Supplementary material

Green Synthesis, In Silico Modeling, and Biological Evaluation of N-substituted (Z)-5-Arylidene imidazolidine /thiazolidine-2,4-dione/4-thione Derivatives Catalyzed by Bu SO_3H Core–Shell Nanostructures

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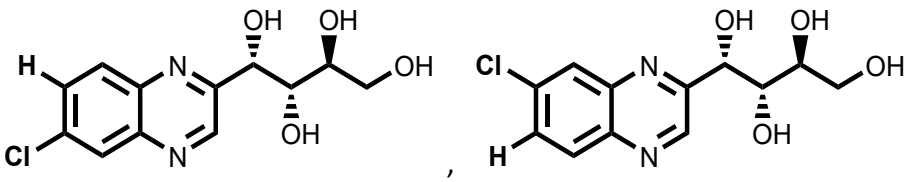
Section 1: The analytical and spectroscopic data for the intermediate compound.



Yield: 85%: mp: 183-187 ºC

$C_{12}H_{13}ClN_2O_4$, MW: 284.70

IR (KBr, cm^{-1}) ν_{max}: 1042.95, 1094.38 (C-OH str.), 3310.2 (O-H str), 2910.8 (C-H str)

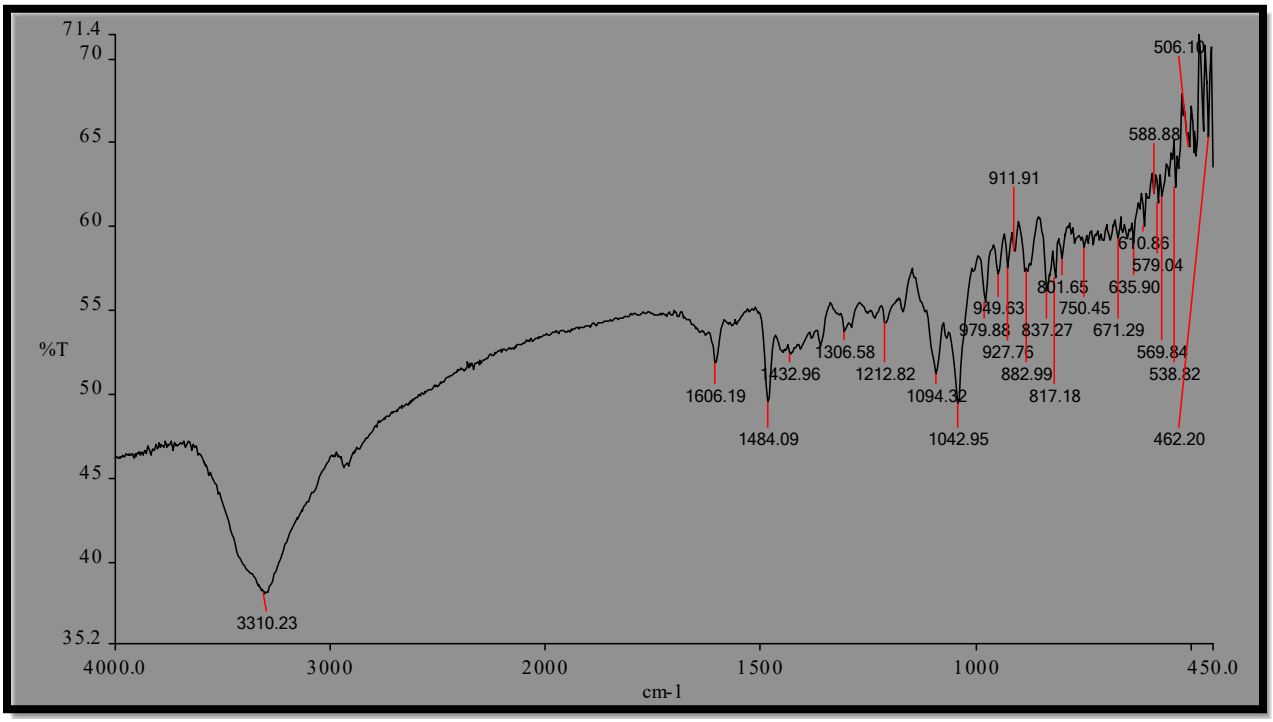


Fig S1. (FT-IR). (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol

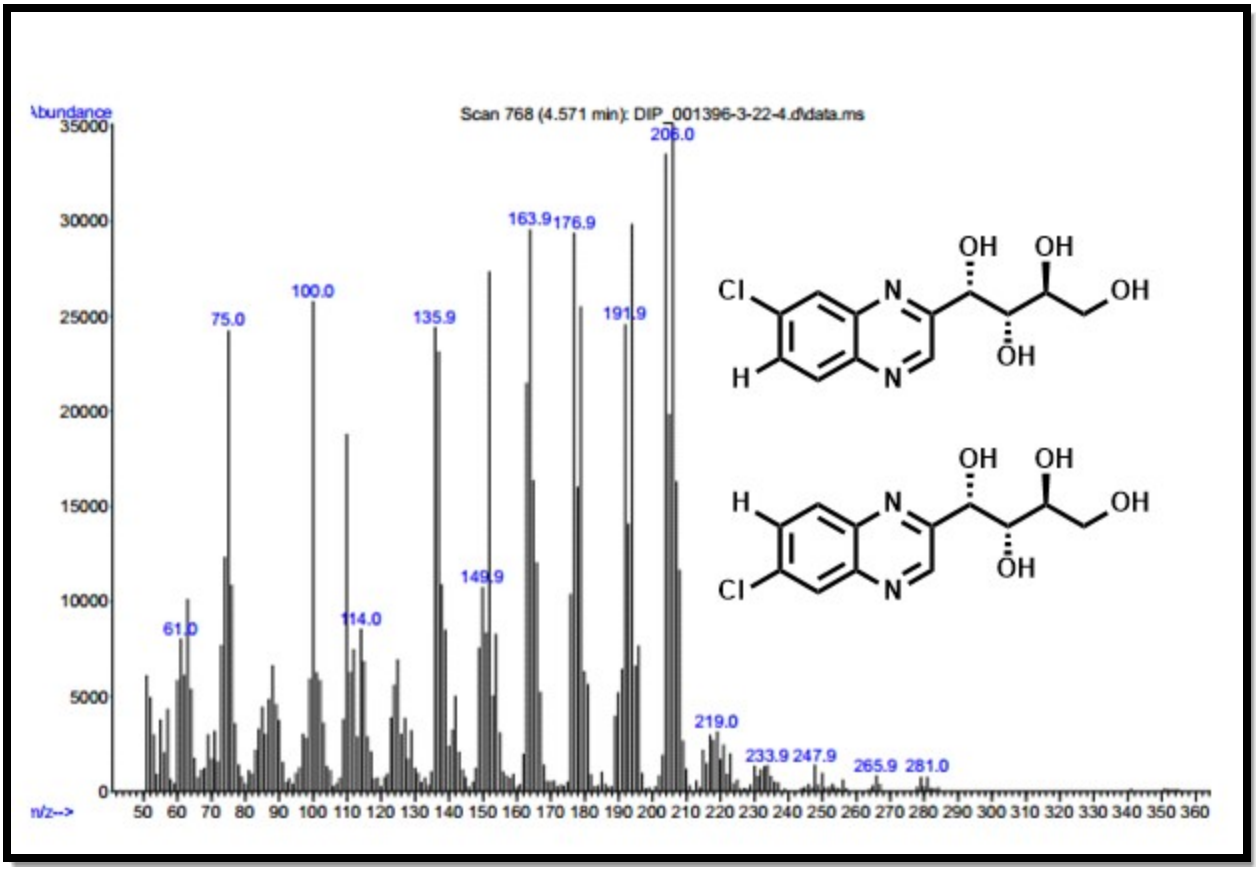


Fig S2. Mass Spectra. (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol

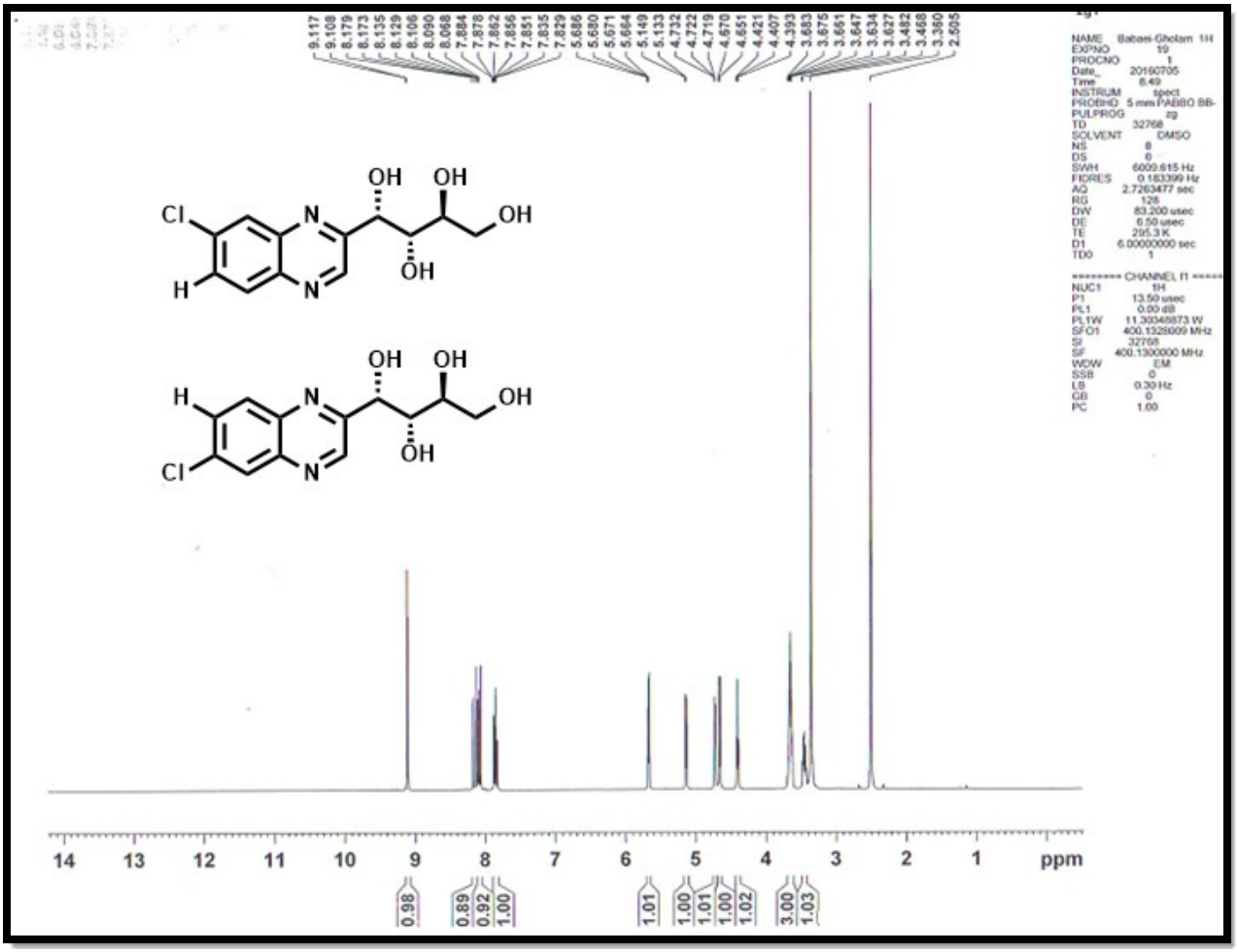


Fig S3. ^{1}HNMR spectra. (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol

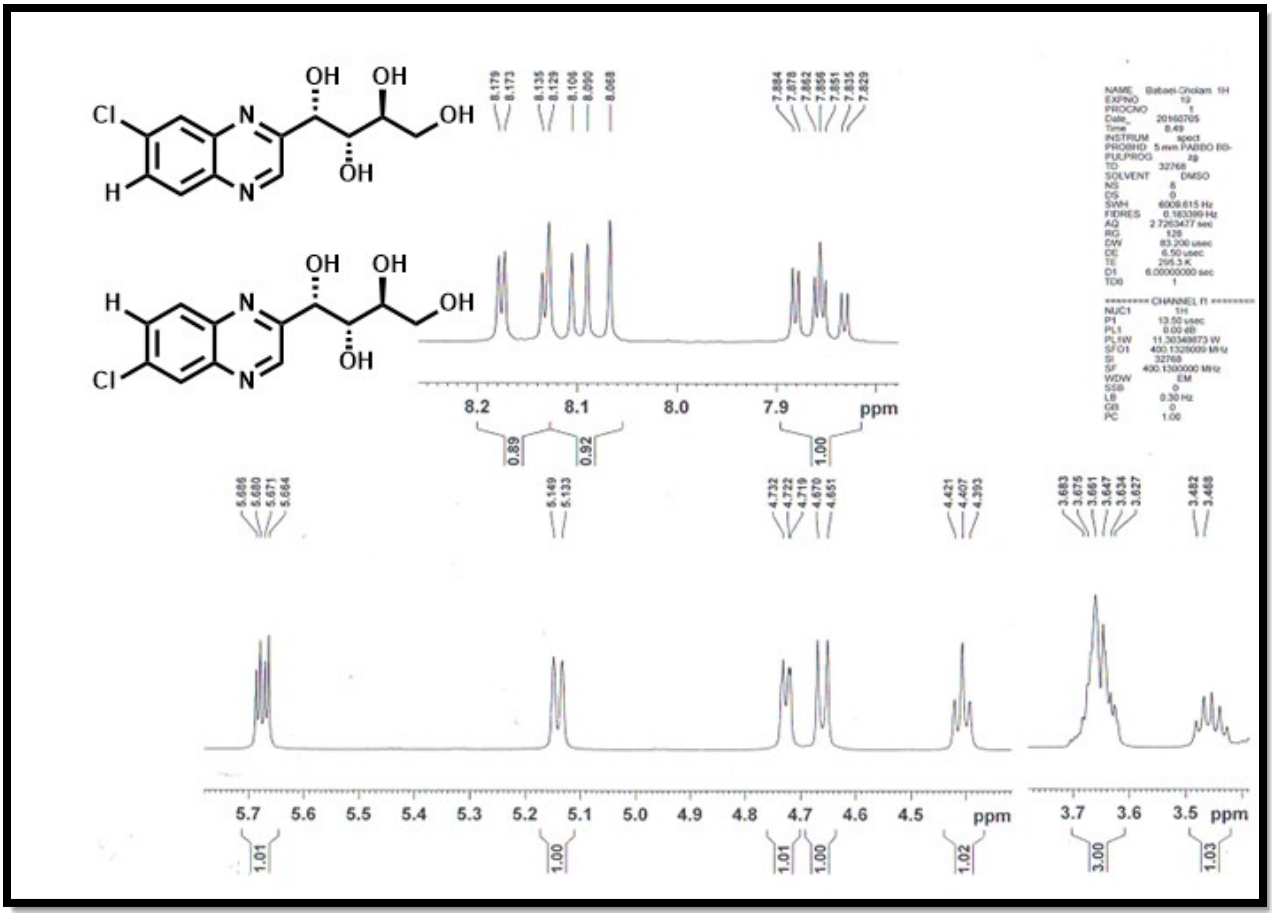


Fig S4. [1]HNMR expand spectra. (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol

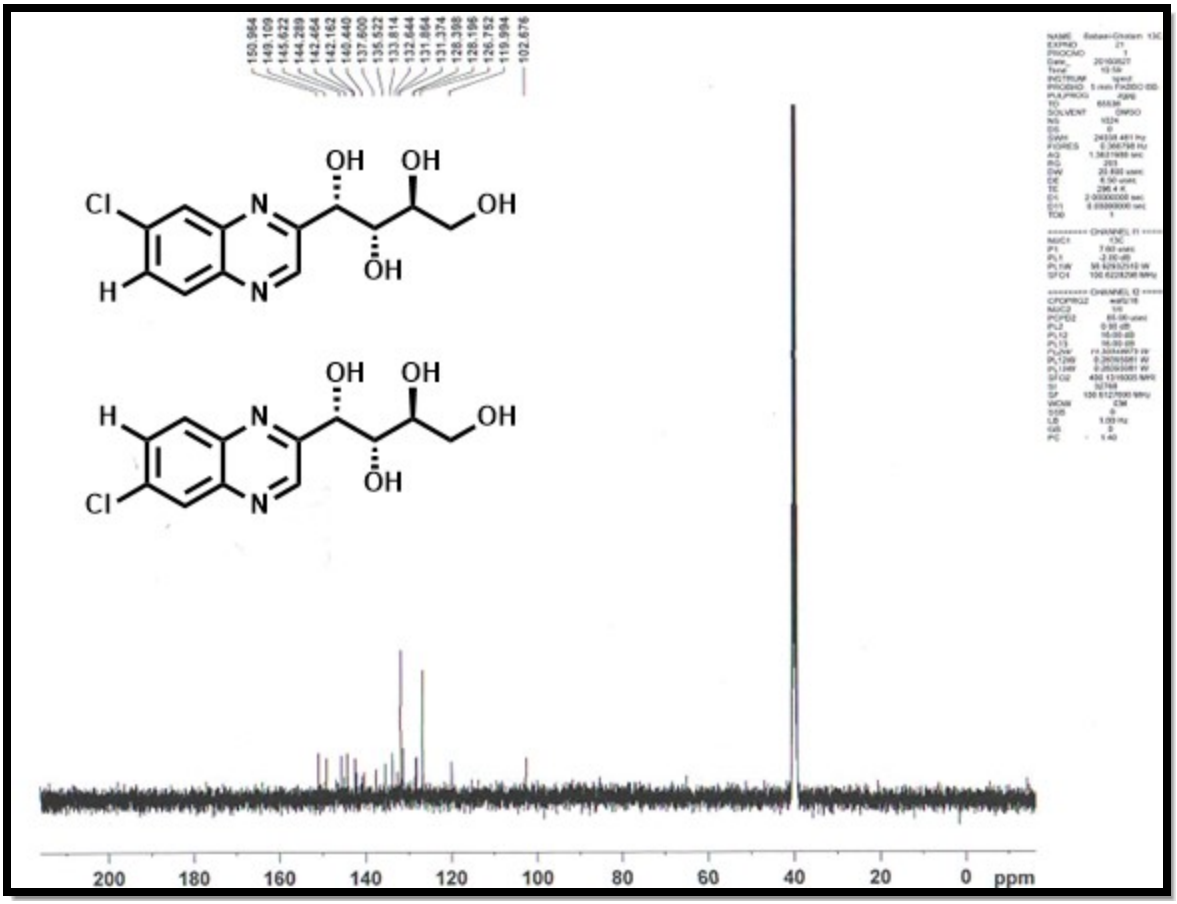


Fig S5. ^{13}CNMR spectra. (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol

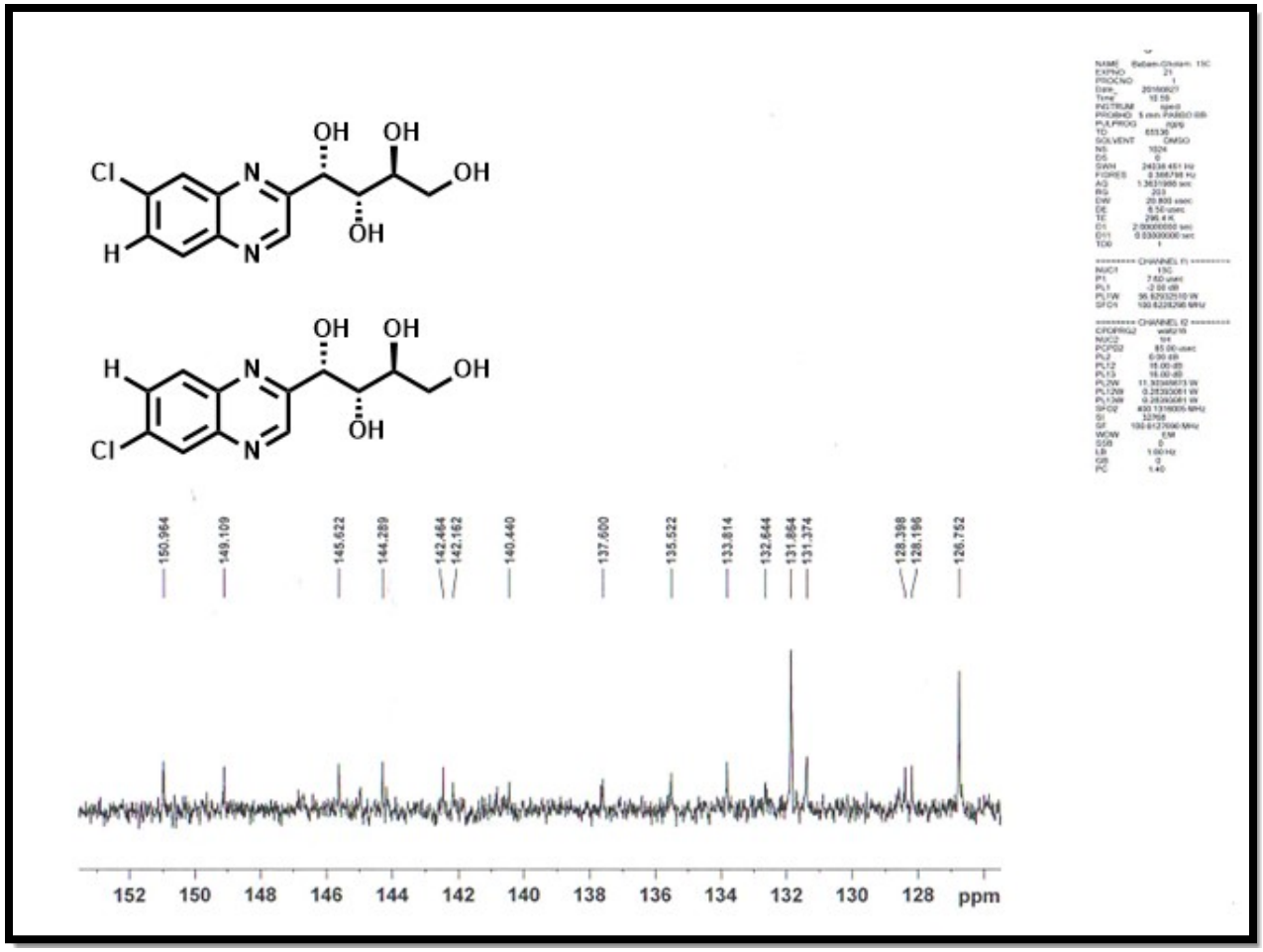
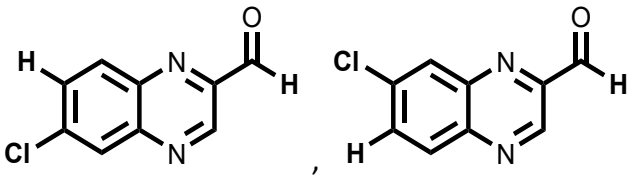


Fig S6. ^{13}CNMR expand spectra. (6-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol و (7-chloroquinoxalin-2-yl) butane-1, 2, 3, 4-tetraol.

