(trifluoromethyl)phenyl) ureido) quinoxalin-6-yl) acetamide (**7g**) (DMSO- d_6 /50MHz/TMS)

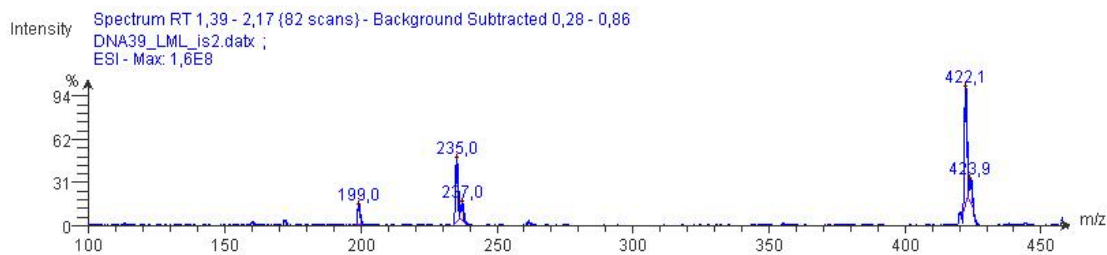


Figure S65. Mass spectrometry of compound 2-chloro-*N*-(3-(3-(3-(trifluoromethyl)phenyl) ureido) quinoxalin-6-yl) acetamide (**7g**) in negative mode (ESI-).



Figure S66. Infra red spectrum (ATR-FTIR) do 2-chloro-*N*-(3-(3-(3-(trifluoromethyl)phenyl) ureido) quinoxalin-6-yl) acetamide (**7g**) (bands in cm⁻¹).

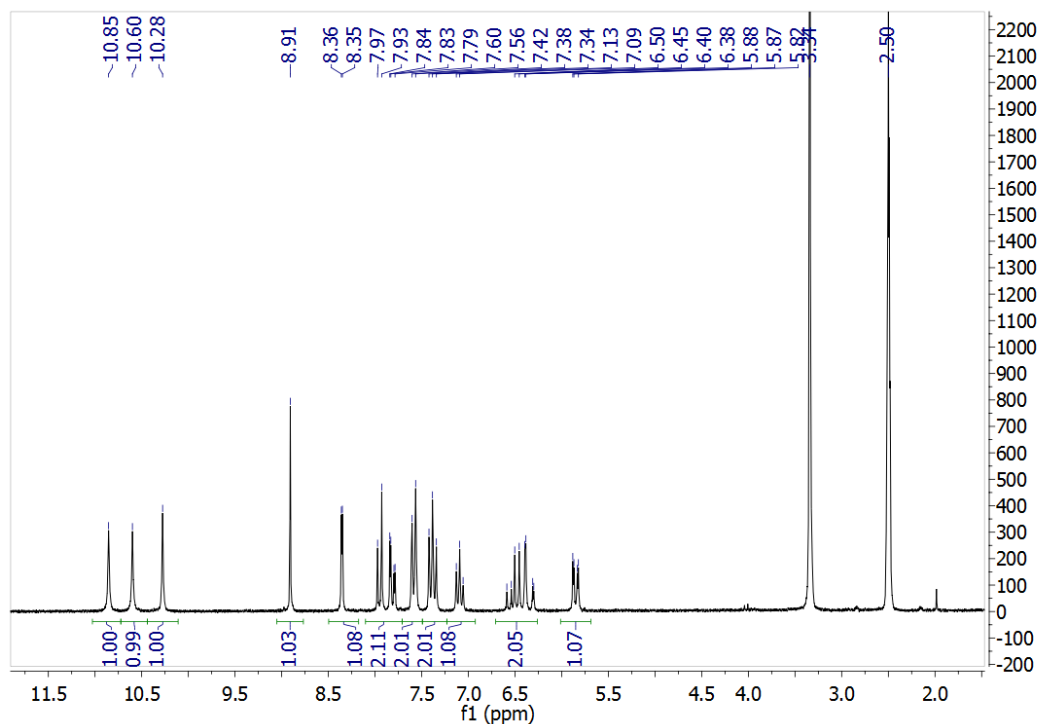


Figure S67. ¹H NMR spectrum of compound *N*-(3-(3-phenylureido)quinoxalin-6-yl)acrylamide (**7h**) (DMSO-*d*₆/200MHz/TMS)

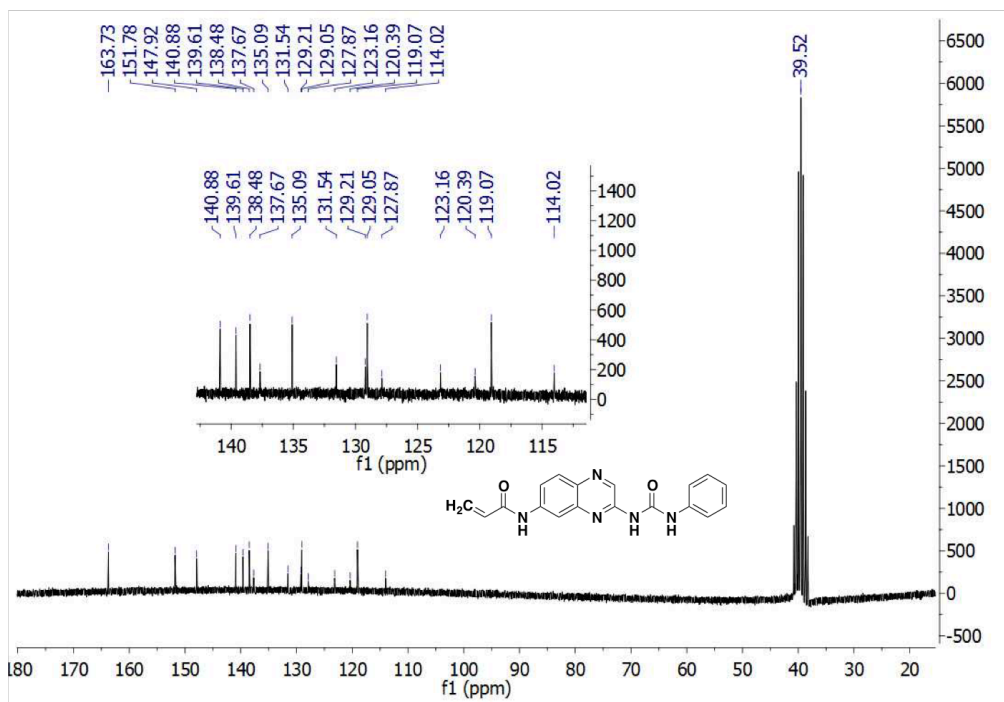


Figure S68. ¹³C NMR spectrum of compound *N*-(3-(3-phenylureido)quinoxalin-6-yl)acrylamide (**7h**) (DMSO-d₆/50MHz/TMS)

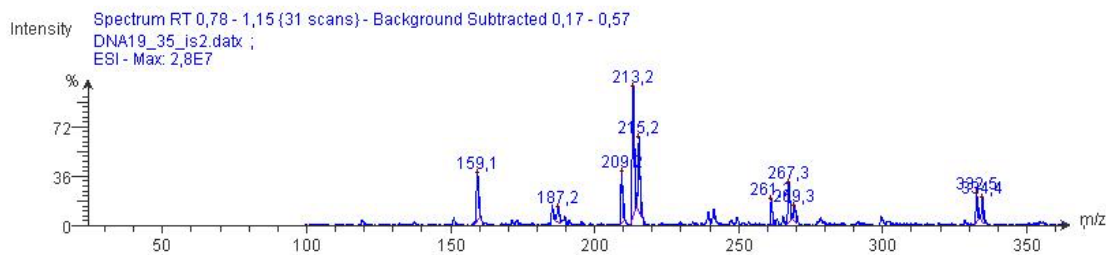


Figure S69. Mass spectrometry of compound *N*-(3-(3-phenylureido)quinoxalin-6-yl)acrylamide (**7h**) in negative mode (ESI-).