6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde



Yield: 86%: mp: 175-183 ºC

$C_9H_5ClN_2O$, MW: 192.60

IR (KBr, cm^{-1}) ν_{max}: 1713.83 (C=O STR.).

^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.17 (s, 2H, H Aldehyde), 9.38 (s, 1H, 3-H Quinoxaline (compound 4)), 8.41 (d, 1H, J = 2.4 Hz, 8-H Quinoxaline (compound 4)), 8.34 (d, 1H, J = 2.4 Hz, 5-H Quinoxaline), 8.32 (d, 1H, J = 8.8 Hz, 5-H Quinoxaline (compound 4)), 8.25 (d, 1H, J = 8.8 Hz, 8-H Quinoxaline), 8.08 (dd, 1H, J = 8.8 and J = 2.4, 6-H Quinoxaline), 8.05 (dd, 1H, J = 8.8 and J = 2.4, 7-H Quinoxaline).

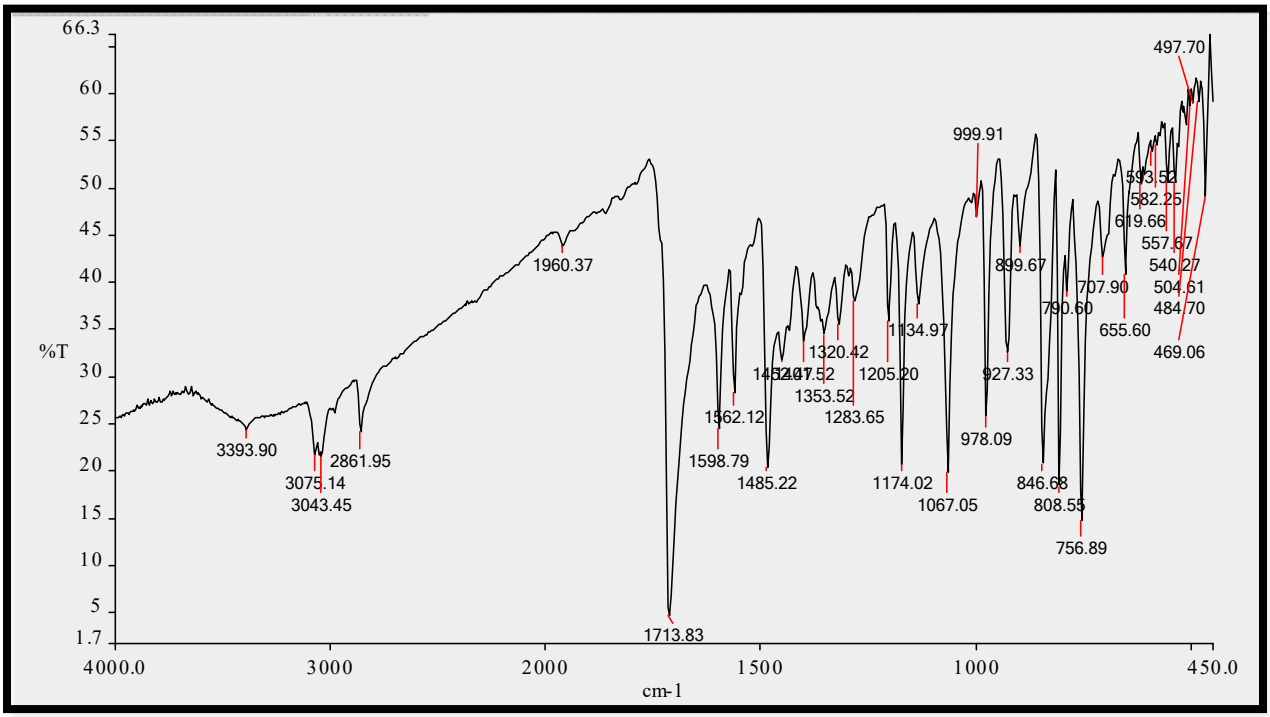


Fig S7. (FT-IR). 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde

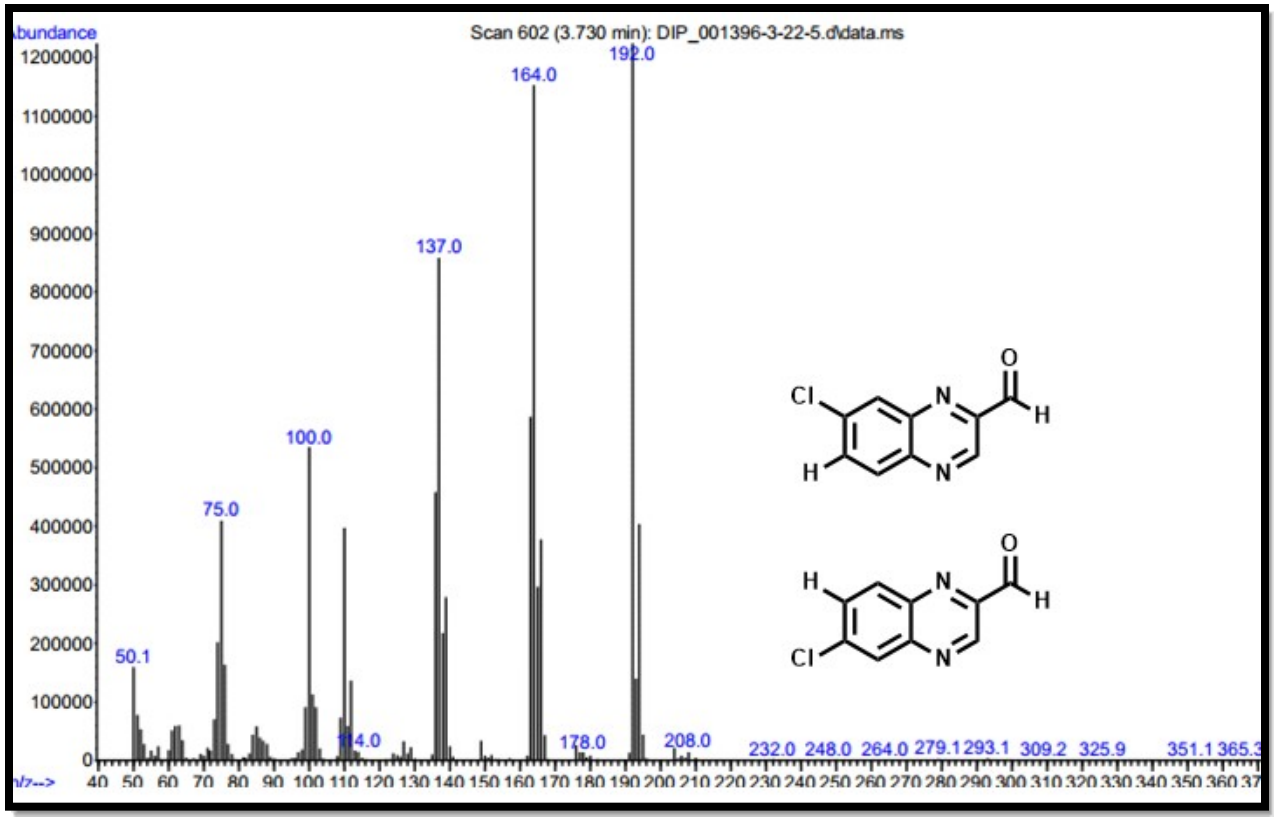


Fig S8. Mass Spectra. 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde

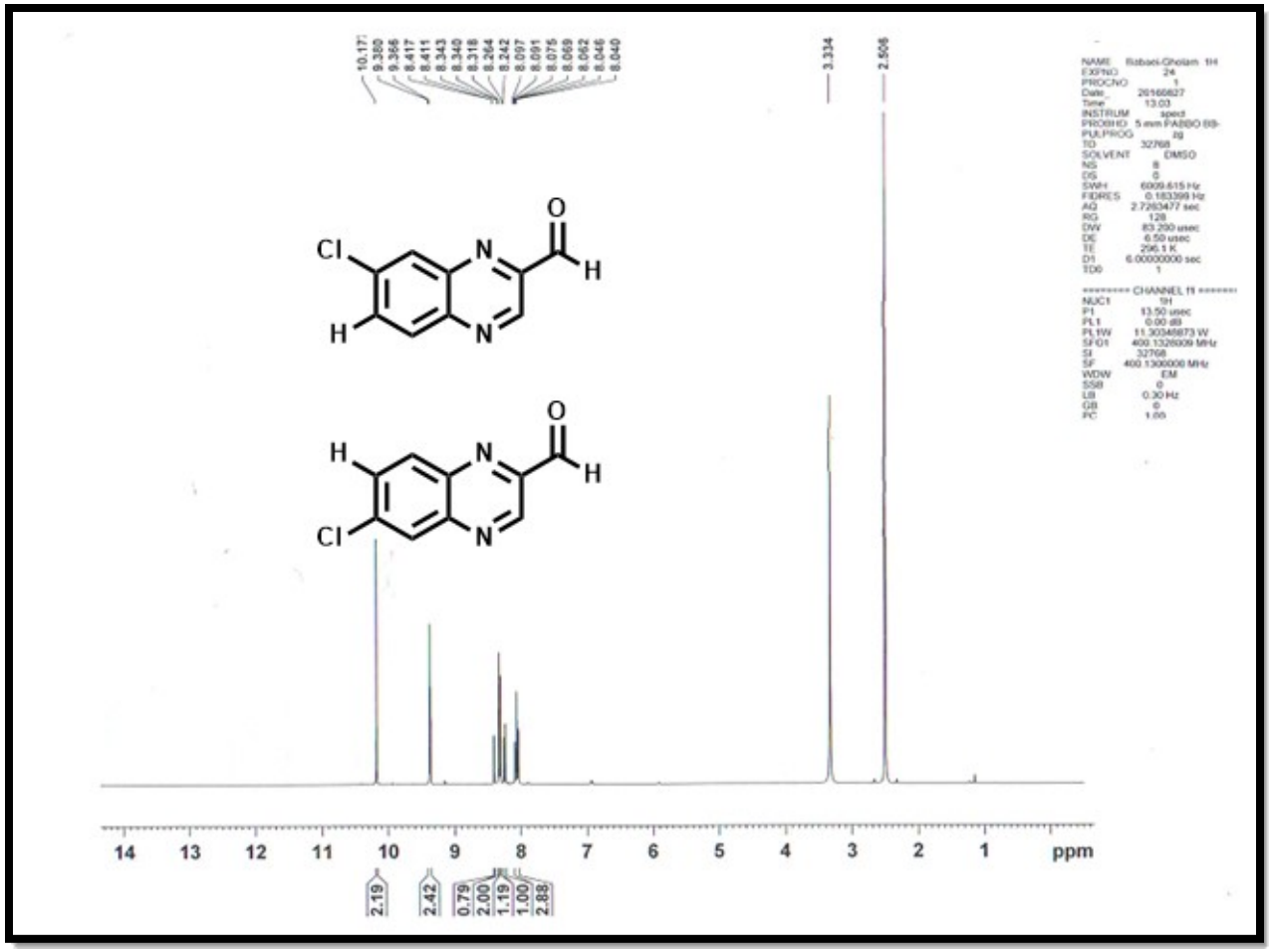


Fig S9. ^{1}HNMR spectra. 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde

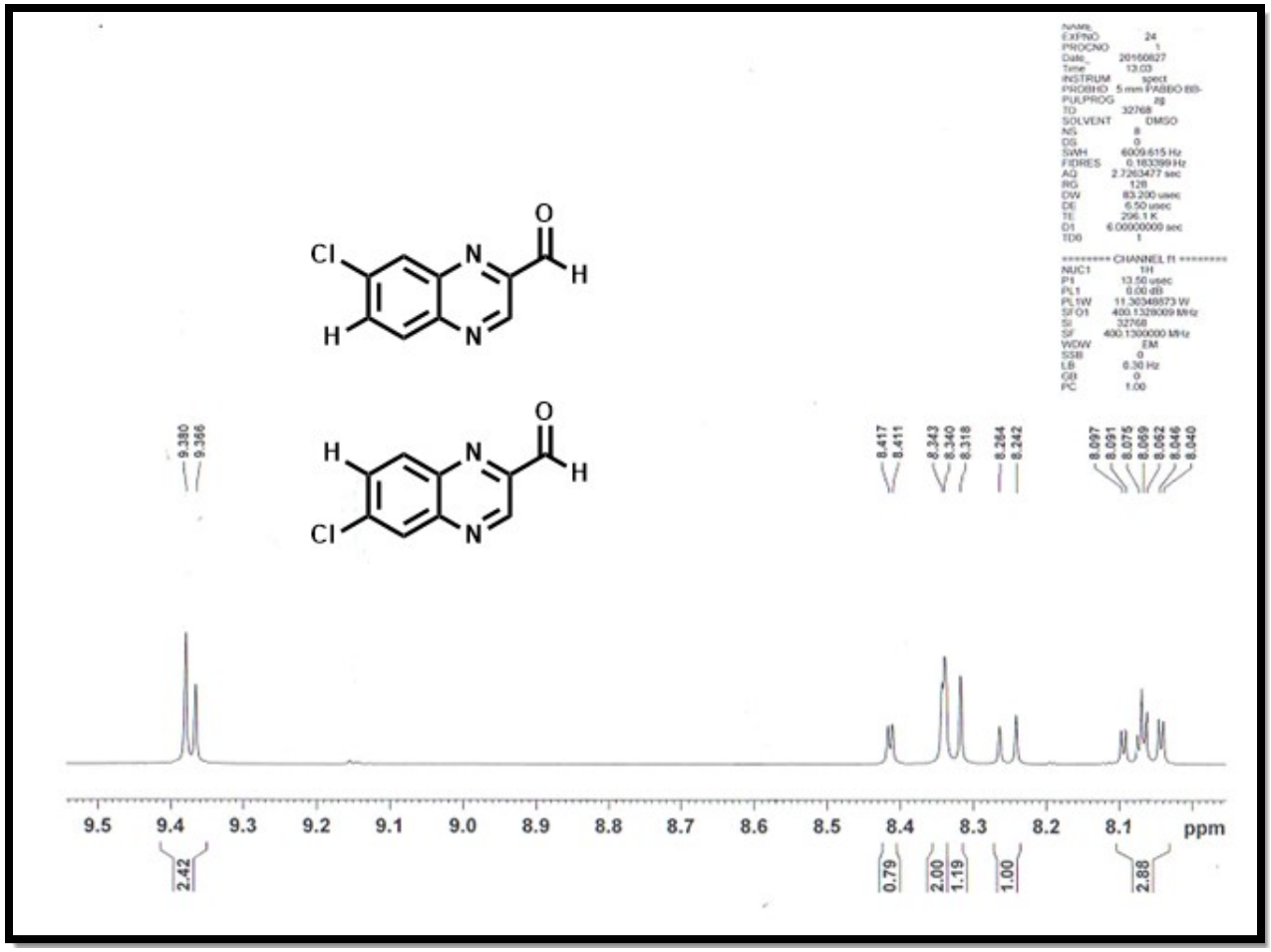


Fig S10. [1]HNMR expand spectra. 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde.

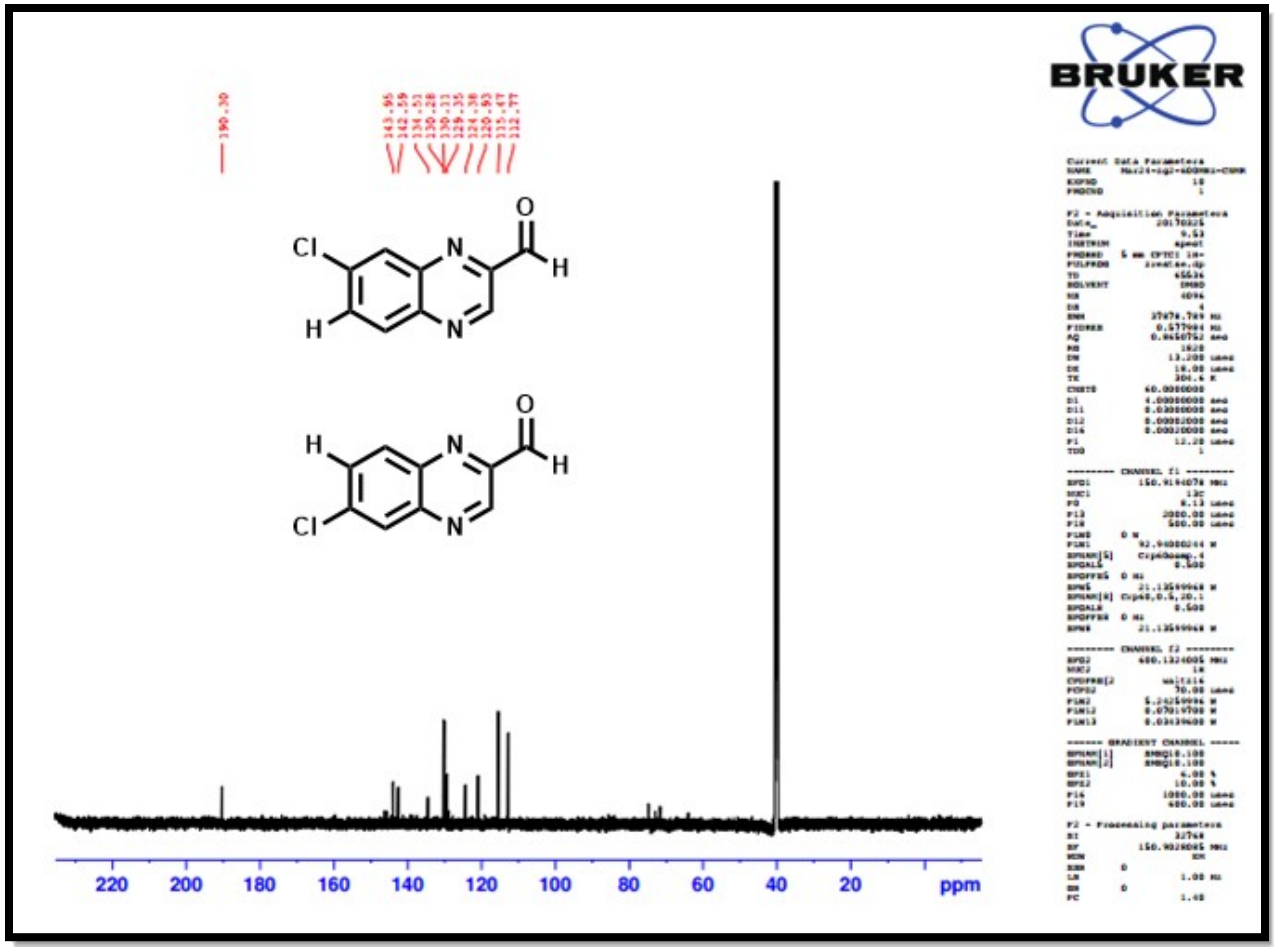


Fig S11. ^{13}CNMR spectra. 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde.

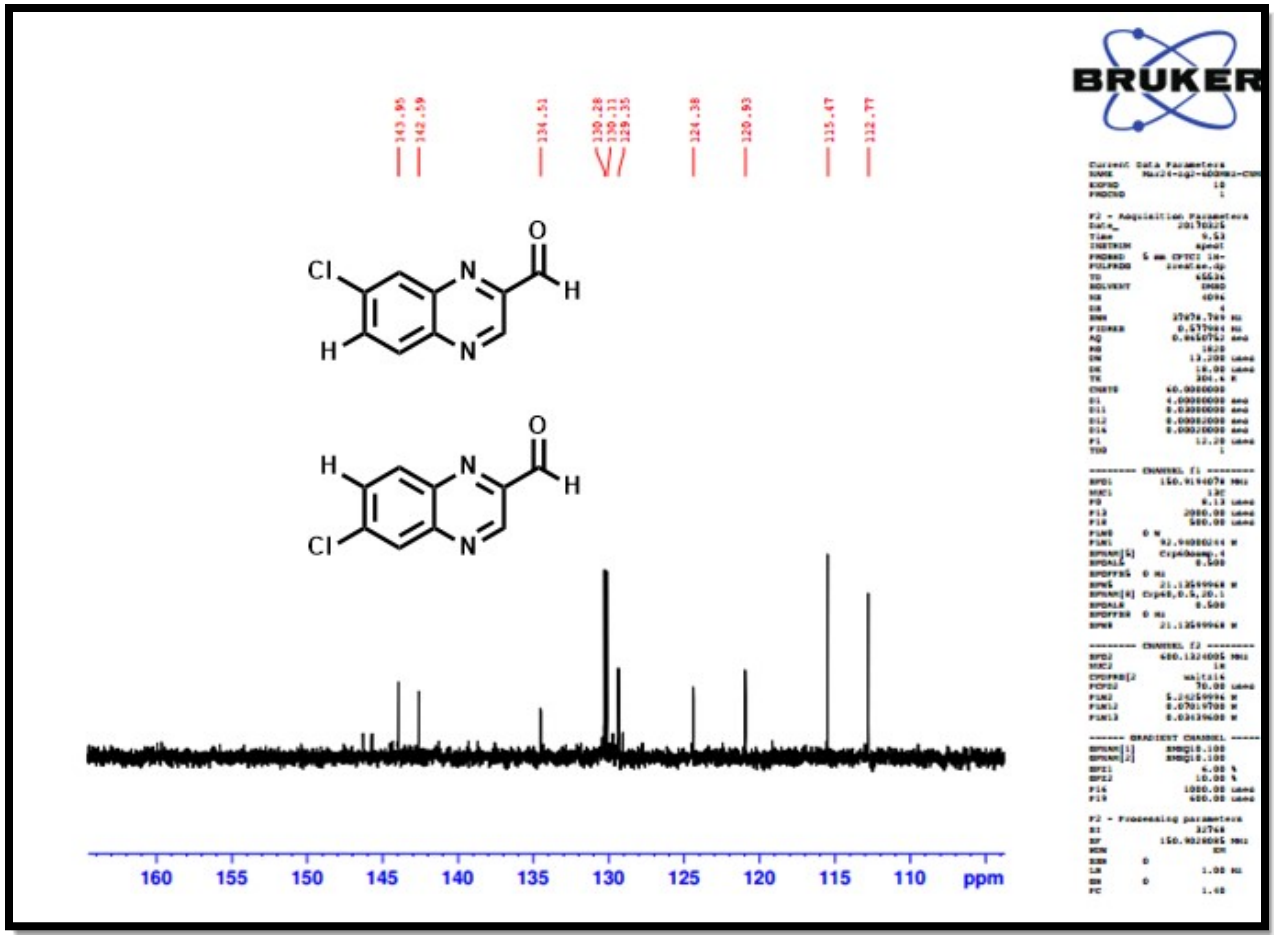
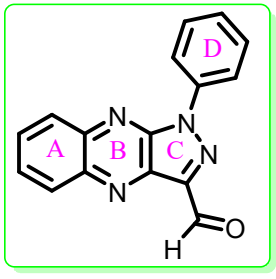


Fig S12. ^{13}CNMR expand spectra. 6-chloroquinoxaline-2-carbaldehyde and 7-chloroquinoxaline-2-carbaldehyde.