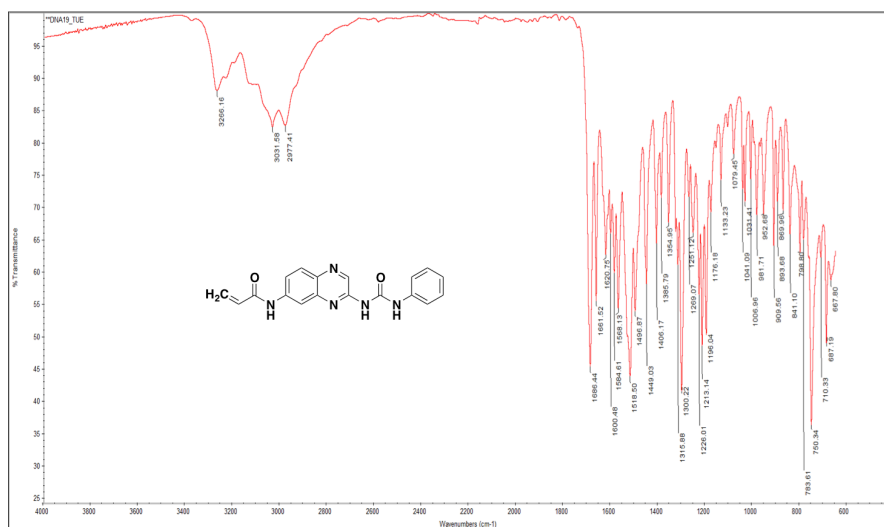


Figure S70. Infra red spectrum (ATR-FTIR) of compound *N*-(3-(3-phenylureido)quinoxalin-6-yl)acrylamide (**7h**) (bands in cm⁻¹).

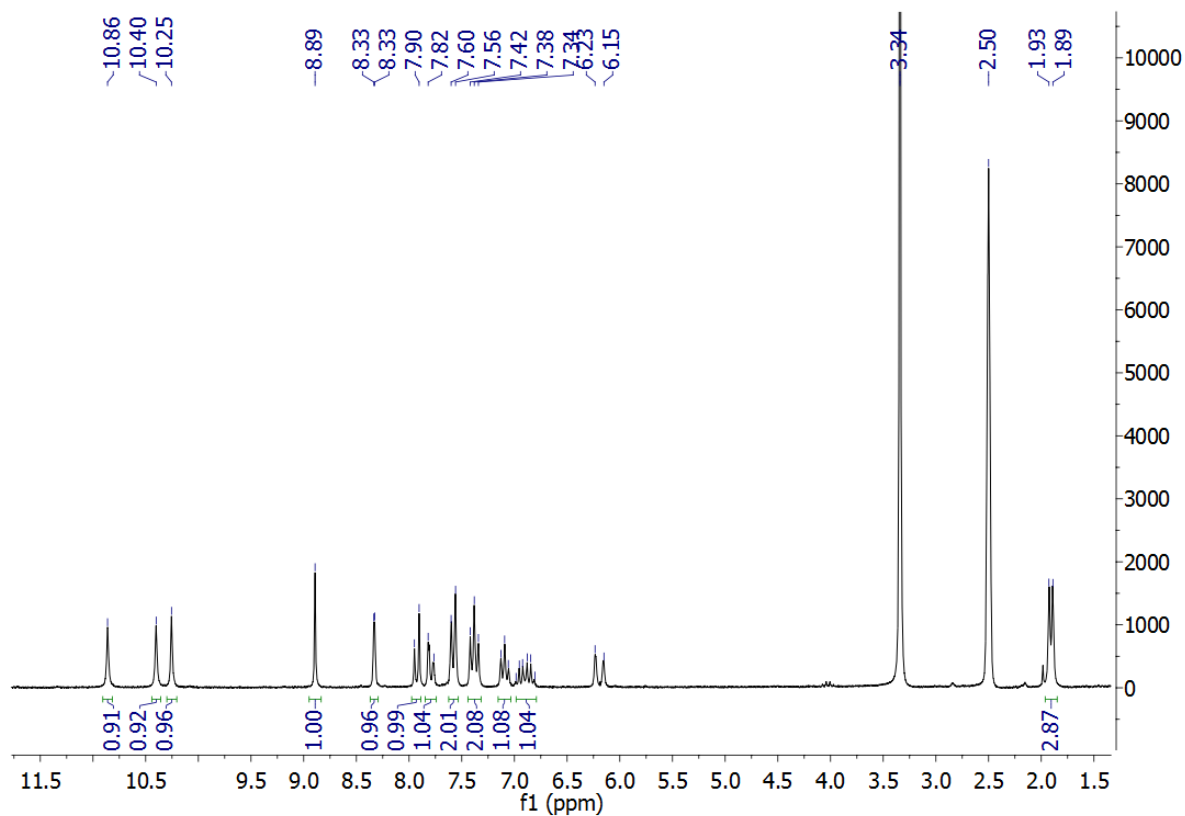


Figure S71. ^1H NMR spectrum of compound 1(*E*)-*N*-(3-(3-phenylureido)quinoxalin-6-yl)but-2-enamide (**7i**) (DMSO- d_6 /200MHz/TMS)

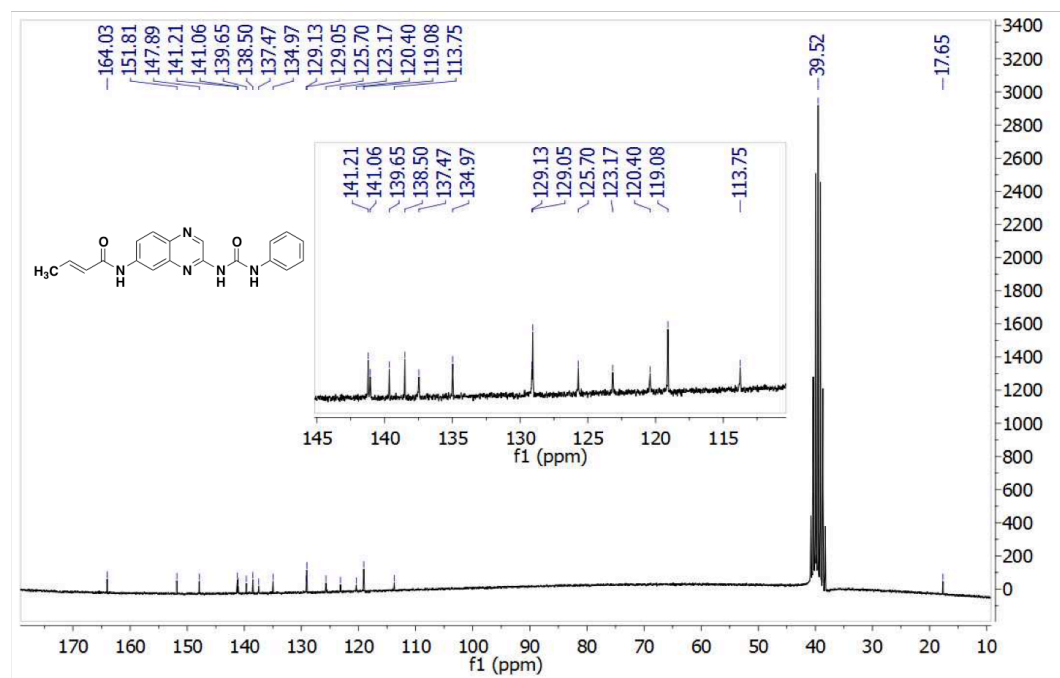


Figure S72. ^{13}C NMR spectrum of compound (*E*)-*N*-(3-(3-phenylureido)quinoxalin-6-yl)but-2-enamide (**7i**) (DMSO- d_6 /50MHz/TMS)

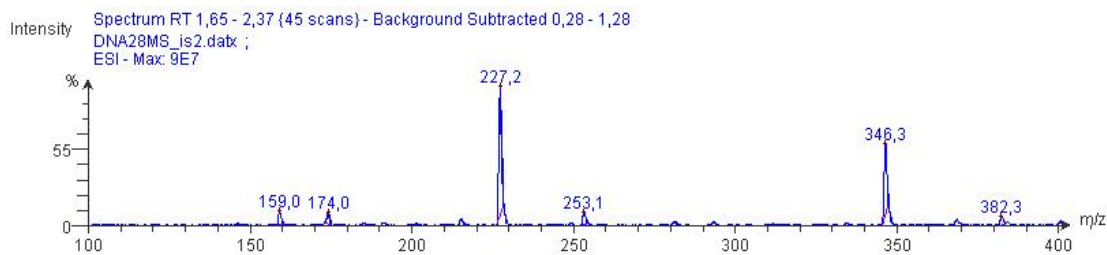


Figure S73. Mass spectrometry of compound (*E*)-*N*-(3-(3-phenylureido)quinoxalin-6-yl)but-2-enamide (**7i**) in negative mode (ESI-).

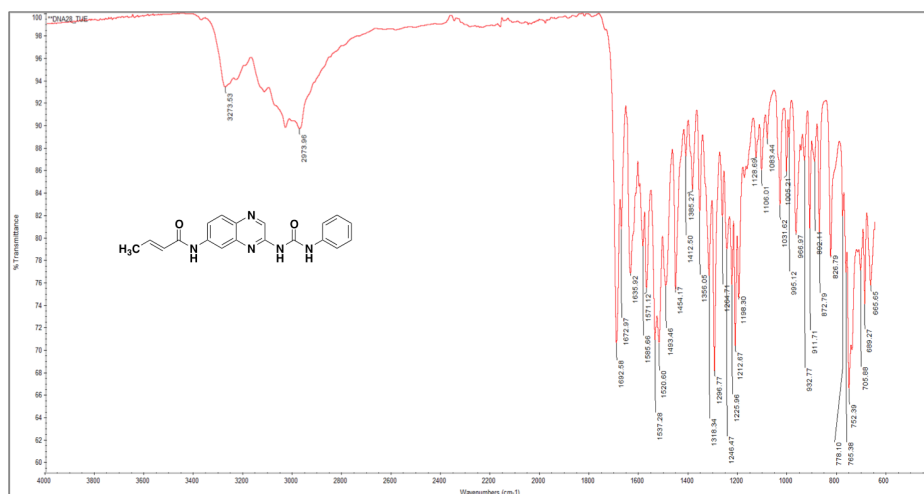


Figure S74. Infra red spectrum (ATR-FTIR) of compound (*E*)-*N*-(3-(3-phenylureido)quinoxalin-6-yl)but-2-enamide (**7i**) (bands in cm⁻¹).

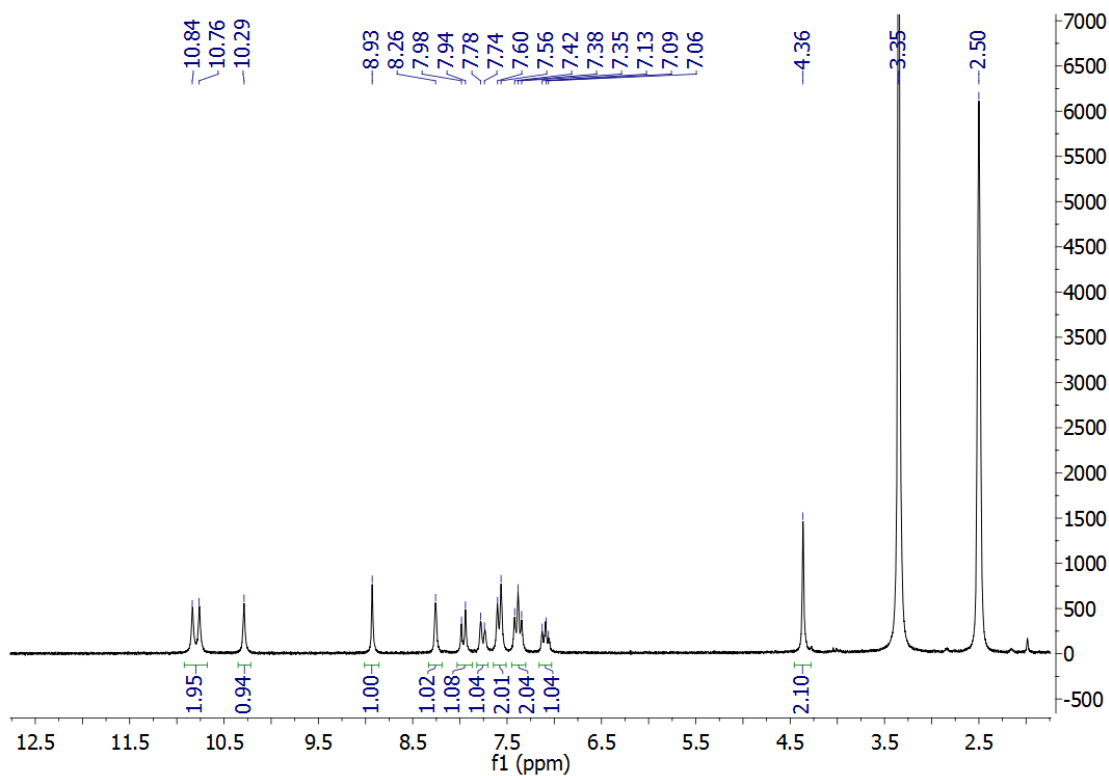


Figure S75. ¹H NMR spectrum of compound 2-chloro-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7j**) DMSO-d₆/200MHz/TMS)

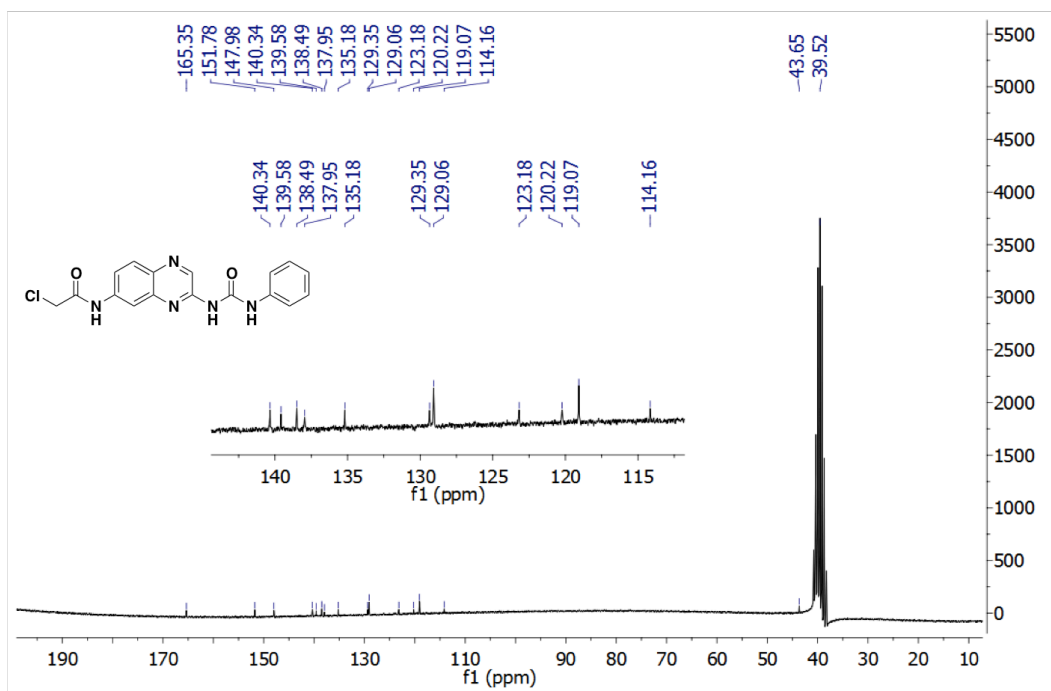


Figure S76. ¹³C NMR spectrum of 2-chloro-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7j**) (DMSO-d₆/50MHz/TMS)

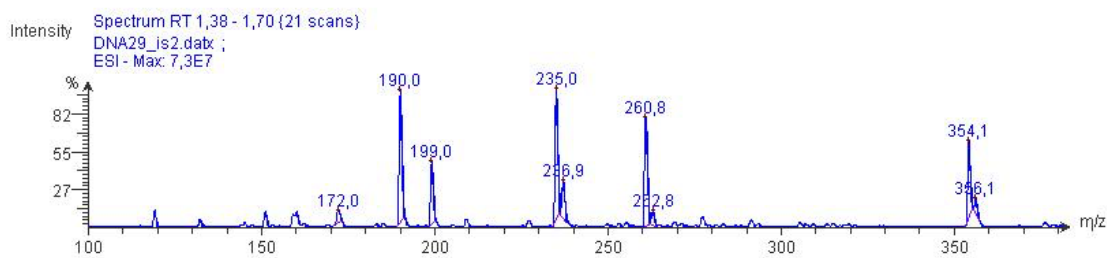


Figure S77. Mass spectrometry of compound 2-chloro-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7j**) in negative mode (ESI).