1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde



Yellow powder; yield: 91%, mp: 107°C.

$C_{16}H_{10}N_4O$, MW: 274.28 g/mole.

R (KBr, cm^{-1}) ν: 2861 (CH aldehyde), 1672 (C=O).

^{1}HNMR (400 MHz, $CDCl_3$) δ (ppm): 10.46 (s, 1H, Aldehyde), 8.39-8.46 (m, 3H, H-8 Quinoxaline, H-2 and H-6 ring D), 8.31 (d, 1H, *J* = 8.4 Hz, H-5 Quinoxaline), 7.98-8.12 (m, 2H, H-7 and H-6 Quinoxaline), 7.71-7.88 (AB quartet, 2H, J = 7.2 Hz, H-3 and H-5 ring D), 7.55 (tt, 1H, H-4 ring D, *J* = 7.2 and 1.2 Hz). ^{13}C-NMR (400 MHz, DMSO d_6) δ (ppm): 114, 116, 122 (Aromatic carbons ring D); 125, 130, 132, 136, 142, 144, 190.0 (C Aldehyde).

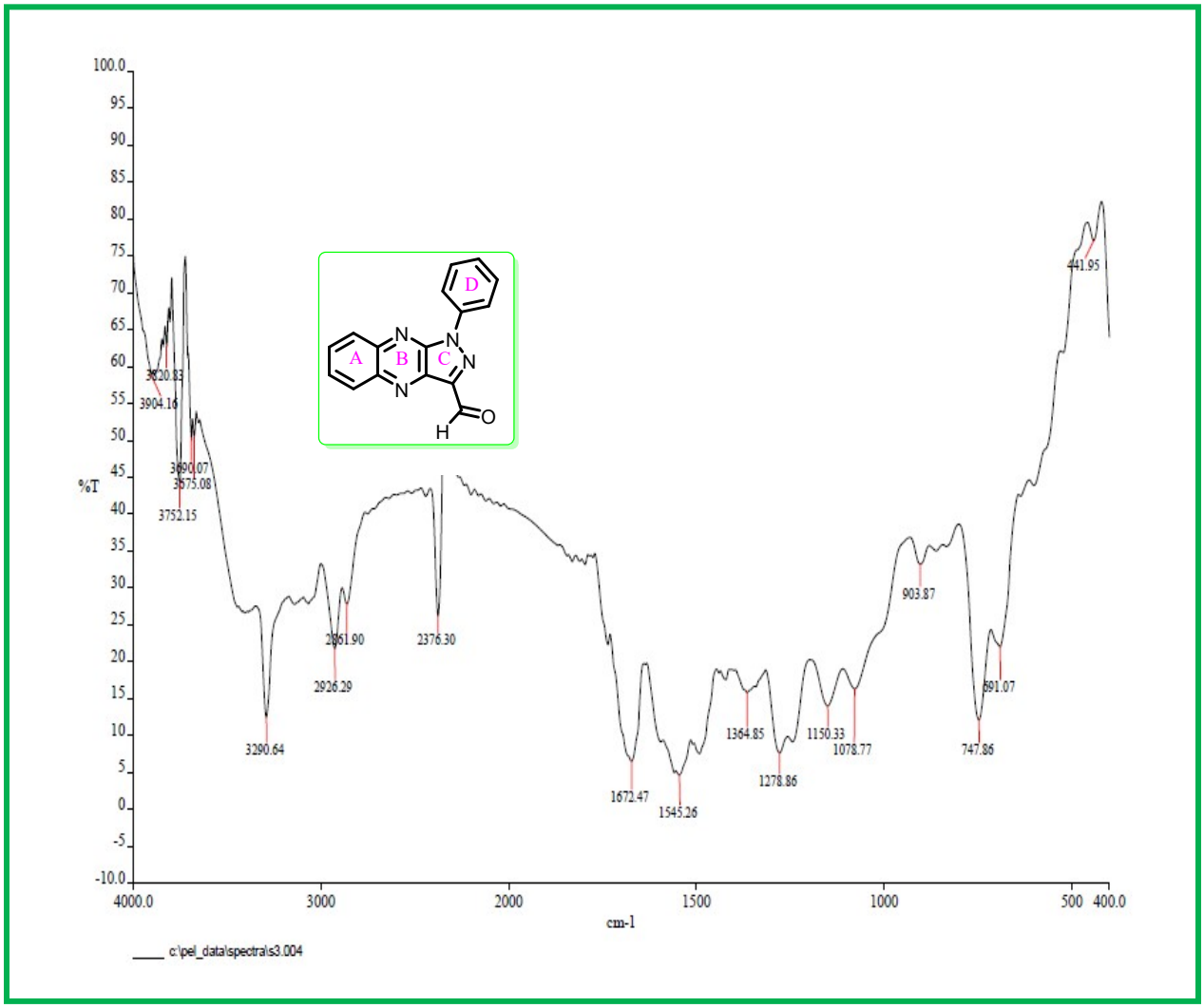


Fig S13. (FT-IR). 1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde .

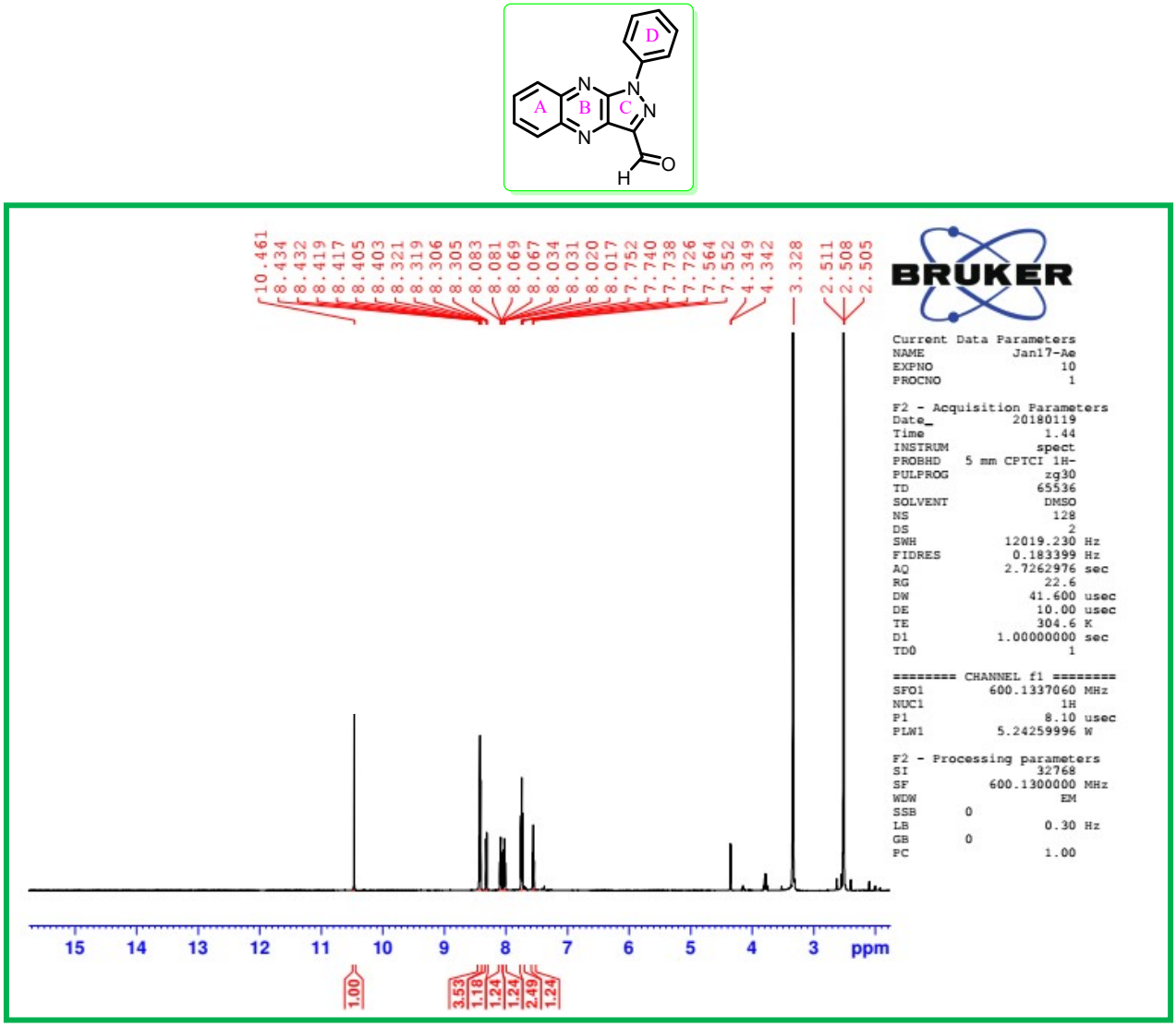


Fig S14. ^{1}HNMR spectra. 1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde .

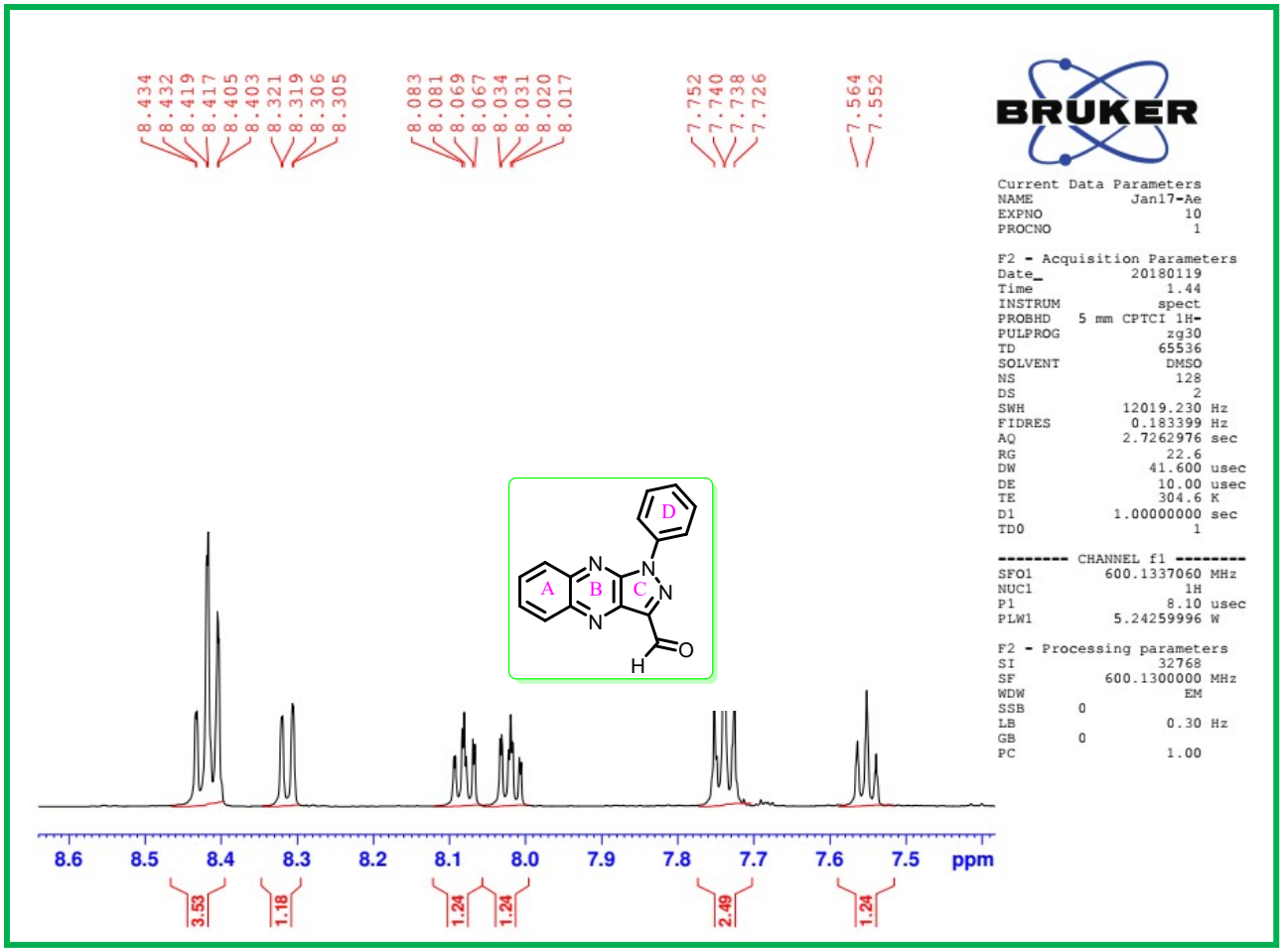


Fig S15. ^{1}HNMR expand spectra. 1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde .

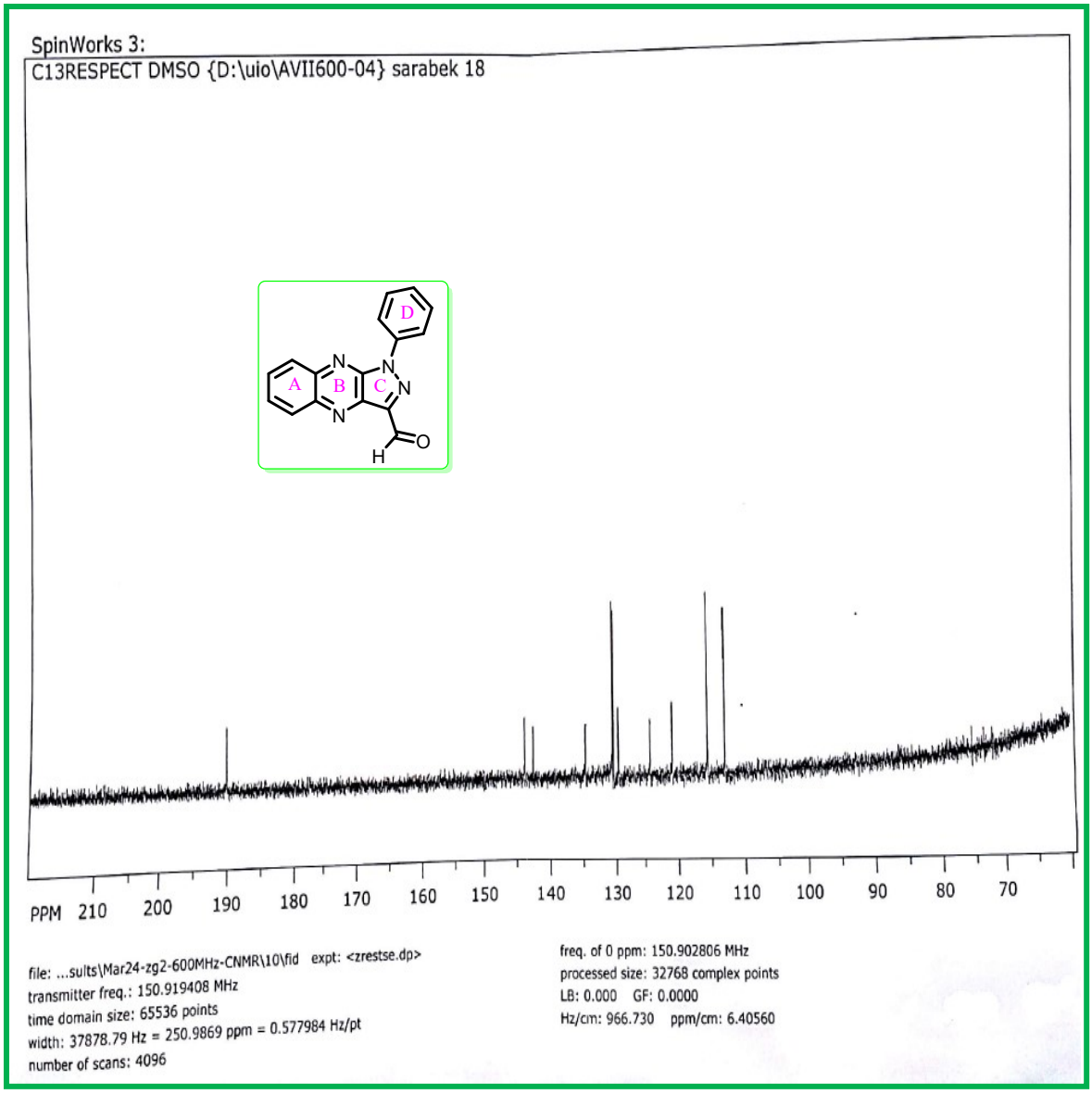


Fig S16. ^{13}CNMR expand spectra. 61-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde

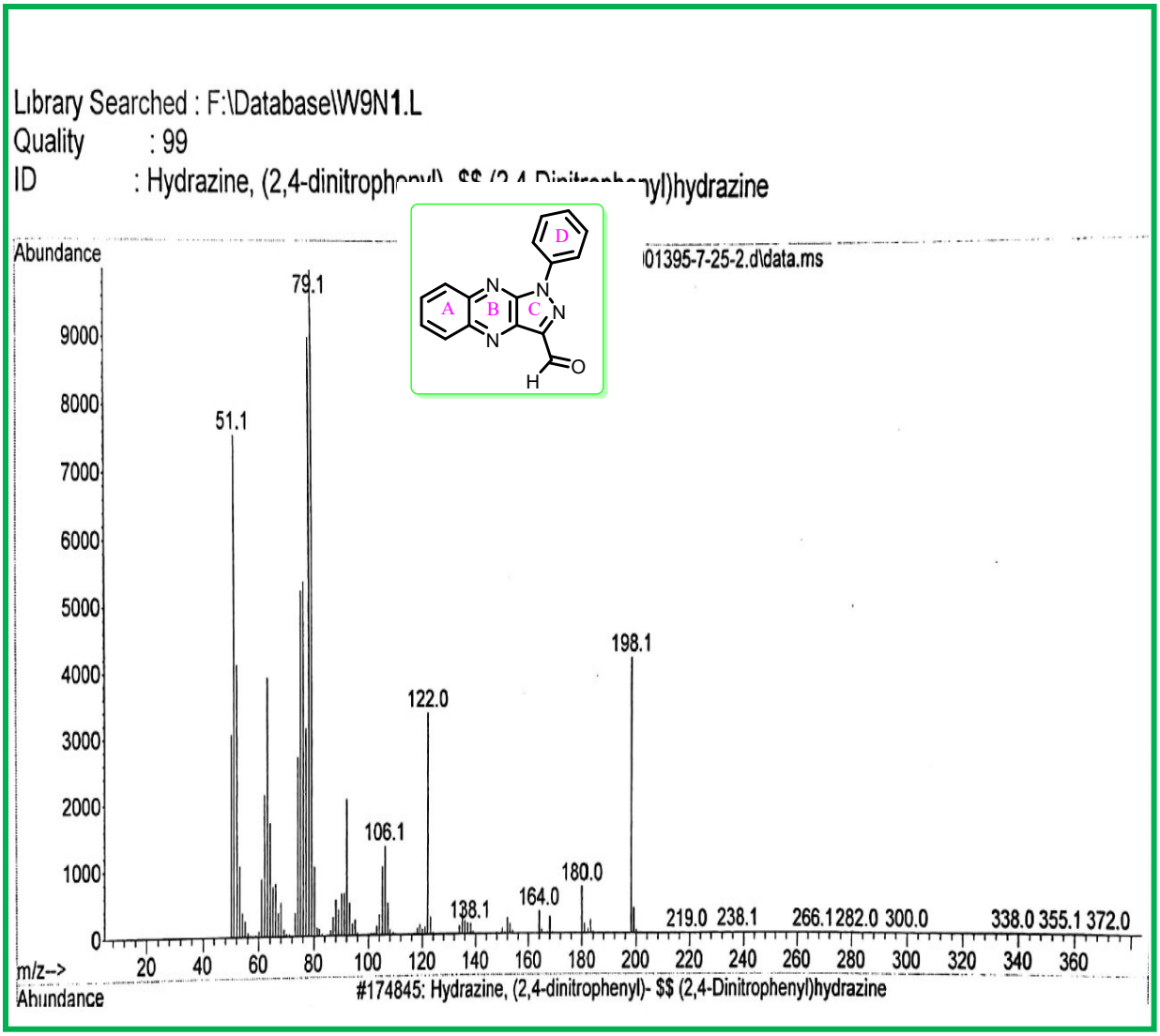


Fig S17. Mass Spectra. 1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxaline-3-carbaldehyde

3-(2-(4-Bromophenyl)-2-oxoethyl) imidazolidine-2,4-dione*:* IR (KBr): ν_{max} = 3400 (NH), 2950 (CH aliphatic), 1740-1690 (3 C=O), 1560-1463 (CH aromatic), 667 (C-Br) cm^{-1};^{1}H NMR (400 MHz, DMSO): δ4.93 (s, 1H, NH), 5.20 (s, 2H, CH_2), 7.77-7.80 (m, 3H, Ar-H), 7.89-7.94 (m, 3H, Ar-H) ppm.

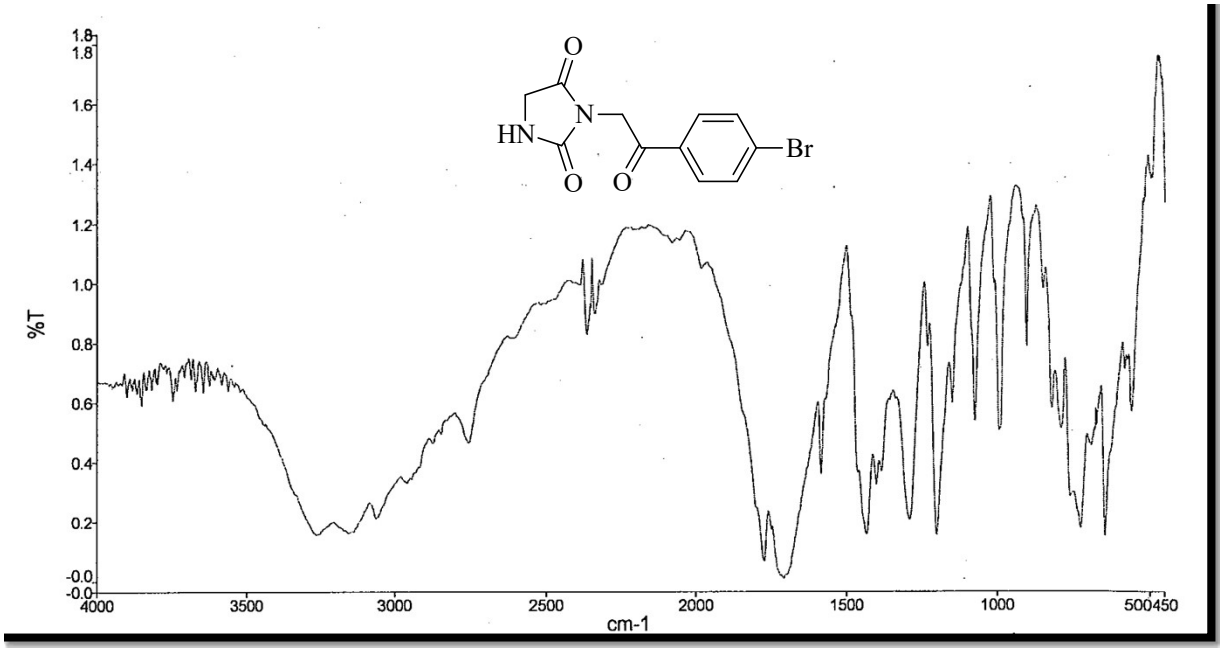


Fig S18. (FT-IR). 3-(2-(4-bromophenyl)-2-oxoethyl) imidazolidine-2,4-dione

(Z)-5-(Quinoxalin-2-ylmethylene) imidazolidine-2,4-dione: IR (KBr): ν_{max} = 3500-3100 (NH, br), 2920 (CH aliphatic), 1735, 1694 (2 C=O), 1690-1475 (CH aromatic&olefinic, C=N), 1275 (C-N) cm^{-1}; ^1H NMR (400 MHz, DMSO): δ4.94 (s, 1H, NH), 7.72 (s, 1H, CH), 7.79 (d, 2H, J = 8.4 Hz, Ar-H), 7.98 (d, 2H, J = 8.4 Hz, Ar-H), 8.25 (s, 1H, NCH),10.62 (s, 1H, NH) ppm.

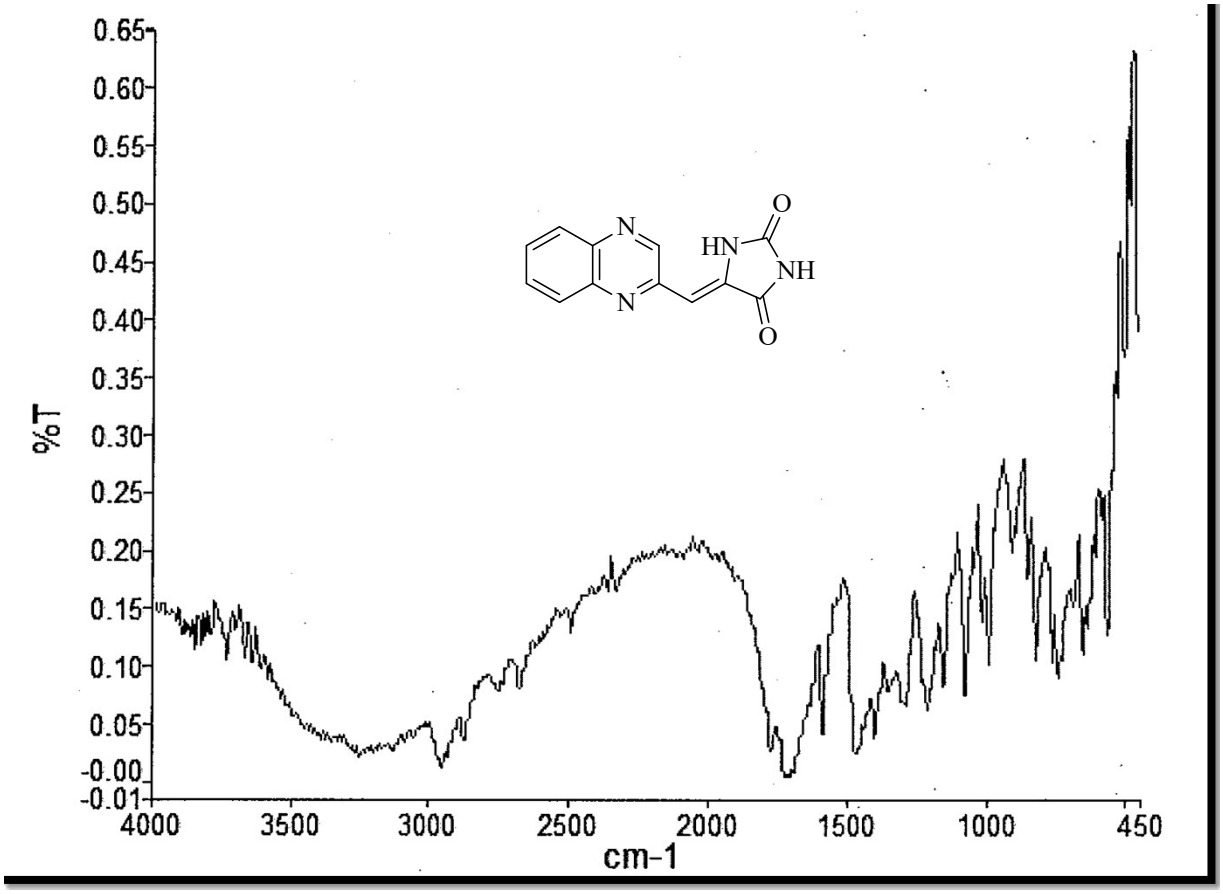


Fig S19. (FT-IR). (Z)-5-(Quinoxalin-2-ylmethylene) imidazolidine-2,4-dione.

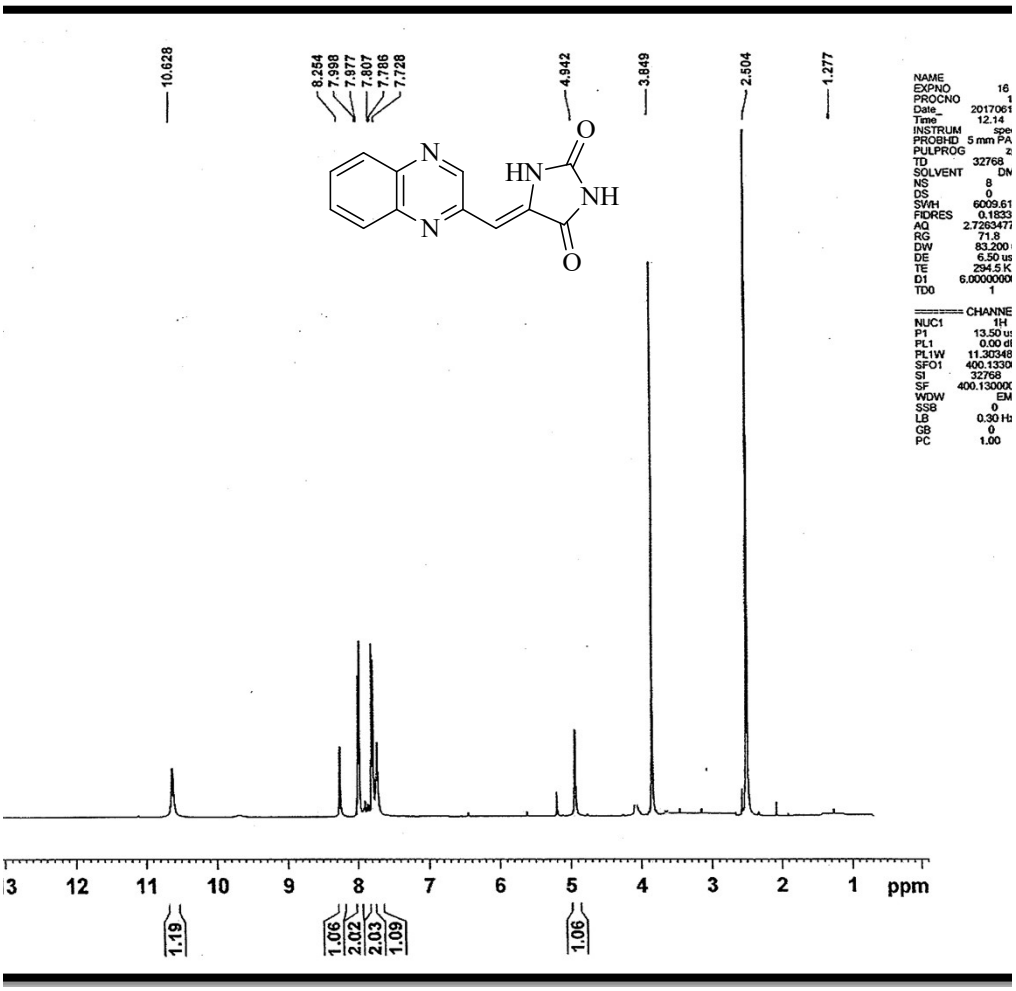


Fig S20. ^{1}HNMR expand Spectra. (Z)-5-(Quinoxalin-2-ylmethylene) imidazolidine-2,4-dione

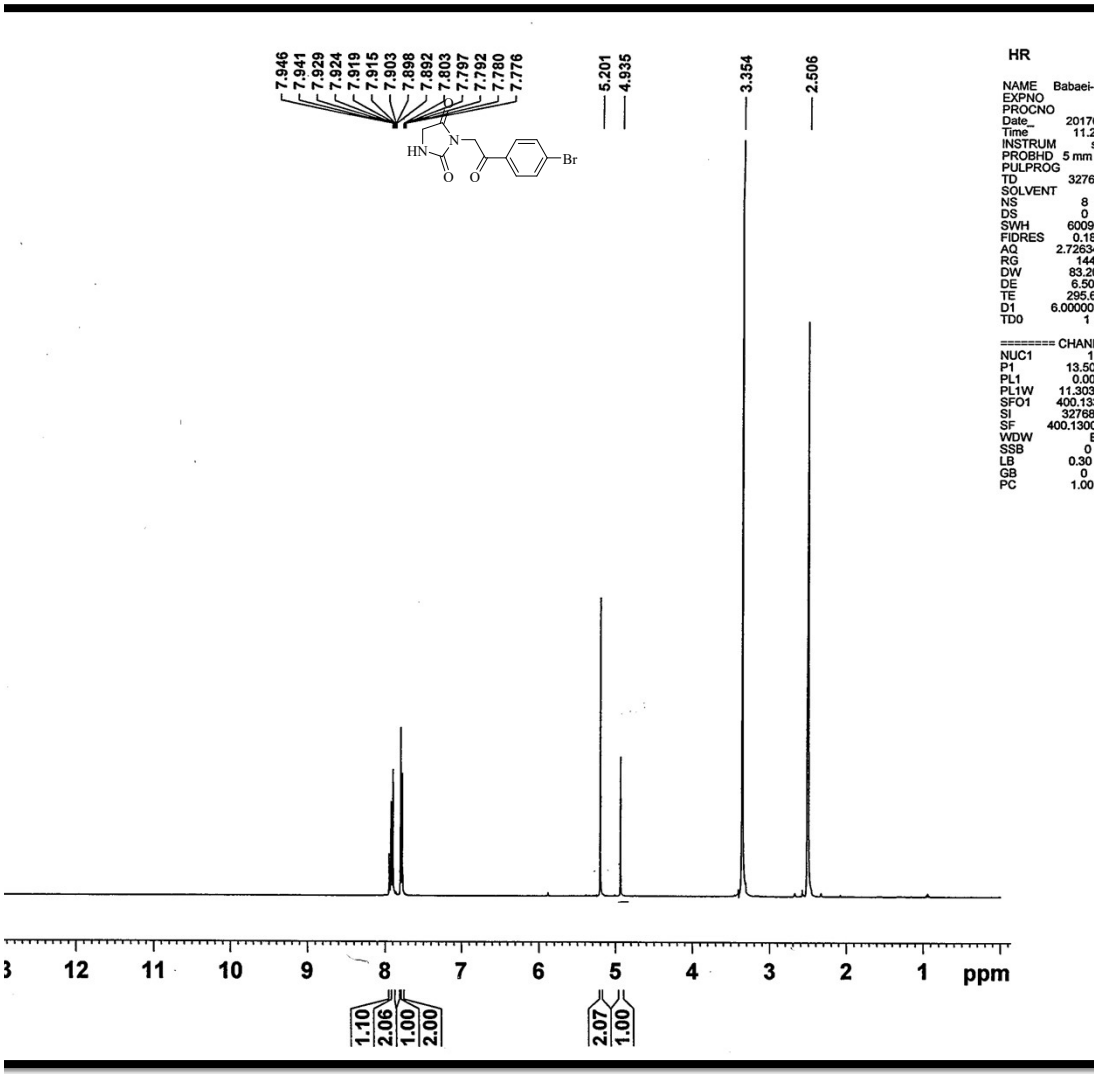
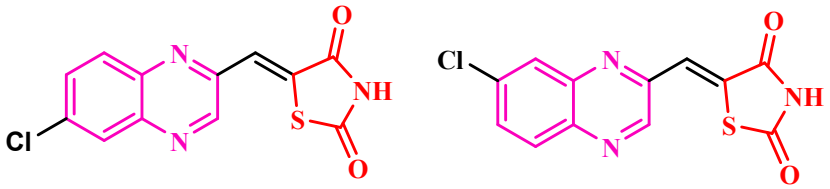


Fig S21. [1]HNMR Spectra. 3-(2-(4-bromophenyl)-2-oxoethyl) imidazolidine-2,4-dione



7 **and** 8

IR (KBr): 3448 (NH), 3100 (C-H_{vinyl}), 2918 (CH str.), 1701 (C=O), 1640 (C=N), 1244 (C=C) cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 8.45 (d, 1H, J = 2 Hz, 8-H Quinoxaline (Compound 8)), 8.17 (d, 1H, J = 2 Hz, 5-H Quinoxaline (Compound 7)), 8.30 (d, 1H, J = 8.8 Hz, 5-H Quinoxaline (Compound 8)), 8.12 (d, 1H, J = 8.8 Hz, 8-H Quinoxaline (Compound 7)), 7.99 (dd, 1H, J = 8.8 Hz and J = 2.4 Hz, 6 -H Quinoxaline (Compound 8)), 7.88 (dd, 1H, J = 8.8 Hz and J = 2.4 Hz, 7 -H Quinoxaline (Compound 7)), 7.63 (s, 1H, NH), 7.23 (s, 1H, H_{vinyl}), 9.40 (s, 1H, 3-H Quinoxaline); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 191 ($C_{C=O}$), 172 ($C_{C=O}$), 166 ($C_{C=O}$), 152 (C-2 Quinoxaline), 147 (C-3 Quinoxaline), 147 (C_{C-Cl}) 145 (C-4a Quinoxaline), 142 (C-8a Quinoxaline), 139(C-6 Quinoxaline), 134 (C-8 Quinoxaline), 132 (C-5 Quinoxaline), 130 (C-4 phenyl), 130 (C-1 phenyl), 130 (C-2 and C-6 phenyl), 129 (C-3 and C-5 phenyl), 127 and 128 (C=C vinyl), 47 (CH_2), 34 (CH_3).

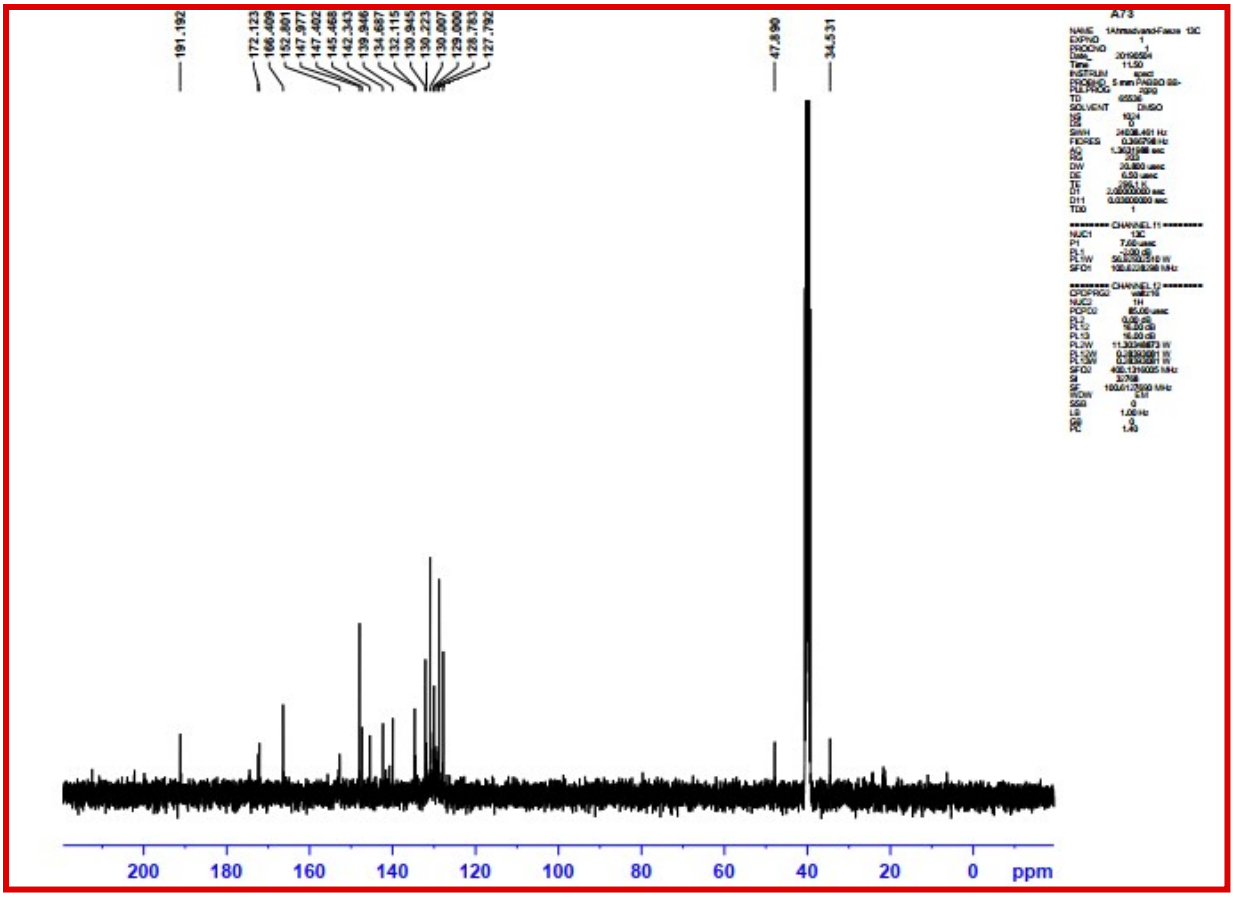


Fig S22. ^{13}CNMR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene) thiazolidine-2,4-dione