Figure S78. Infra red spectrum (ATR-FTIR) of compound 2-chloro-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7j**) (bands in cm⁻¹).

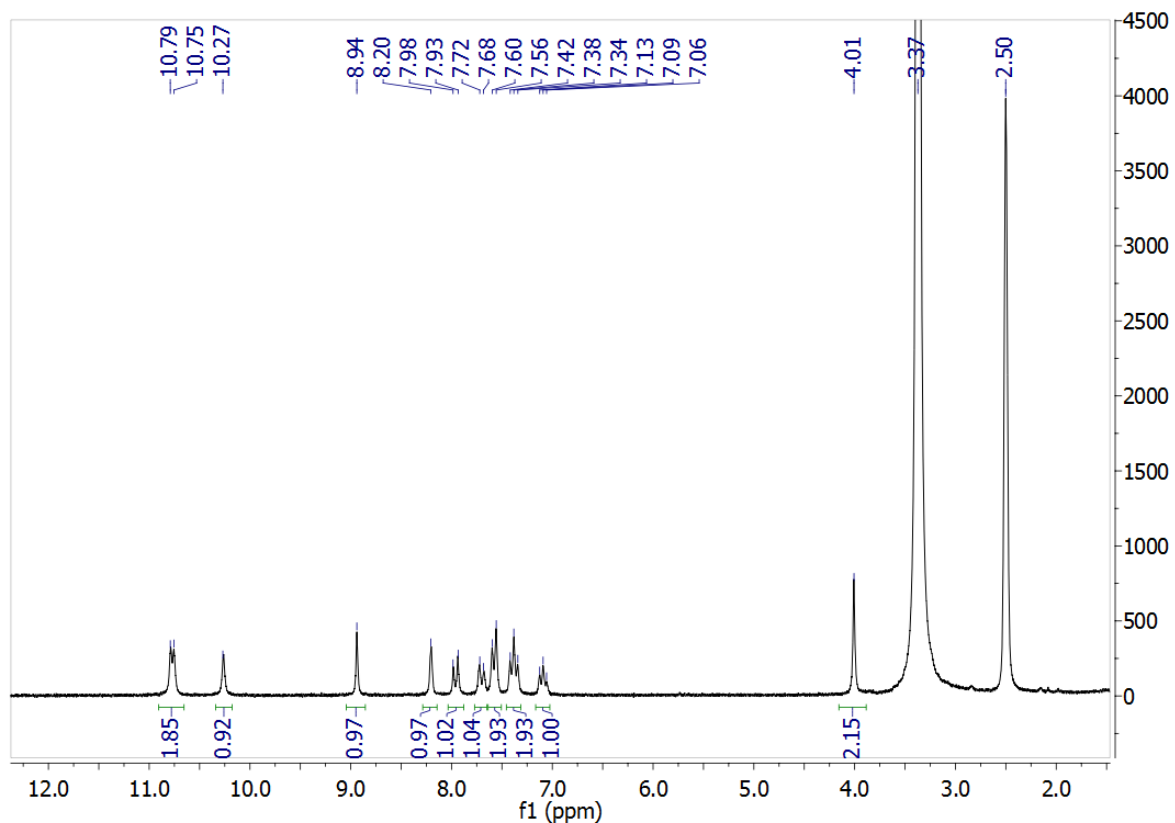


Figure S79. ^1H NMR spectrum of compound 2-ciano-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7k**) (DMSO- d_6 /200MHz/TMS)

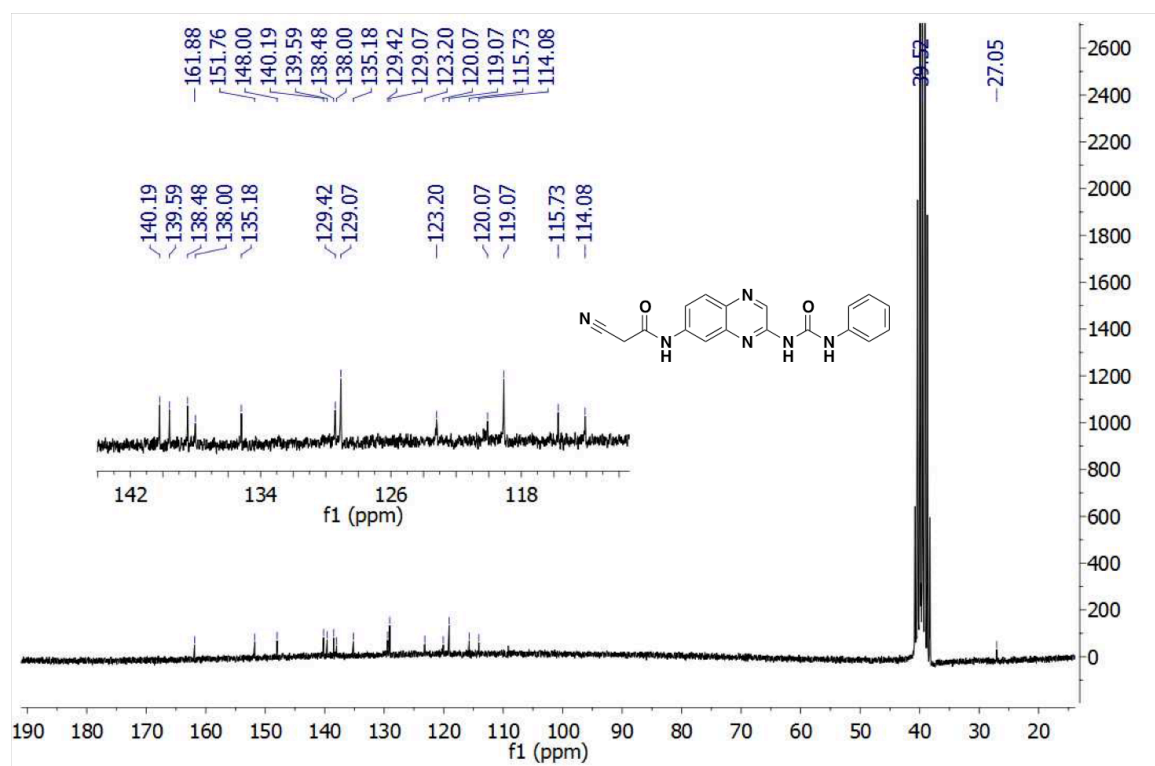


Figure S80. ^{13}C NMR spectrum of compound 2-ciano-*N*-(3-(3-phenylureido)quinoxalin-6-yl)acetamide (**7k**) (DMSO- d_6 /50MHz/TMS)

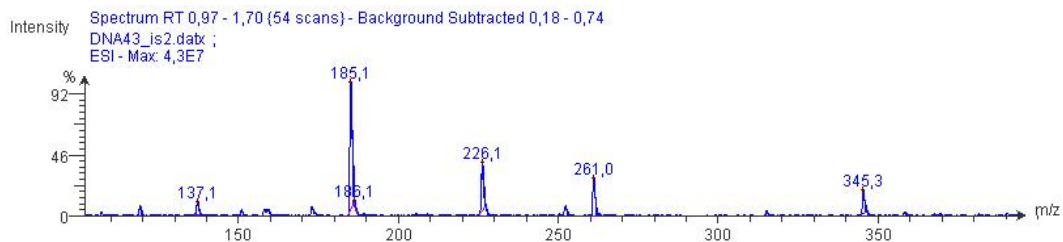


Figure S81. Mass spectrometry of compound 2-ciano-*N*-(3-(3-phenylureido)quinoxalin-6-yl) acetamide (**7k**) in negative mode (ESI-).