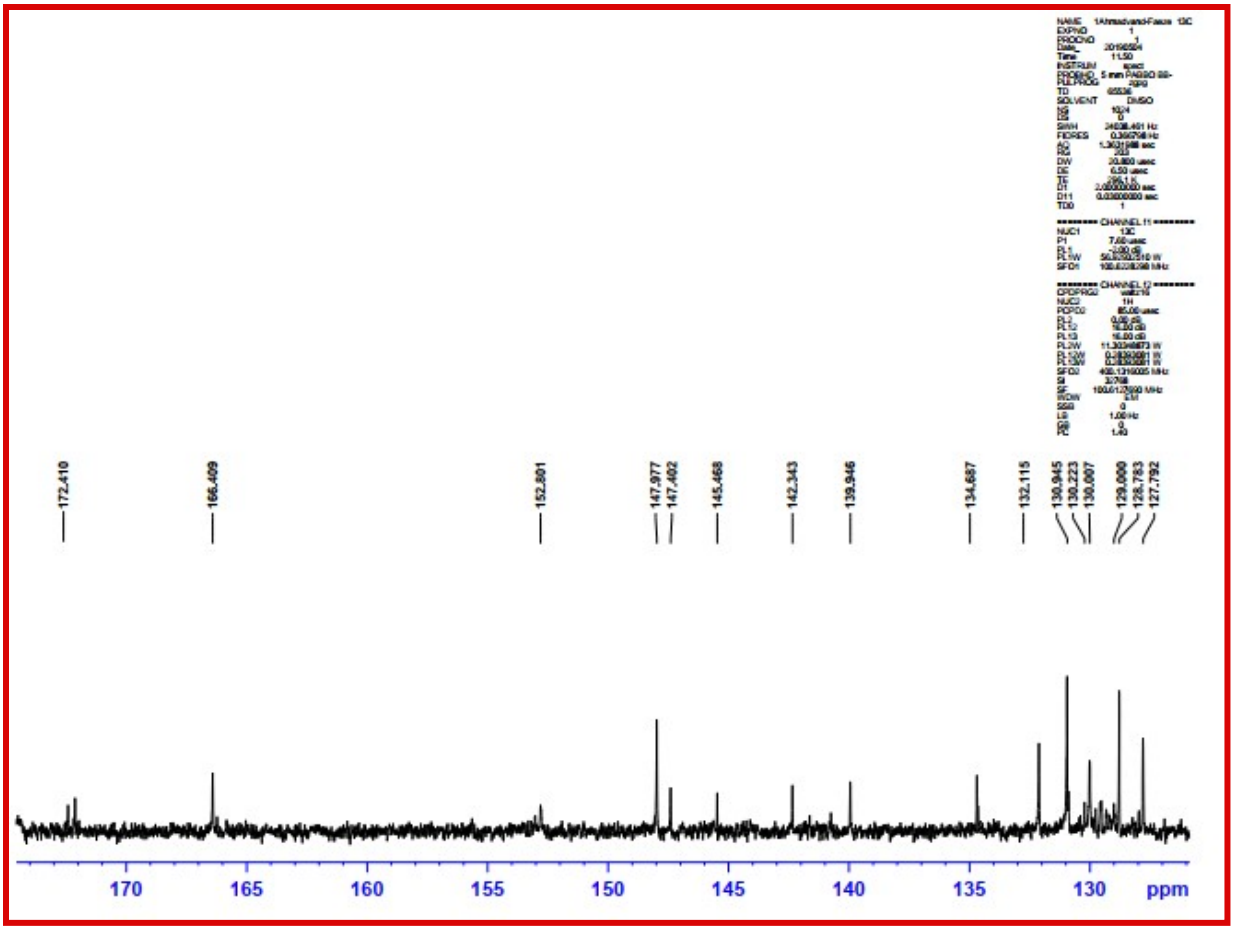


Fig S23. ^{13}CNMR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene) thiazolidine-2,4-dione

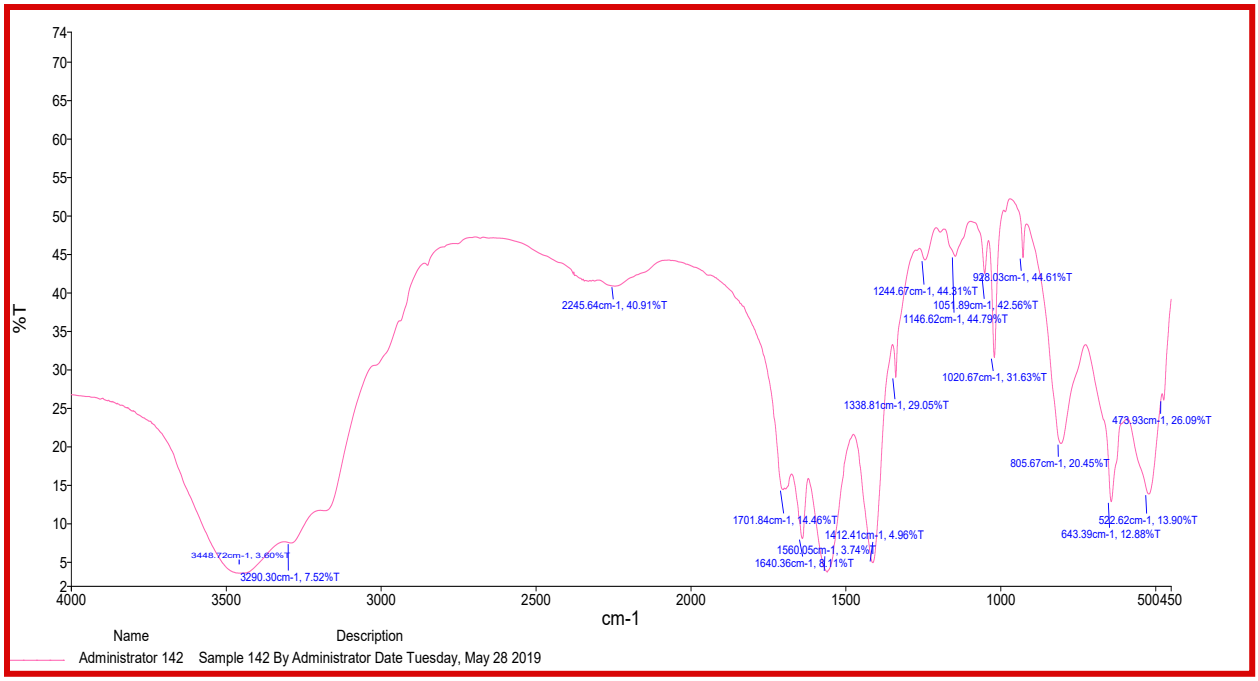


Fig S24. FTIR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene) thiazolidine-2,4-dione

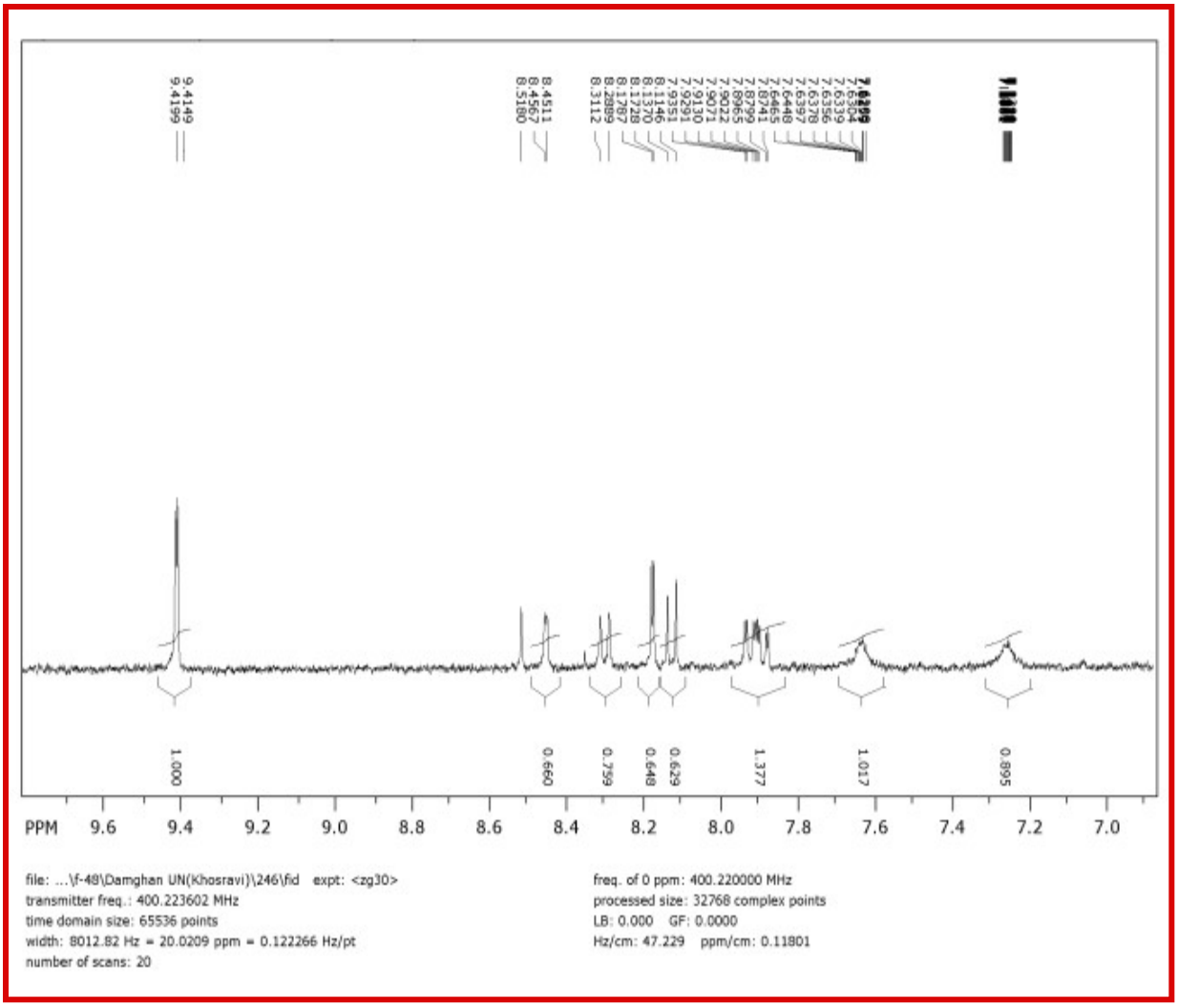


Fig S25. ^{1}HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene) thiazolidine-2,4-dione

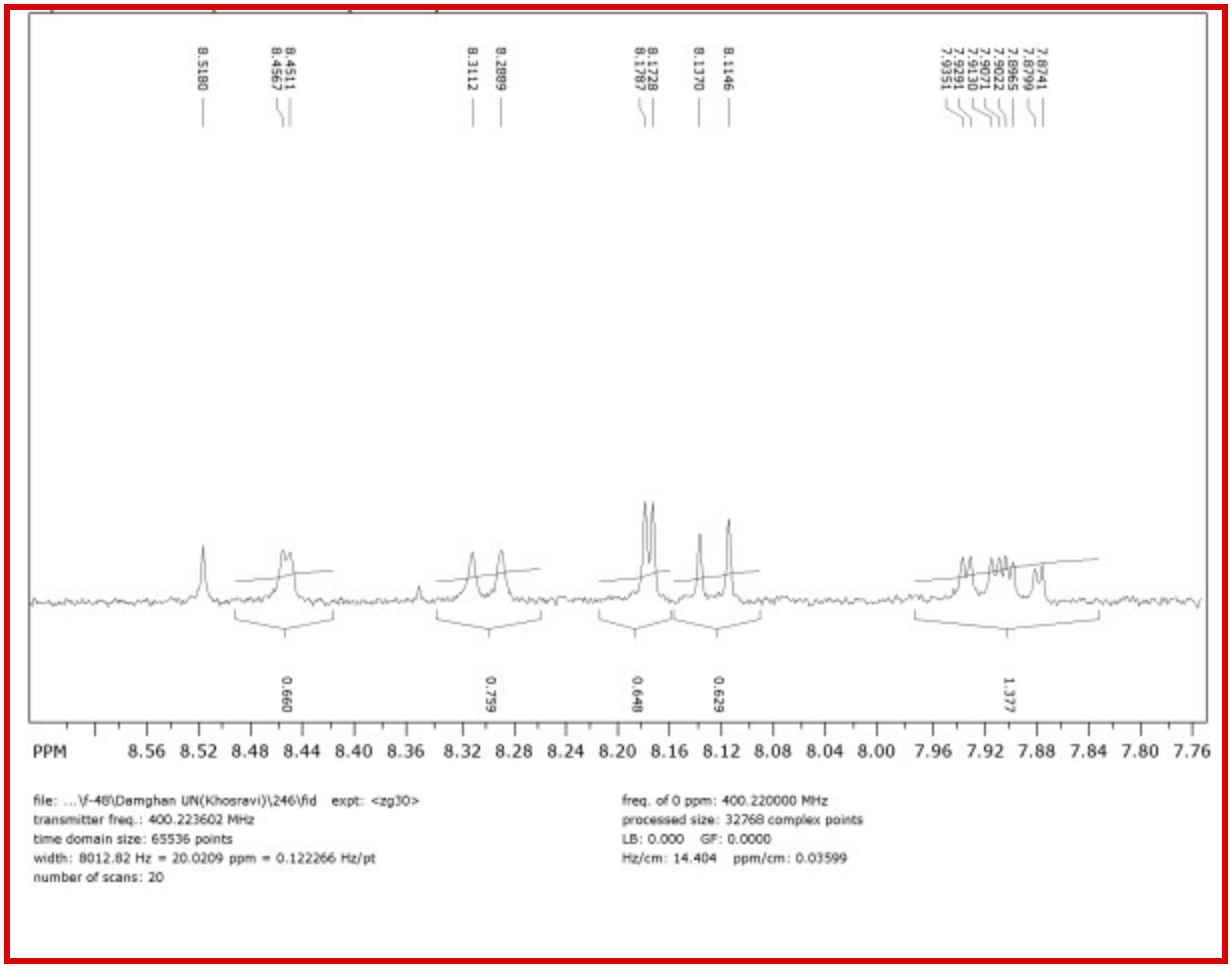
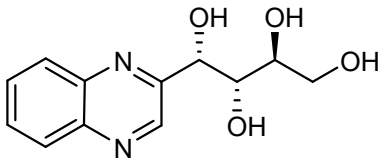


Fig S26. ^{1}HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene) thiazolidine-2,4-dione



IR (KBr): ν_{max} = 3451-3243 (4 OH, br), 2910 (CH aliphatic), 1663-1562 (CH aromatic, C=N), 1370 (C-N), 1125, 1108, 1044 (3 C-OH) cm^{-1}.

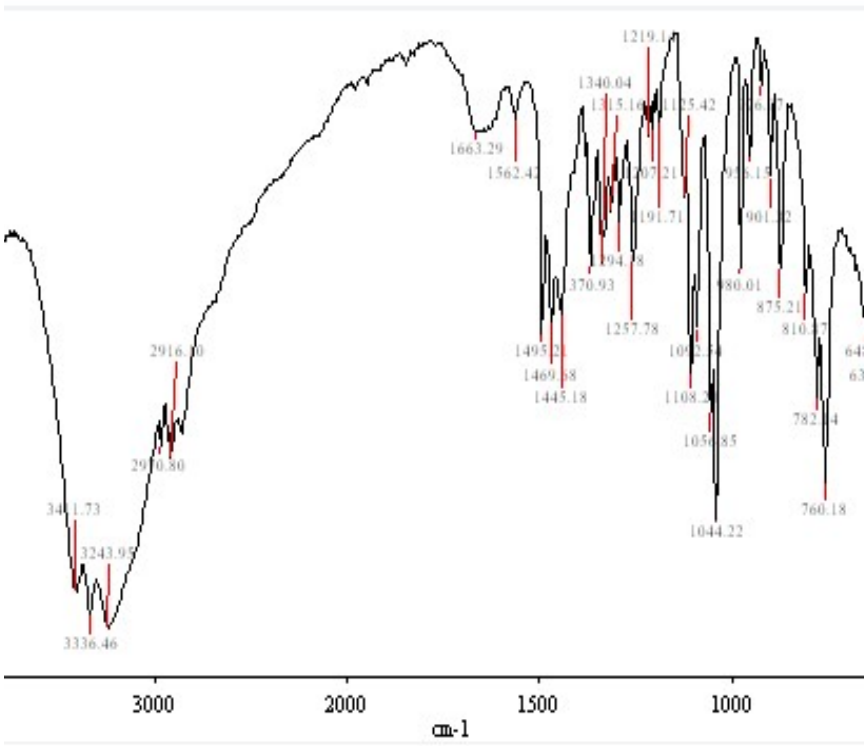
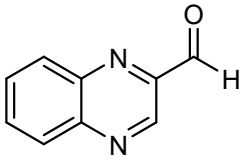


Fig S27. (FT-IR). (1S,2R,3S)-1-(quinoxalin-2-yl) butane-1,2,3,4-tetraol



IR (KBr): ν_{max} = 2862 (CH aldehyde), 1699 (C=O), 1640-1609 (CH aromatic&olefinic, C=N), 1359-1329 (2 C-N) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.80-7.98 (m, 2H, Ar-H), 8.22-8.29 (m, 2H, ArH),9.49 (s, 1H, $CH_{olefinic}$), 10.33 (s, 1H, CHO) ppm. MS (m/z, %): 158 (M^+,100).

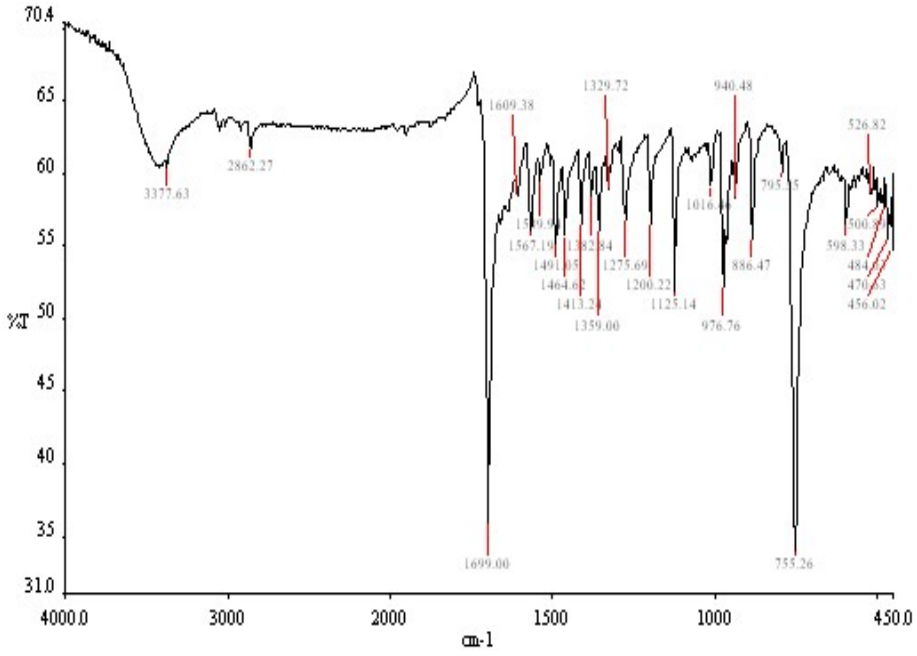


Fig S28. (FT-IR). quinoxaline-2-carbaldehyde

yellow crystal (94%); mp: 168-169 °C; IR (KBr, v_{max}, cm^{-1}): 3468, 3135, 3039, 2703, 1731, 1643, 1395, 1347, 1205, 1174, 897, 876, 788, 787, 662, 542 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$): δ (ppm) 4.26 (s, 2H, CH_2), 12.88 (bs, 1H, NH); ^{13}C-NMR (100 MHz, $CDCl_3$); 40.6, 175.5, 201.

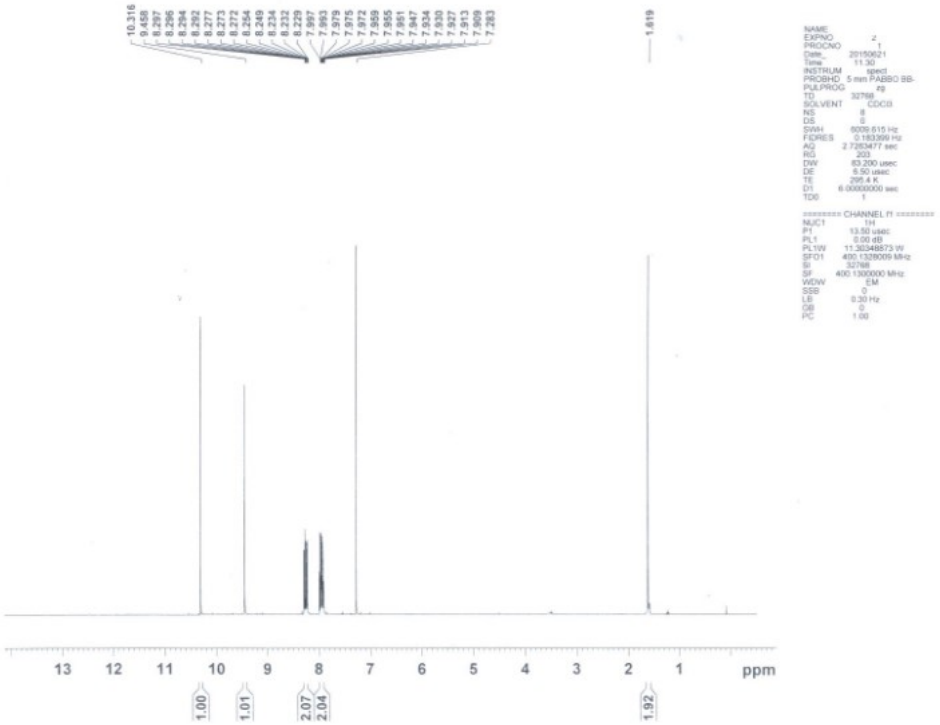
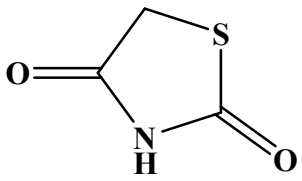


Fig S29. ^{1}HNMR expand spectra. quinoxaline-2-carbaldehyde



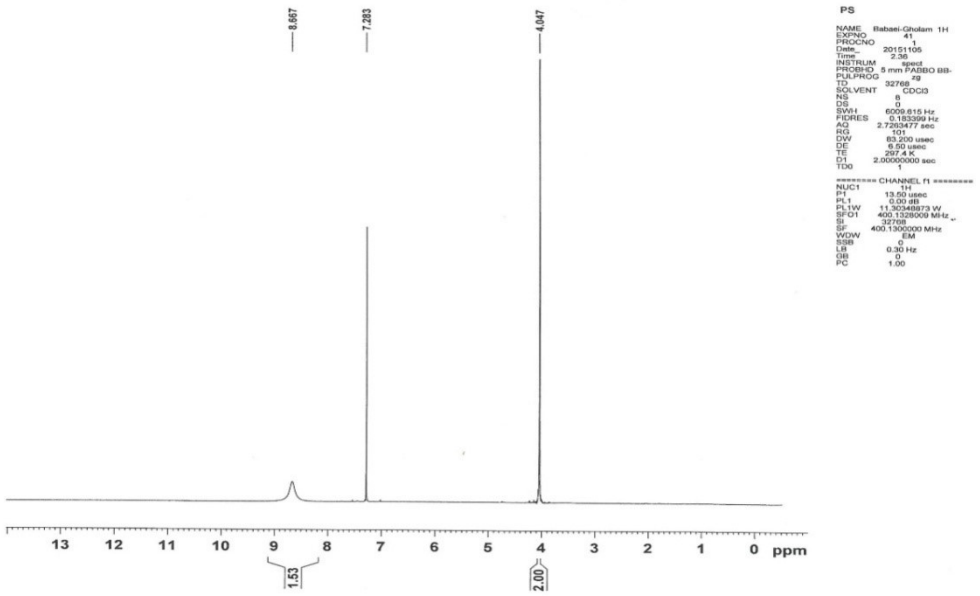


Fig S30. ^{1}HNMR spectra. Thiazolidine-2,4-dion

Section 2: The analytical and spectroscopic data for the unknown final products.