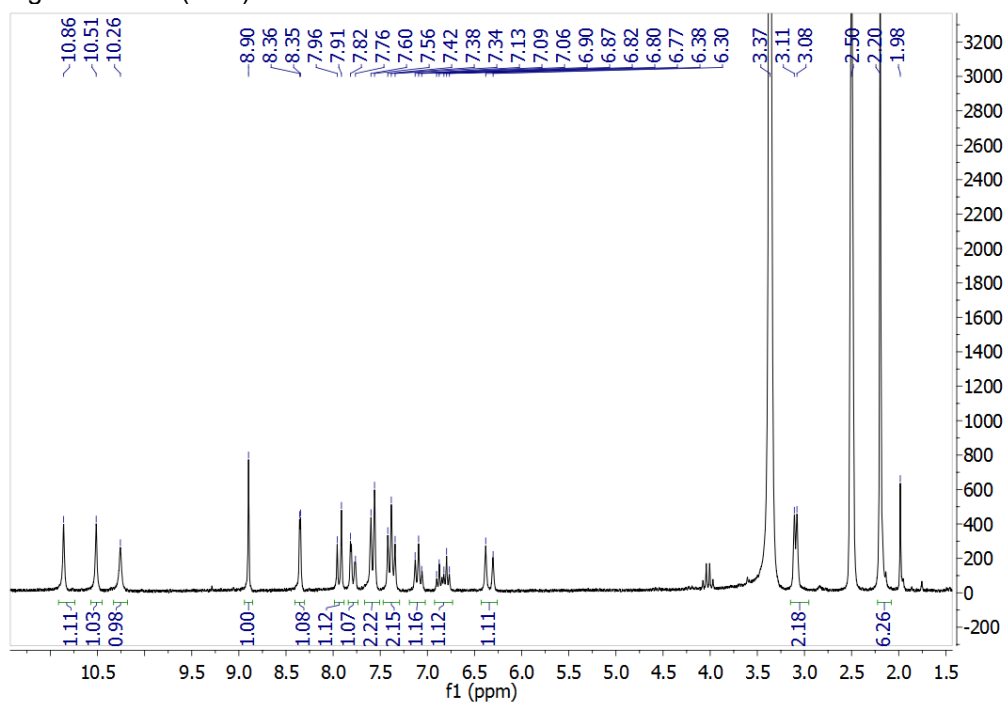


Figure S82. ^1H NMR spectrum of compound (*E*)-4-(dimethylamino)-*N*-(3-(3-phenylureido) quinoxalin-6-yl)but-2-enamide (**7l**) (DMSO- d_6 /200MHz/TMS)

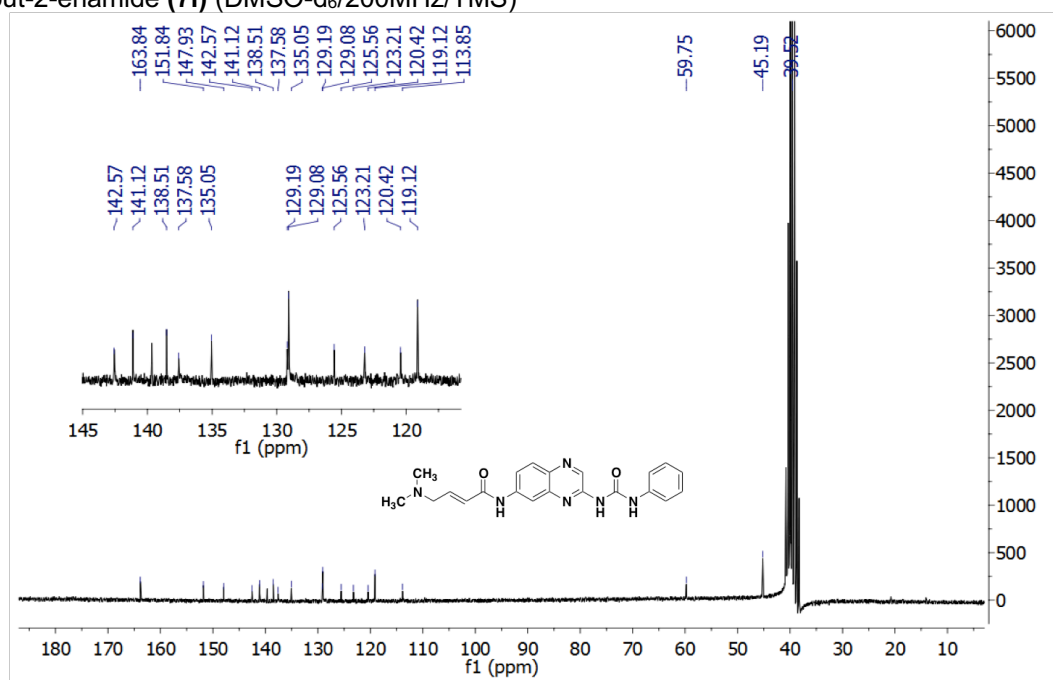


Figure S83. ^{13}C NMR spectrum of compound (*E*)-4-(dimethylamino)-*N*-(3-(3-phenylureido) quinoxalin-6-yl)but-2-enamide (**7l**) (DMSO- d_6 /50MHz/TMS)

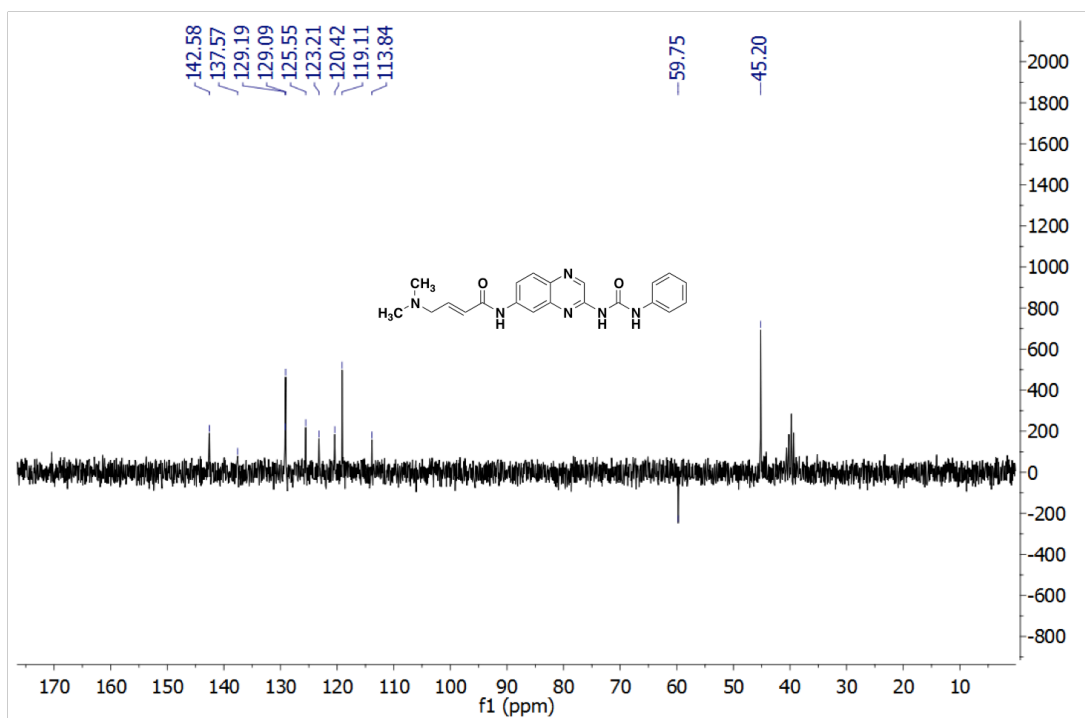


Figure S84. Espectro de DEPT 135 of compound *E*-4-(dimethylamino)-*N*-(3-(3-phenylureido)quinoxalin-6-yl)but-2-enamide (**7I**) (DMSO- d_6 /50MHz/TMS).

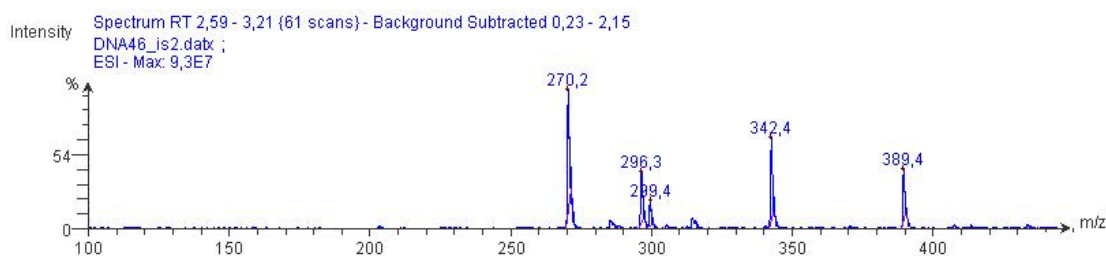


Figure S85. Mass spectrometry of compound *E*-4-(dimethylamino)-*N*-(3-(3-phenylureido) quinoxalin-6-yl)but-2-enamide (**7I**) in negative mode (ESI-).

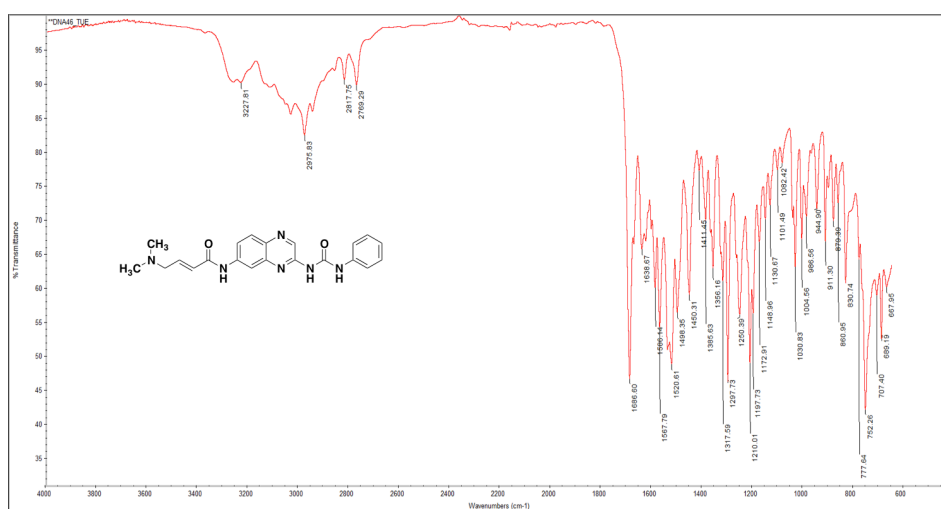


Figure S86. Infra red spectrum (ATR-FTIR) of compound *E*-4-(dimethylamino)-*N*-(3-(3-phenylureido) quinoxalin-6-yl)but-2-enamide (**7I**) (bands in cm⁻¹).

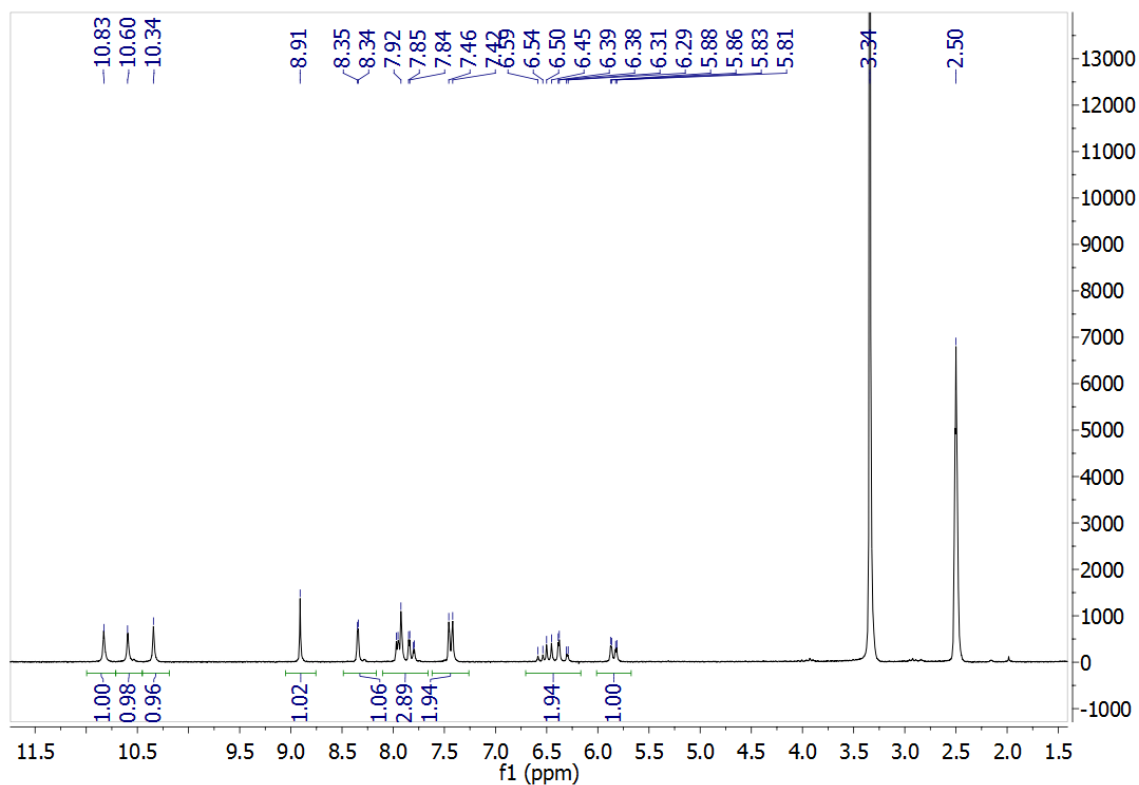


Figure S87. ^1H NMR spectrum of compound *N*-(3-(3-(3-chloro-4-fluorophenyl) ureido)quinoxalin-6-yl) acrylamide (**7m**) (DMSO- d_6 /200MHz/TMS)

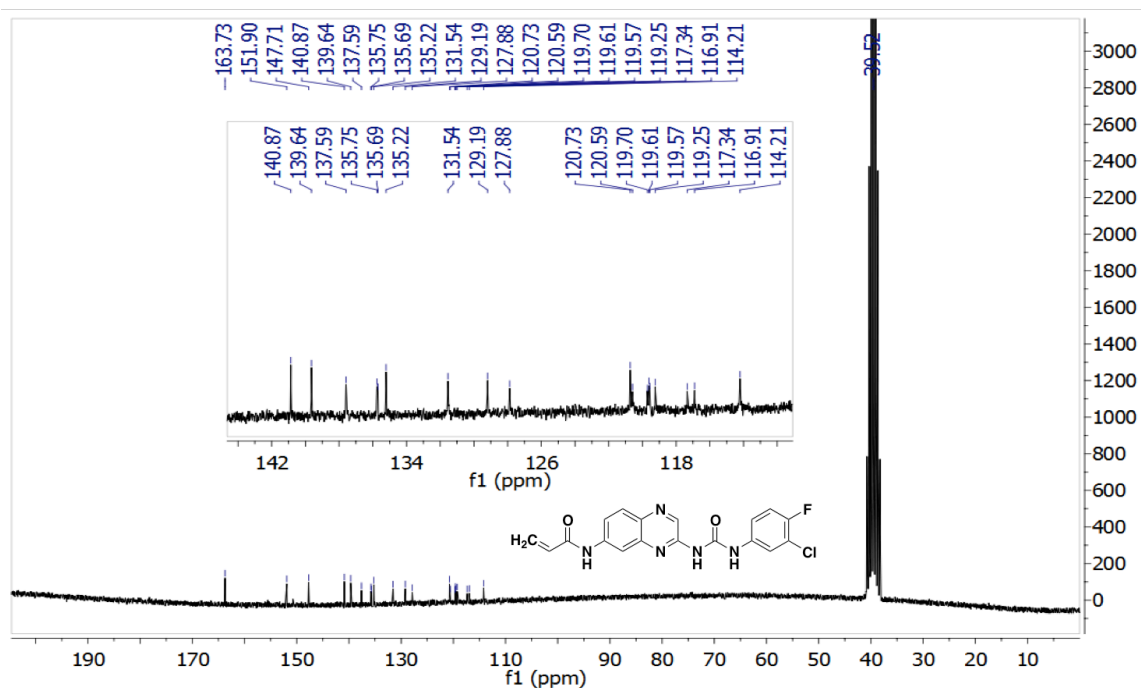


Figure S88. ^{13}C NMR spectrum of compound *N*-(3-(3-(3-chloro-4-fluorophenyl)ureido) quinoxalin-6-yl) acrylamide (**7m**) (DMSO- d_6 /50MHz/TMS)