(Z)-3-phenyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one(L8a); IR (KBr, cm^{-1}): ν =2918.12 (C-H aromatic), 1660 (C=O), 1596 (C=N). ^{1}HNMR (400 MHz, DMSO d_6) δ (ppm): 9.42 (S, 1H, H-3 Quinoxaline), 8.14 (S, 1H, HC═C)),8.28- 8.31 (m, 1H, H-8 Quinoxaline), 8.15-8.17 (m, 1H, H-5 Quinoxaline), 8.03 (S. 1H, HC═C), 7. 94- 8.00 (m, 2H, H-6 and H-7 Quinoxaline), 4.12 (q, 2H, J=7.2 Hz, CH_2), 1.23 (t,3H, J=7.2 Hz, CH).

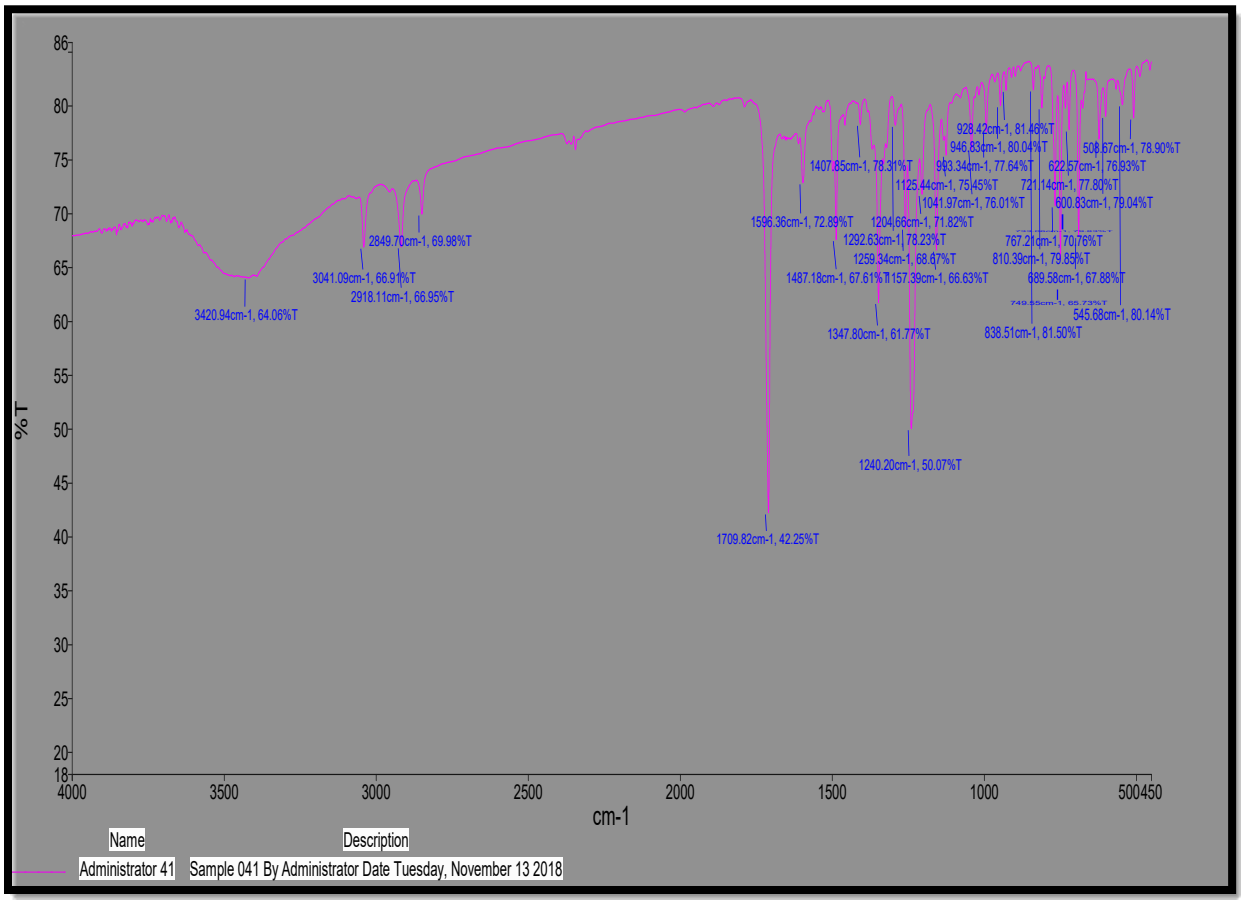


Fig S31. (FT-IR). (Z)-3-phenyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L8a)**

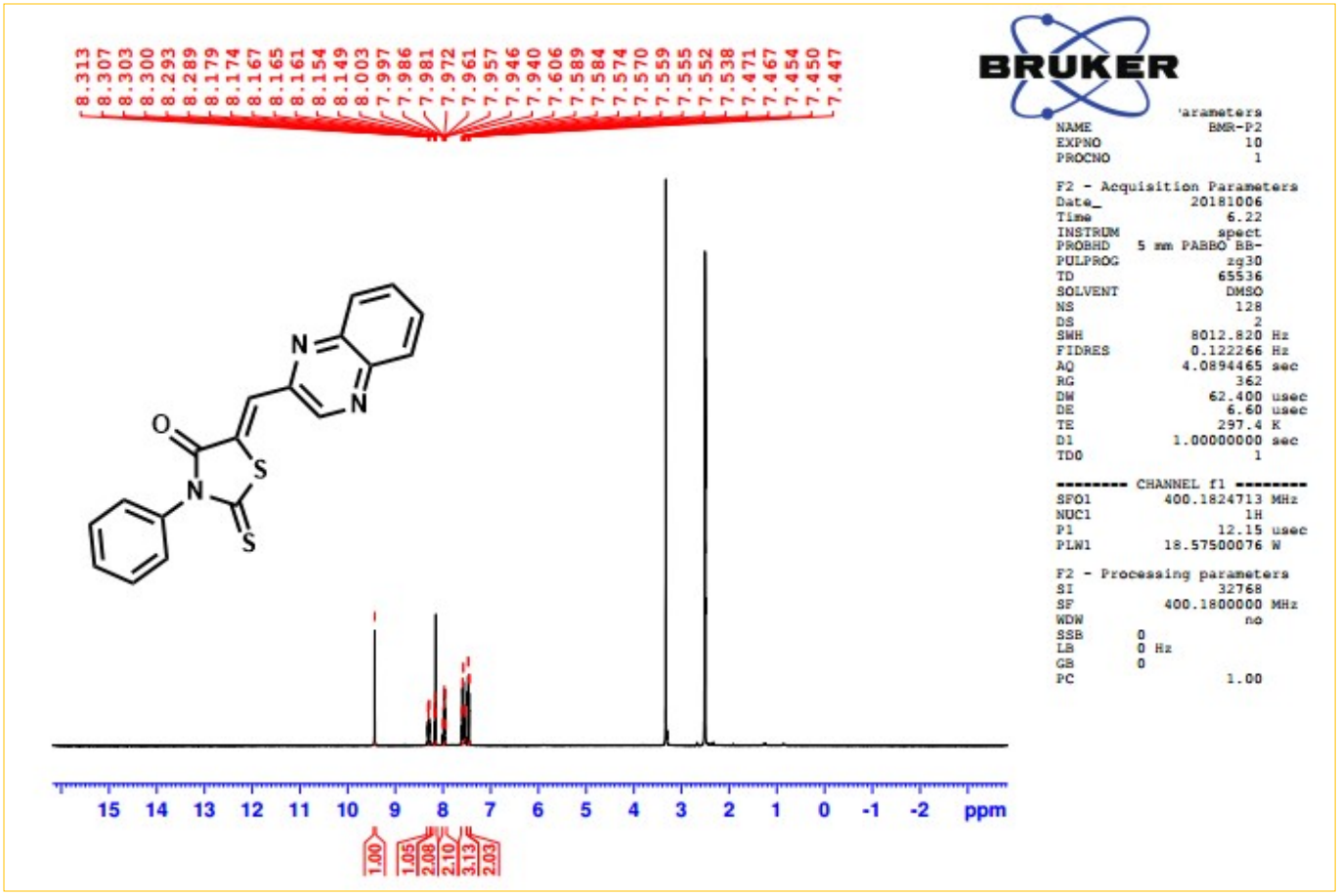


Fig S32. ^{1}HNMR Spectra. (Z)-3-phenyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L8a)**

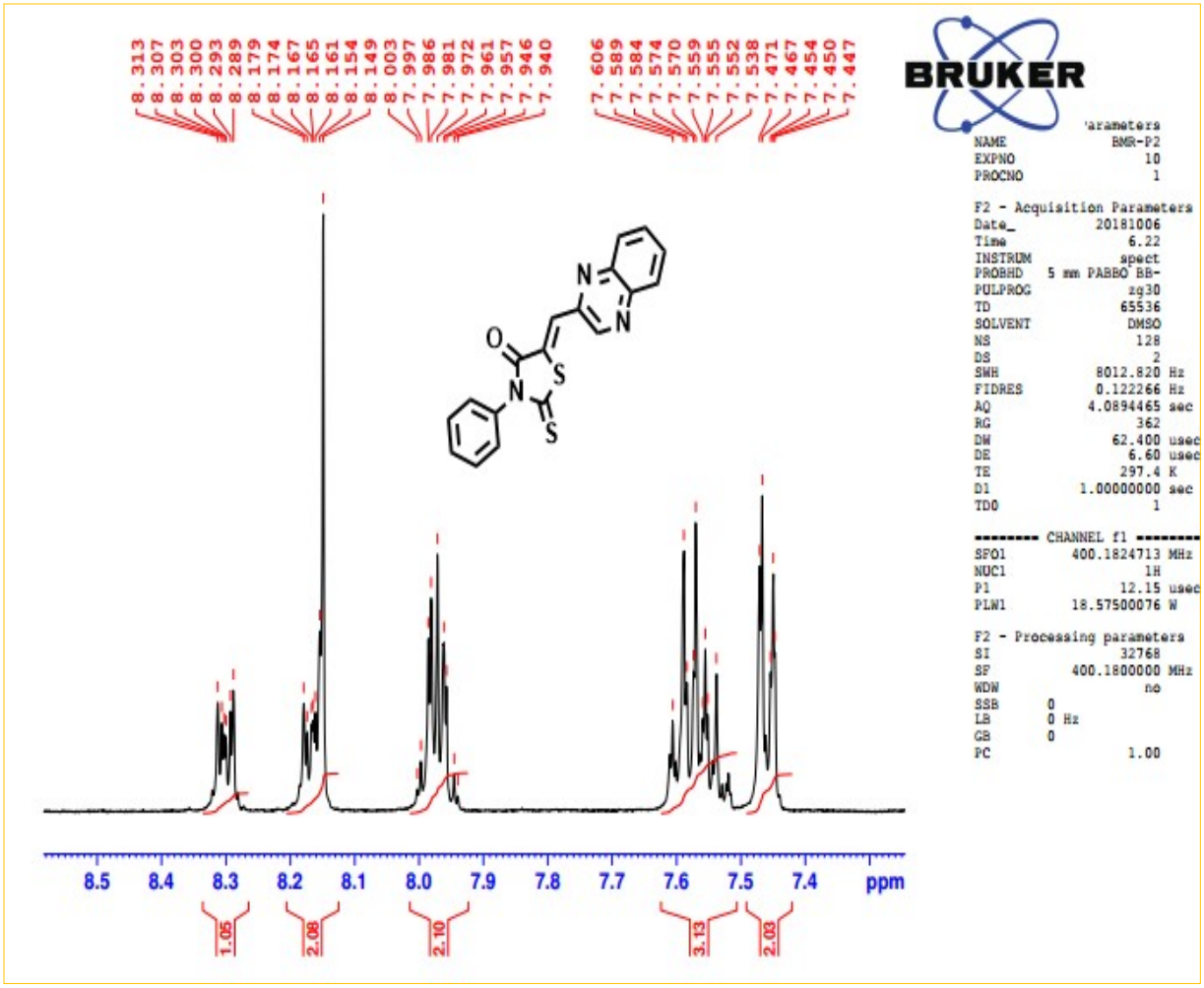


Fig S33. ^{1}HNMR expand spectra. (Z)-3-phenyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L8a)**

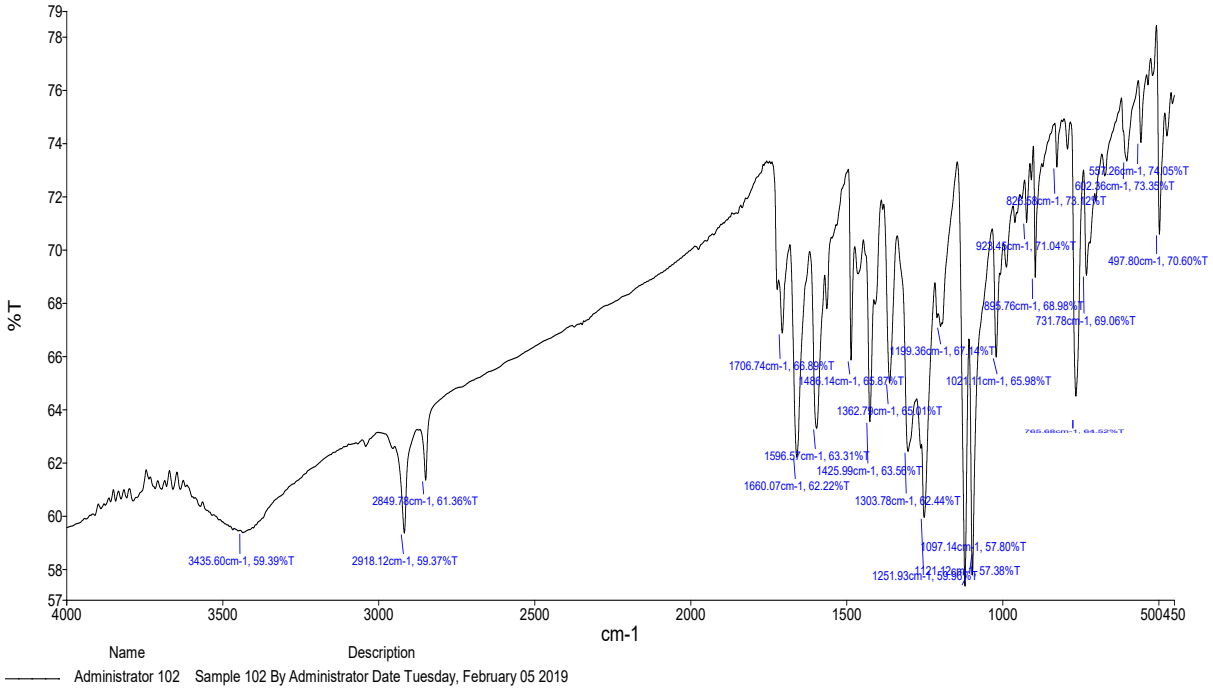


Fig S34. (FT-IR). (Z)-3-methyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L6a**)

(Z)-3-methyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one(L6a); IR (KBr, cm), 2917.91(C– H aromatic), 1239(C=C). 1709(C=O), 1603 (C=N), HNMR (400 MHz, DMSO d_6),[1] HNMR (400 MHz, DMSO d_6) δ (ppm): 9.41 (S, 1H, H-3 Quinoxaline), 8.22- 8.30 (m,1H, H-8 Quinoxaline), 8.14-8.21 (m, 1H, H-5 Quinoxaline), 8.13 (S. 1H, HC═C), 7.29 8.00 (m, 2H, H-6 and H-7 Quinoxaline), 3.46 (t,3H, CH_3).

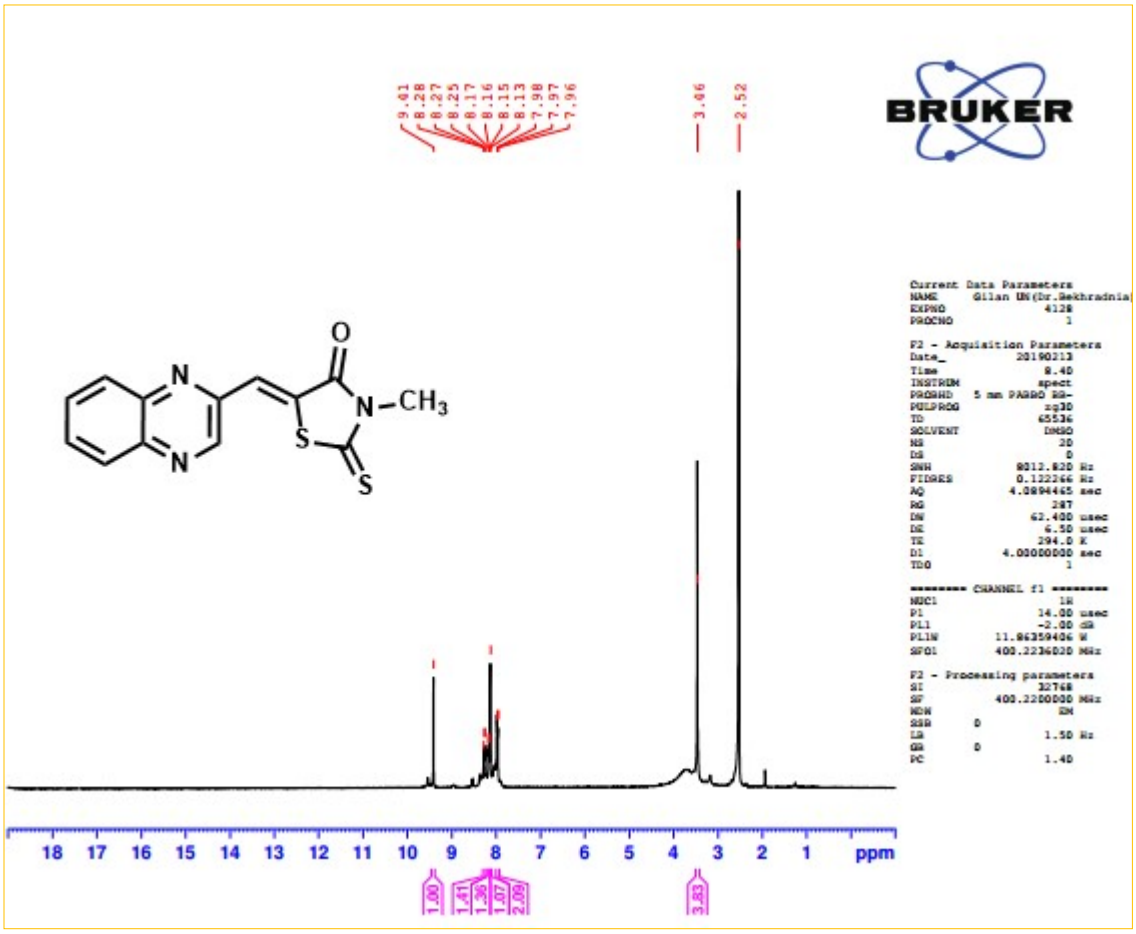


Fig S35. [1]HNMR Spectra. (Z)-3-methyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L6a**)

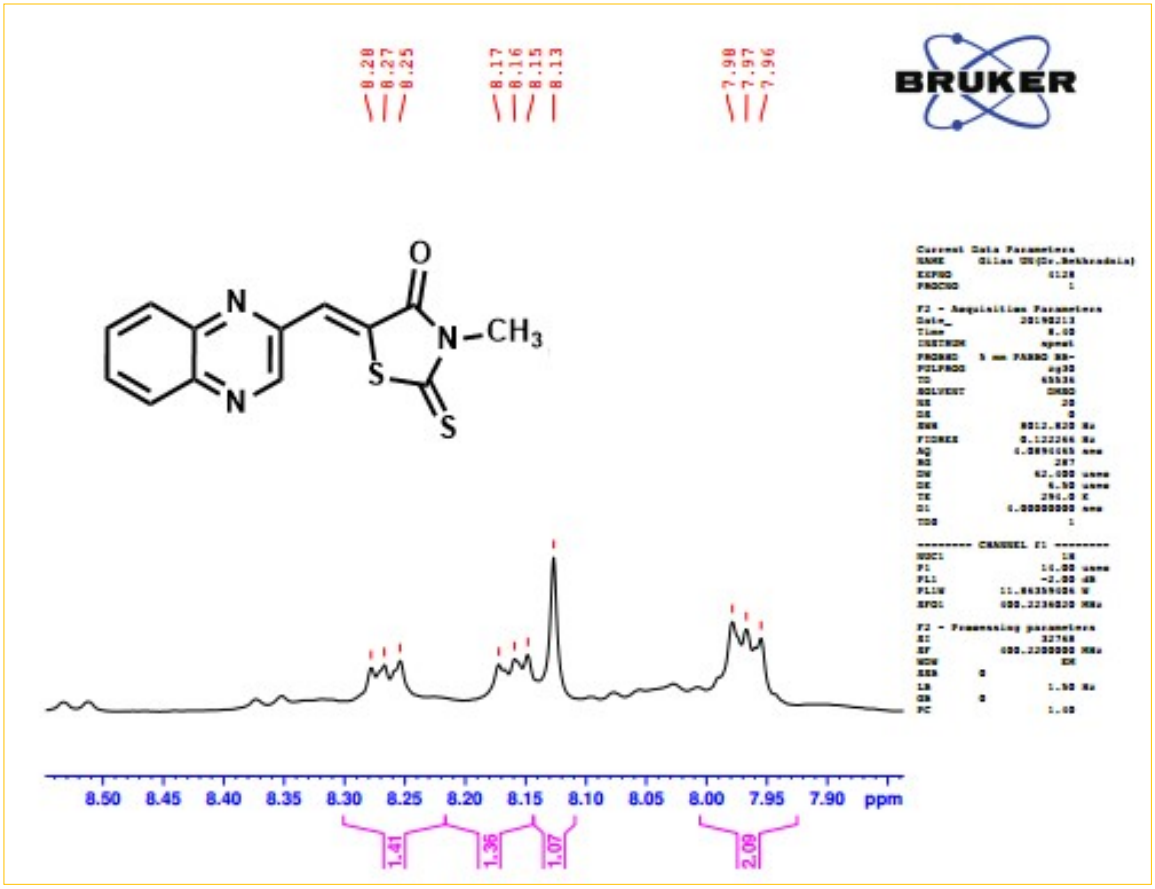


Fig S36. [1]HNMR expand spectra. (Z)-3-methyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L6a**)

(Z)-3-ethyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (L7a): IR (KBr, cm^{-1}): ν =2918.12 (C-H aromatic), 1660 (C=O), 1596 (C=N).[1]HNMR (400 MHz, DMSO d6) δ (ppm): 9.40 (S, 1H, H-3 Quinoxaline), 8.22- 8.30 (m,1H, H-8 Quinoxaline), 8.13-8.20 (m, 1H, H-5 Quinoxaline), 8.03 (S. 1H, HC═C), 7.89-43, 8.01 (m, 2H, H-6 and H-7 Quinoxaline), 4.12 (q, 2H, J=7.2 Hz, CH2), 1.23 (t,3H, J=7.2Hz, CH_3.