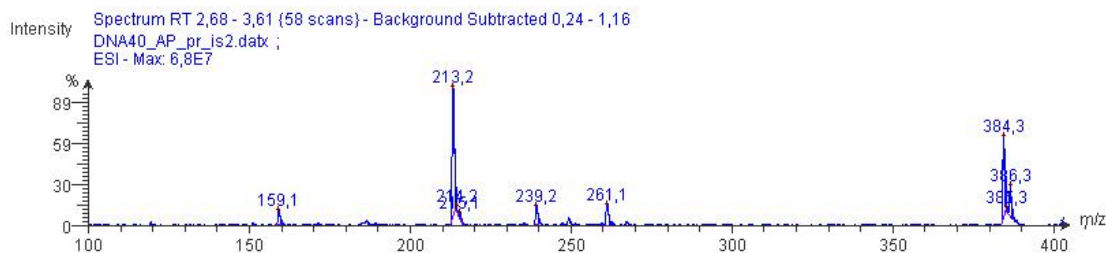


Figure S89. Mass spectrometry of compound *N*-(3-(3-(3-chloro-4-fluorophenyl)ureido) quinoxalin-6-yl) acrylamide (**7m**) in negative mode (ESI-).

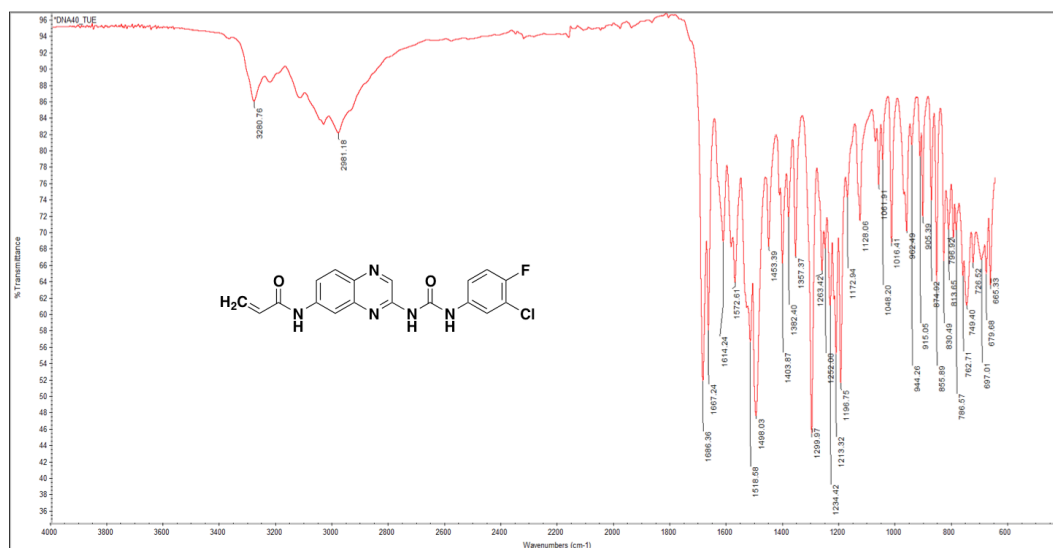


Figure S90. Infra red spectrum (ATR-FTIR) of compound *N*-(3-(3-(3-chloro-4-fluorophenyl)ureido)quinoxalin-6-yl) acrylamide (**7m**) (bands in cm^{-1}).

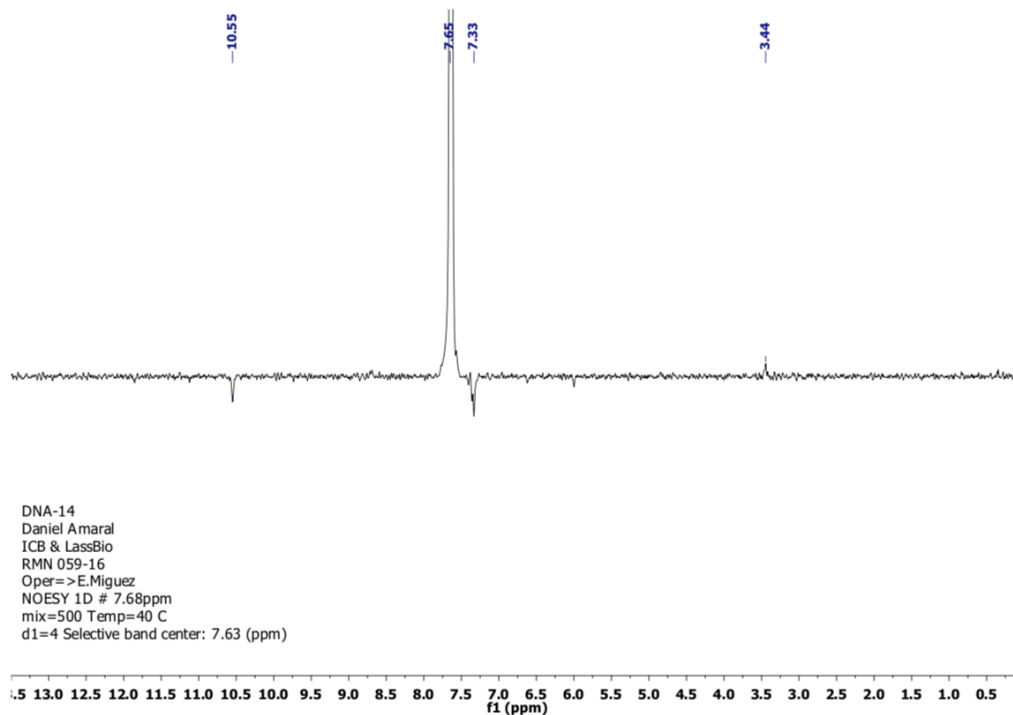


Figure S91. NOESY 1D spectrum of of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) with irradiation at 7.68 ppm (DMSO- d_6 /300MHz/TMS)