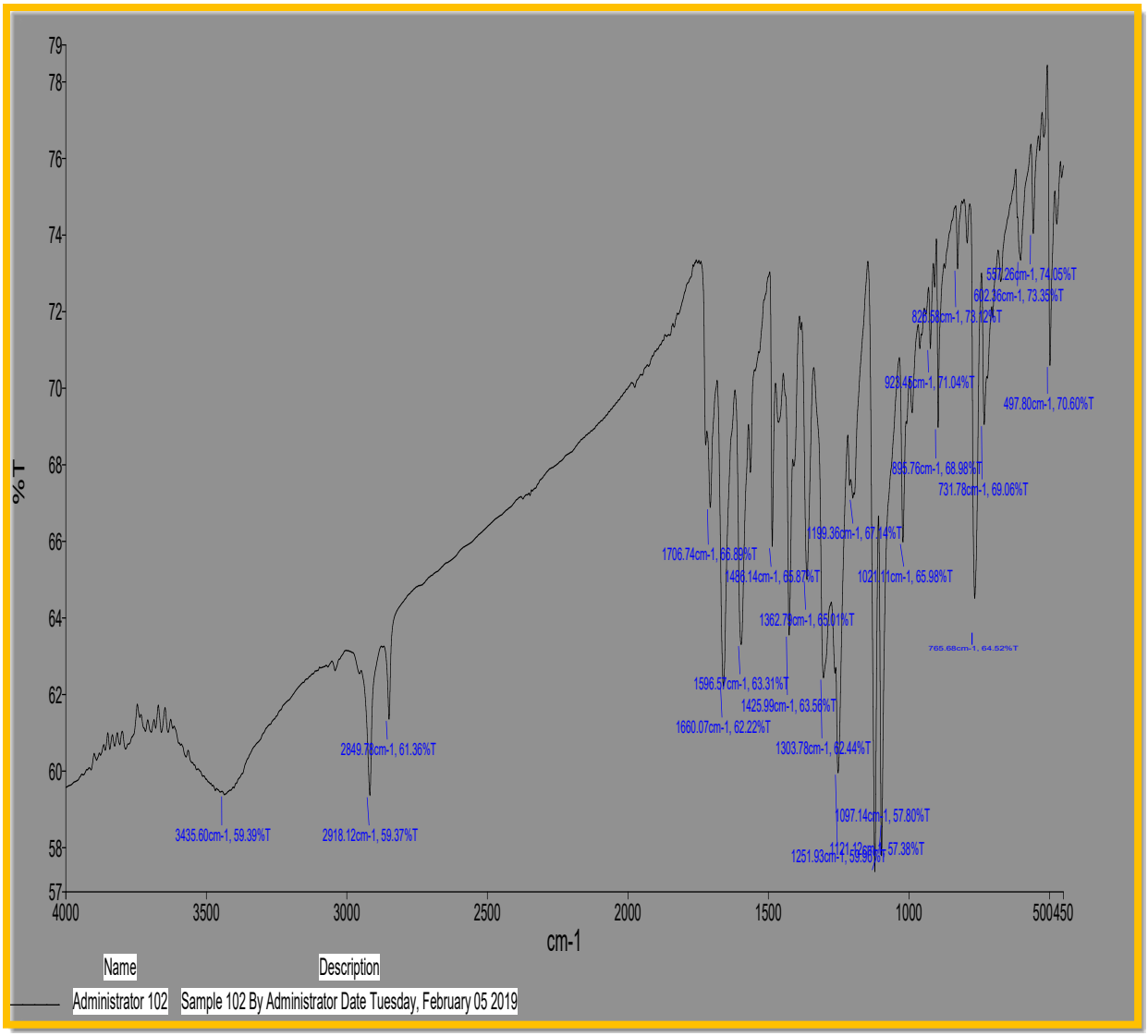


Fig S37. (FT-IR). (Z)-3-ethyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L7a**)

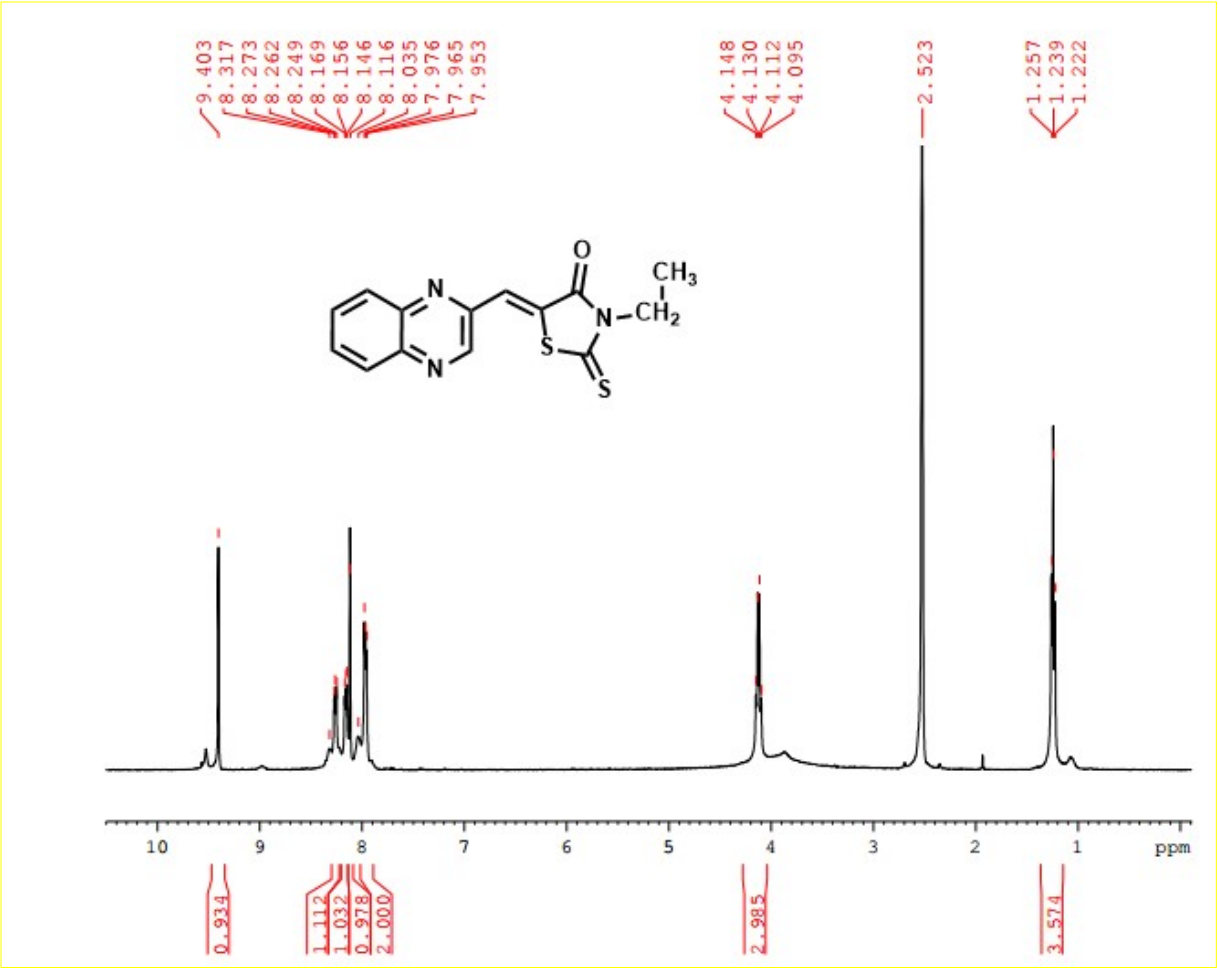


Fig S38. ^{1}HNMR Spectra. (Z)-3-ethyl-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L7a**)

(Z)-3-(4-nitrophenyl)-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one(L2b) ;

IR (KBr, cm^{-1}): ν = 2919 (C-H aromatic), 1680 (C=O), 1597 (C=N)^{1}.HNMR (400 MHz, DMSO d_6) δ: 10.57 (S, 1H, H-3 Quinoxaline), 9.6 (S, 1H, HC═C) 8.4-8.2 ,(m, 2H, H-5 and H-8 Quinoxaline), 8.21(d, 2H, J=8 Hz, H-2 and H-6 phenyl)7.83 ,(d, 2H, J=8 Hz, H-3 and H-5 phenyl), 8.04-8.07 (m, 2H, H-6 and H-7 Quinoxaline).

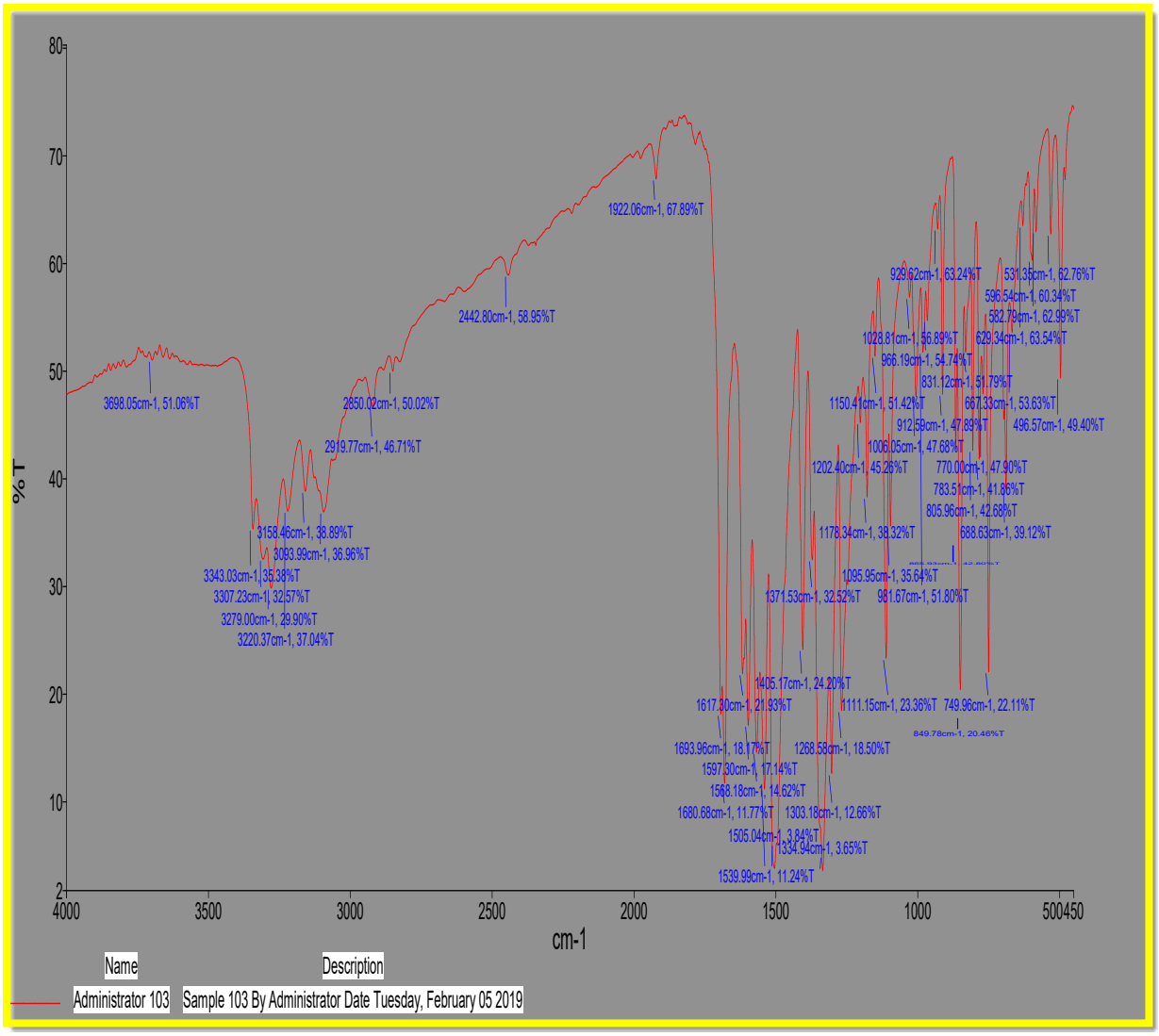


Fig S39. (FT-IR). (Z)-3-(4-nitrophenyl)-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L2b**)

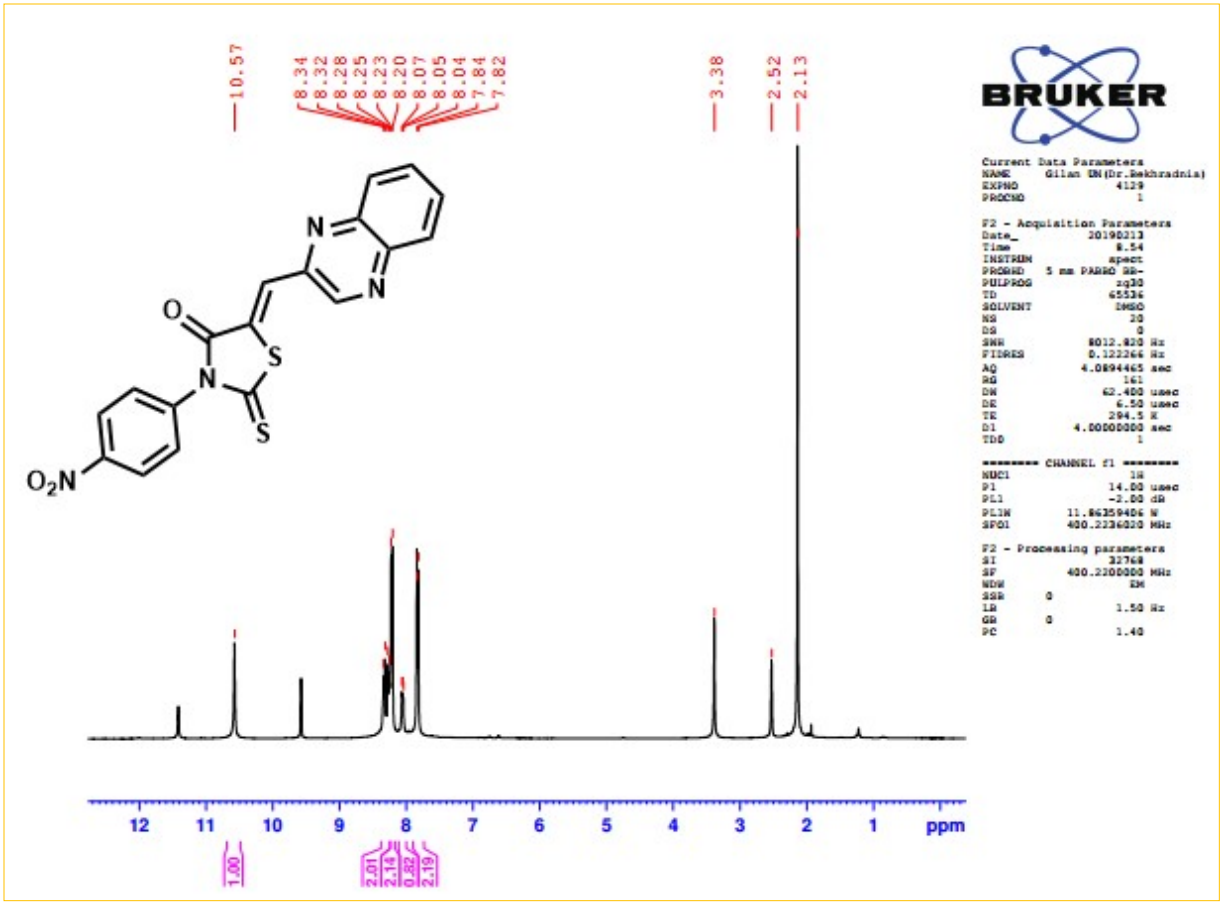
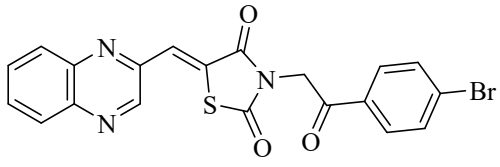


Fig S40. ^{1}HNMR Spectra. (Z)-3-(4-nitrophenyl)-5-(quinoxalin-2-ylmethylene)-2-thioxothiazolidin-4-one (**L2b**)



(3-(2)-4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-Dione(L5b); IR (KBr): 1743 and 1684 cm^{-1} (C=O); ^{1}HNMR (400 MHz, DMSO d_6) δ: 9.38 (s, 1H, H-3 Quinoxaline), 8.32 (s, 2H, CH), 8.23-8.28 (m, 1H, H-8 Quinoxaline), 8.14-8.19 (m, 1H, H-5 Quinoxaline), 8.04 (d, 2H, J = 8.4 Hz, H-2 and H-6 Phenyl), 7.93-8.00 (m, 2H, H-6 and H-7 Quinoxaline), 7.84 (d, 2H, J = 8.4 Hz, H-3 and H-5 Phenyl), 5.37 (s, 2H, CH_2);^{13}C NMR (100 MHz, DMSO d_6) δ: 208, 191, 170, 165, 148, 147, 141, 133, 132, 131, 130, 129, 126, 47

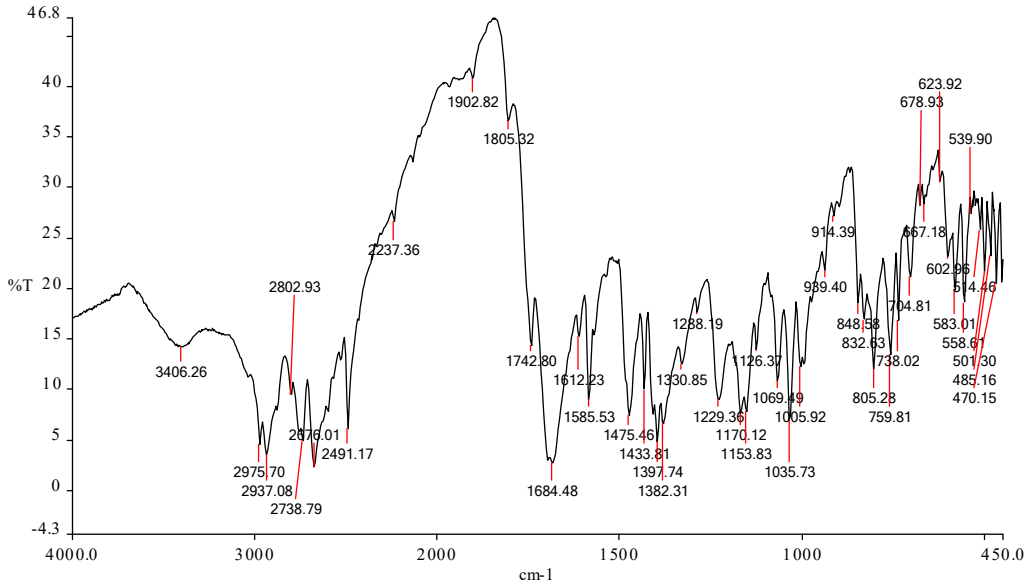


Fig S41. (FT-IR). (3-(2)-4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-Dione (**L5b**)