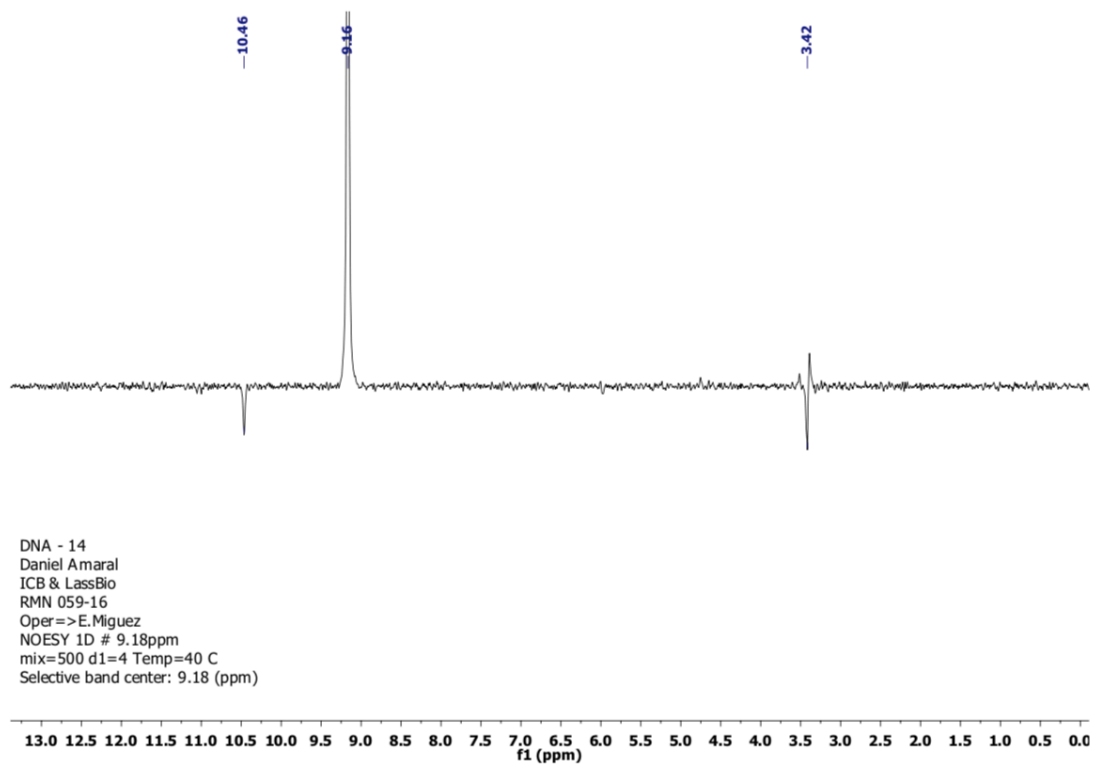


Figure S92. NOESY 1D spectrum of of compound 1-(7-nitroquinoxalin-2-yl)-3-phenylurea (**9c**) with irradiation at 9.18 ppm (DMSO-d₆/300MHz/TMS)

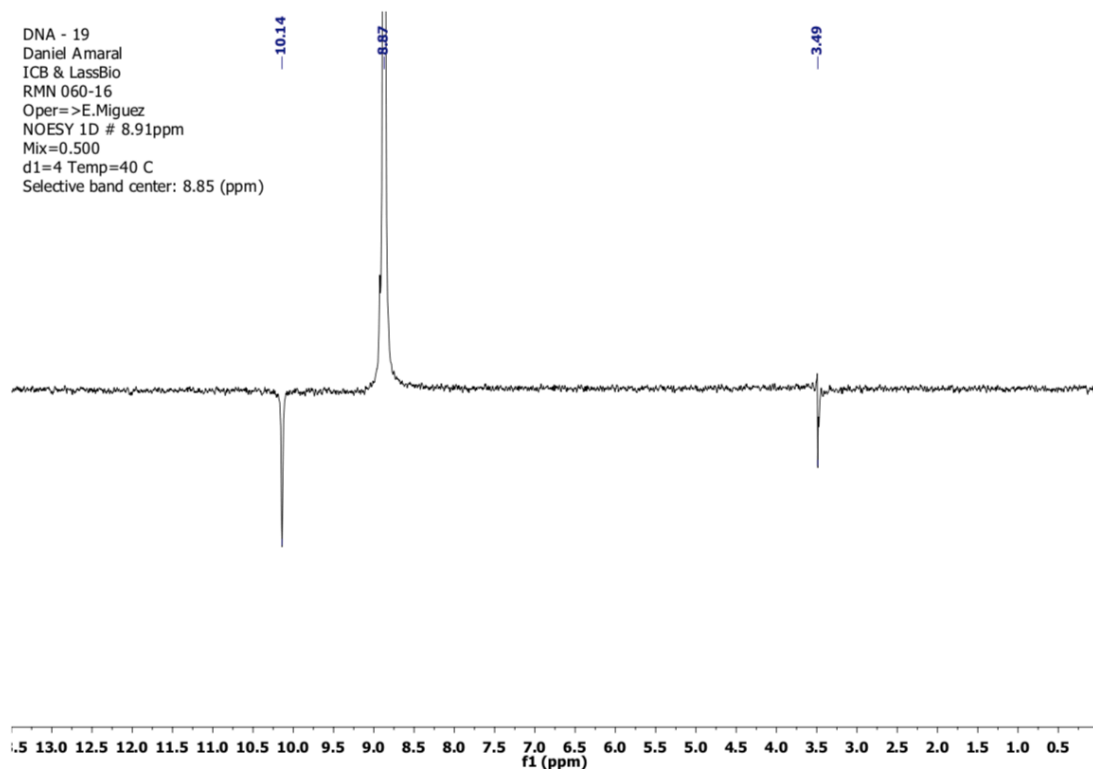


Figure S93. NOESY 1D spectrum of compound N-(3-(3-phenylureido)quinoxalin-6-yl) acrylamide (**7h**) with irradiation at 8.91 ppm (DMSO-d₆/300MHz/TMS)

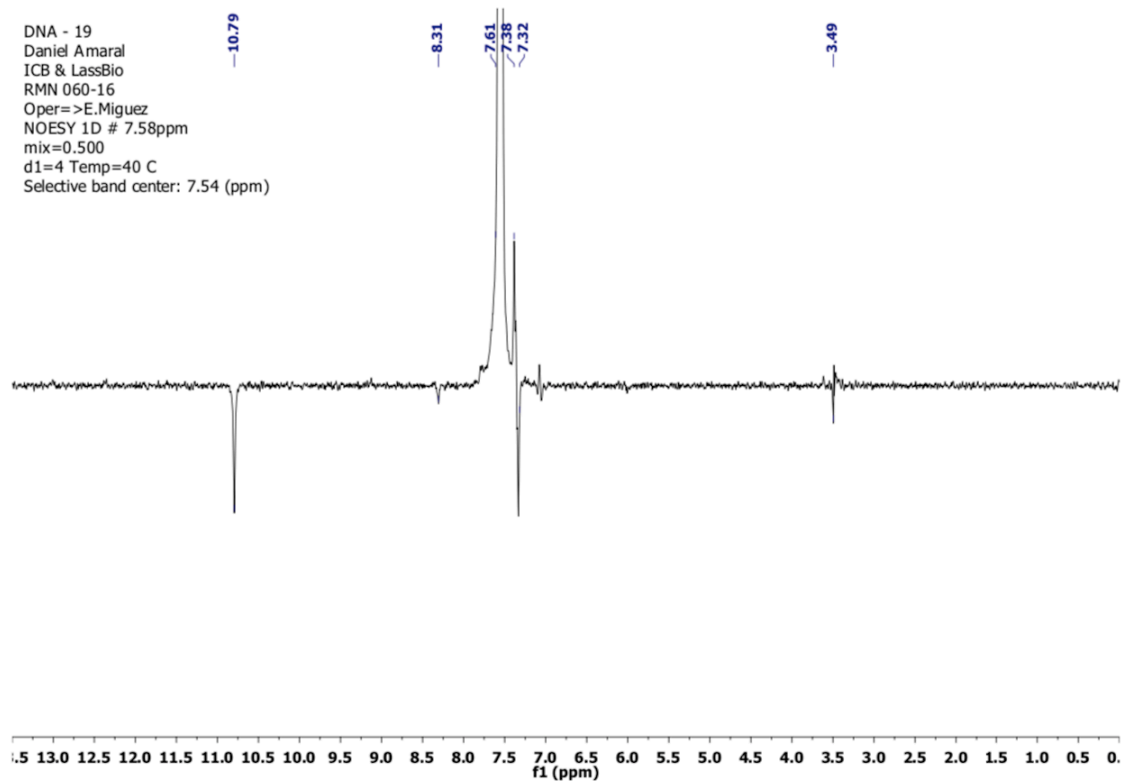


Figure S94. NOESY 1D spectrum of compound *N*-(3-(3-phenylureido)quinoxalin-6-yl) acrylamide (**7h**) with irradiation at 7.58 ppm (DMSO- d_6 /300MHz/TMS)