H-NMR طيف

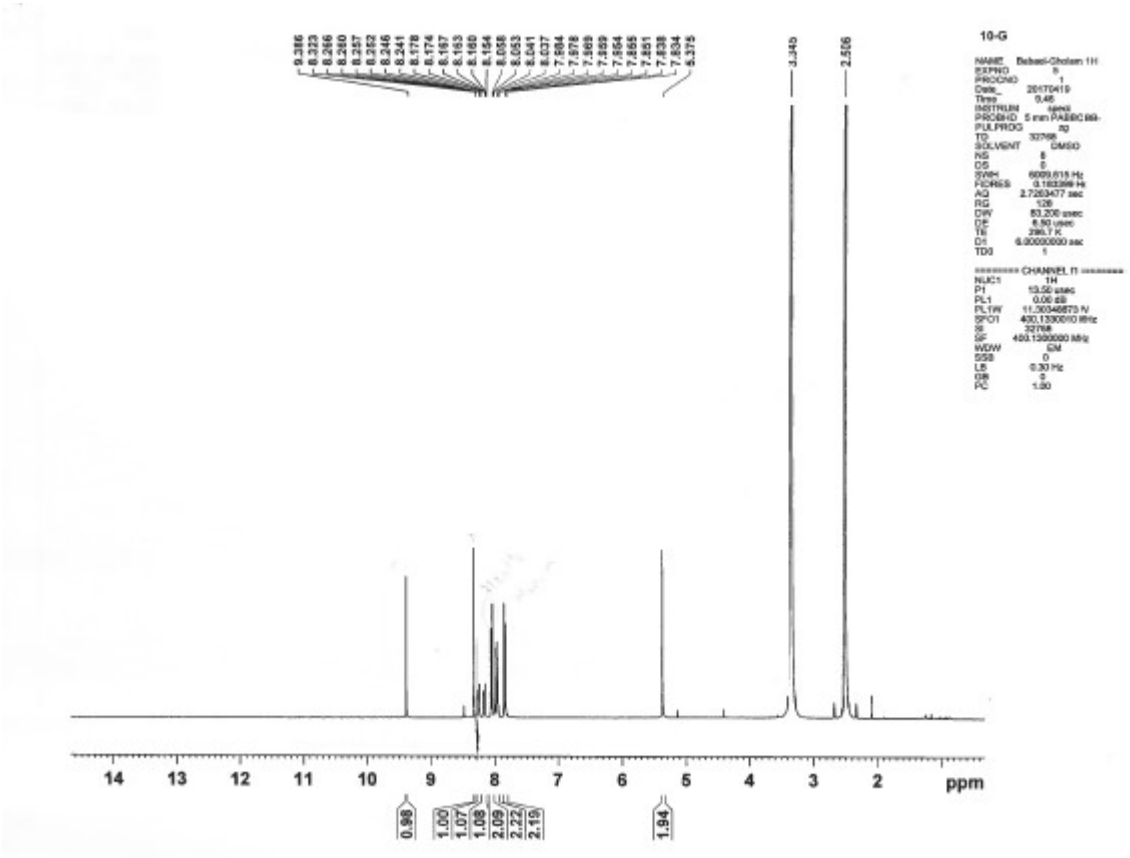


Fig S42. [1]HNMR Spectra. (3-(2)-4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-Dione (**L5b**)

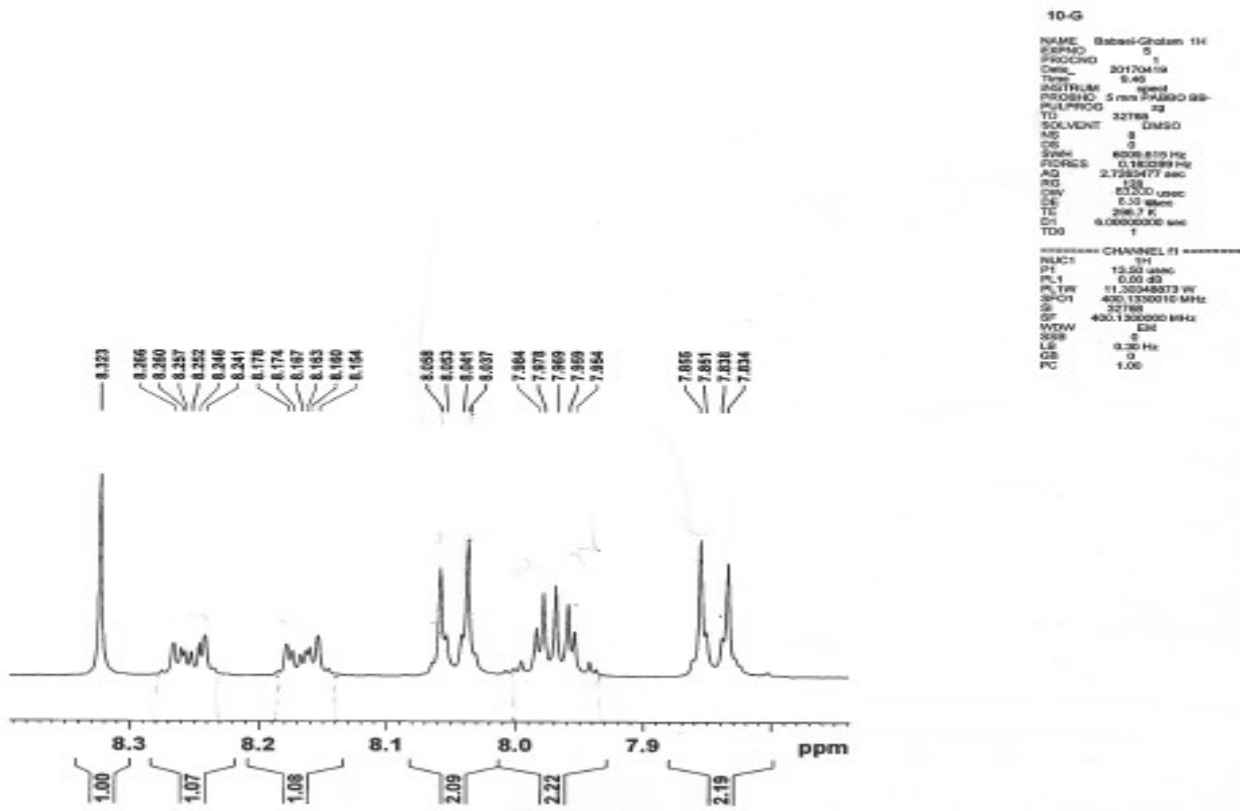
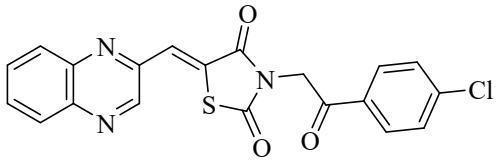


Fig S43. ^{1}HNMR expand spectra. (3-(2)-4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L5b**)



3-(2)-4-chlorophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (L9a); IR (KBr): 1743 and 1684 cm^{-1} (C=O);^{1}HNMR (400 MHz, DMSO d_6) δ: 9.39 (s, 1H, H-3 Quinoxaline), 8.33 (s, 2H, CH), 8.24-8.29 (m, 1H, H-8 Quinoxaline), 8.16-8.20 (m, 1H, H-5 Quinoxaline), 8.13 (d, 2H, J = 8.4 Hz, H-2 and H-6 Phenyl), 7.94-8.001 (m, 2H, H-6 and H-7 Quinoxaline), 7.70 (d, 2H, J = 8.8 Hz, H-3 and H-5 Phenyl), 5.38 (s, 2H, CH_2);

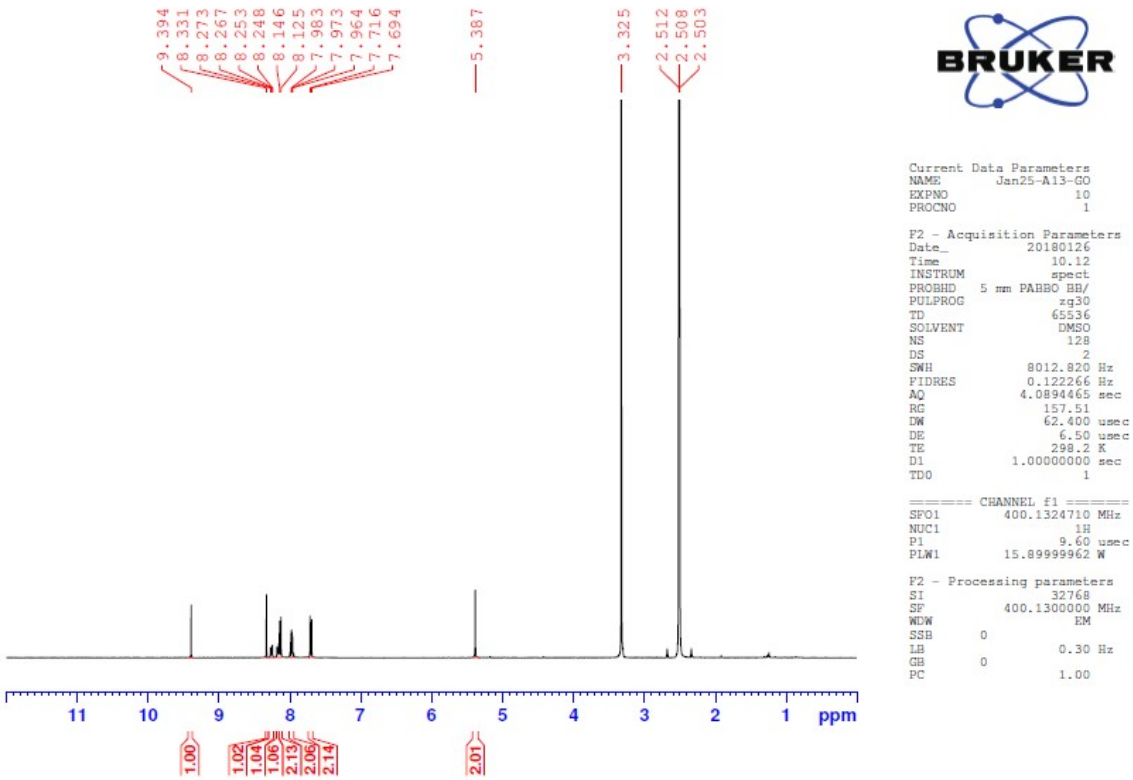


Fig S44. ^{1}HNMR Spectra. 3-(2)-4-chlorophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L9a**)

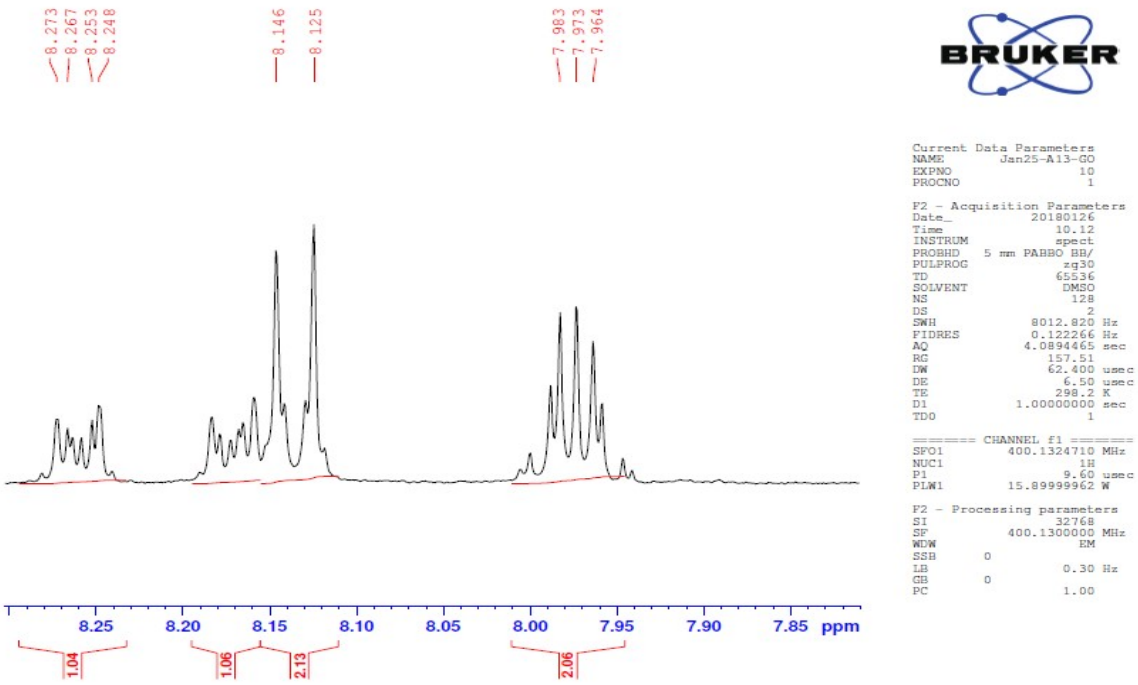


Fig S45. ^{1}HNMR expand spectra. 3-(2)-4-chlorophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L9a**).

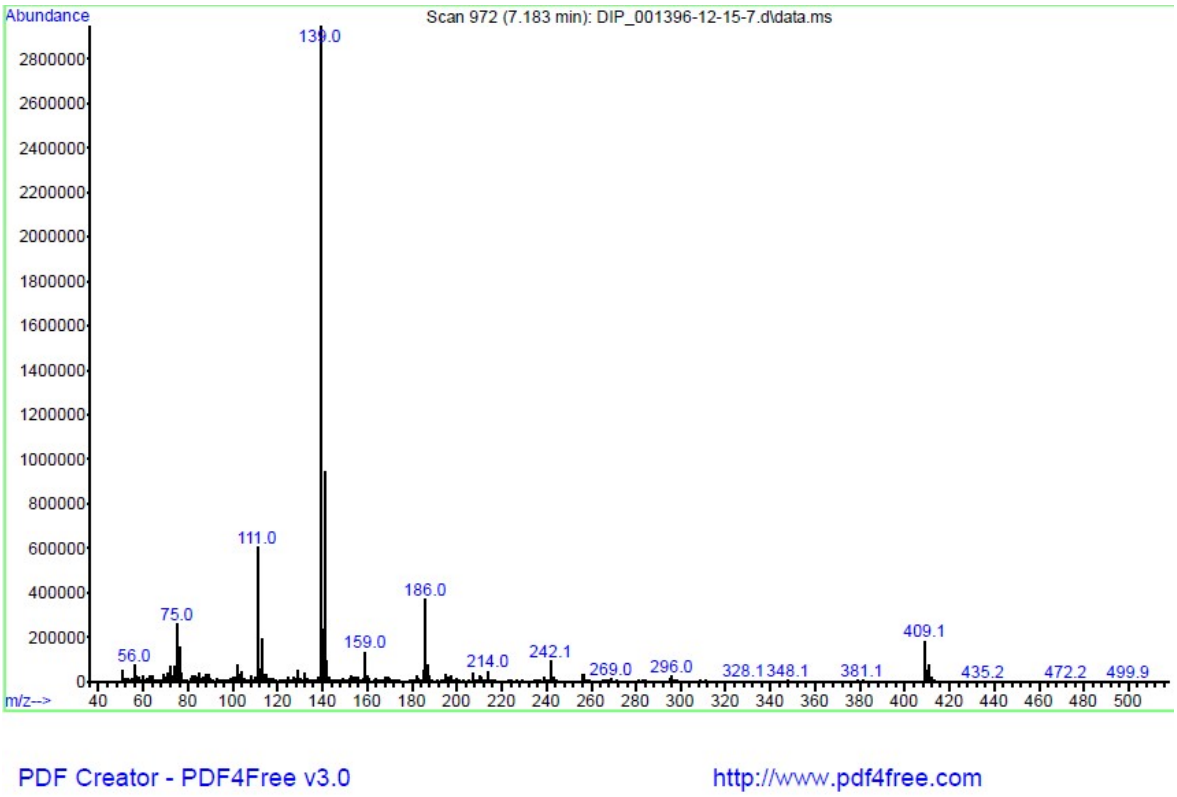


Fig S46. Mass Spectra. 3-(2)-4-chlorophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L9a**)

3-(2)-4-methoxyphenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (L6b); IR (KBr): 1743 and 1684 cm^{-1} (C=O);^{1}HNMR (400 MHz, DMSO d_6) δ: 9.39 (s, 1H, H-3 Quinoxaline), 8.32 (s, 2H, CH), 8.23-8.30 (m, 1H, H-8 Quinoxaline), 8.14-8.20 (m, 1H, H-5 Quinoxaline), 8.09 (d, 2H, J = 8.4 Hz, H-2 and H-6 Phenyl), 7.93-8.01 (m, 2H, H-6 and H-7 Quinoxaline), 7.13 (d, 2H, J = 8.4 Hz, H-3 and H-5 Phenyl), 5.30 (s, 2H, CH_2), 3.89 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO d_6) δ: 208, 191, 170, 165, 148, 147, 141, 133, 132, 131, 130, 129, 126, 47

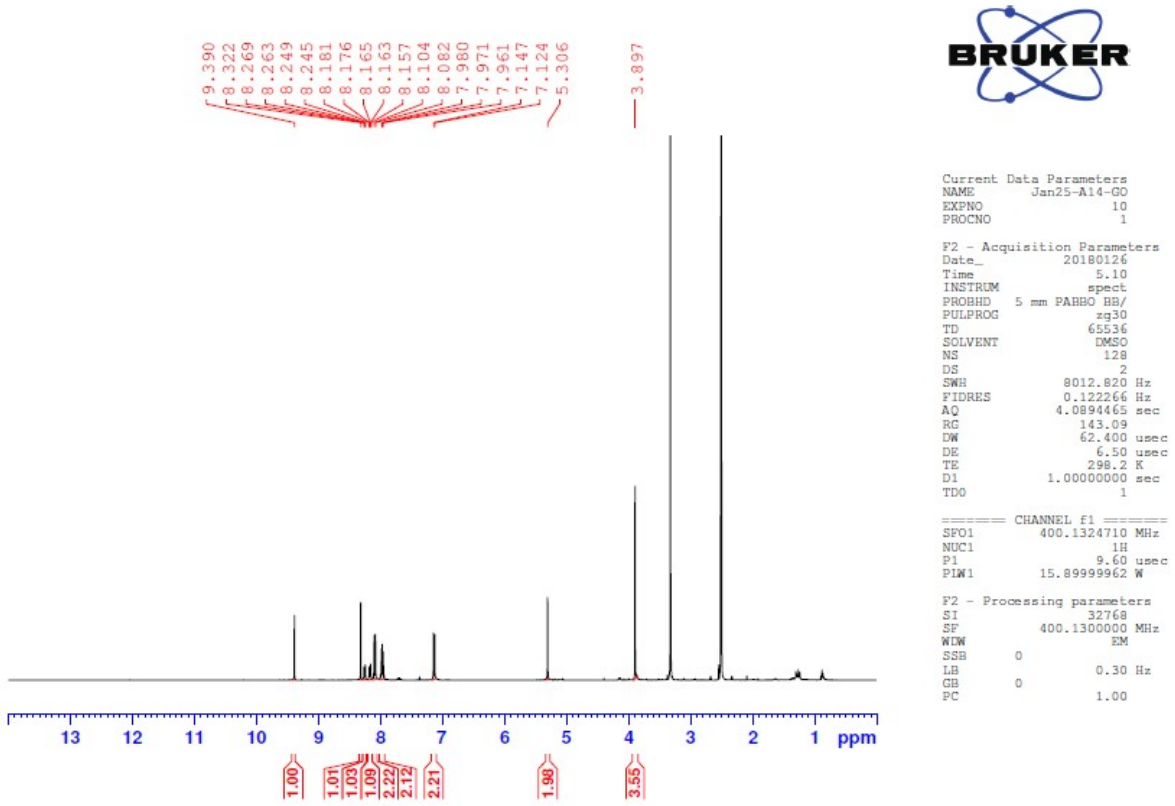


Fig S47. ^{1}HNMR Spectra. 3-(2)-4-methoxyphenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L6b)**

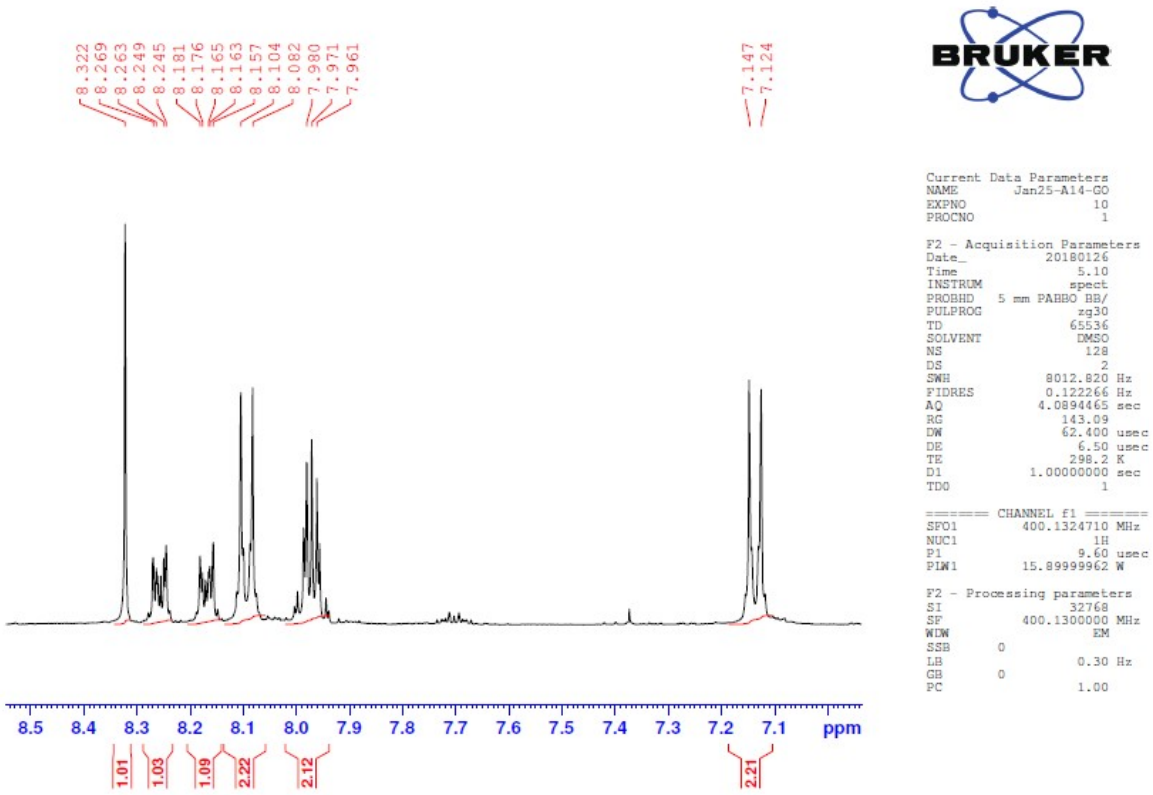


Fig S48. ^{1}HNMR expand spectra. 3-(2)-4-methoxyphenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L6b)**

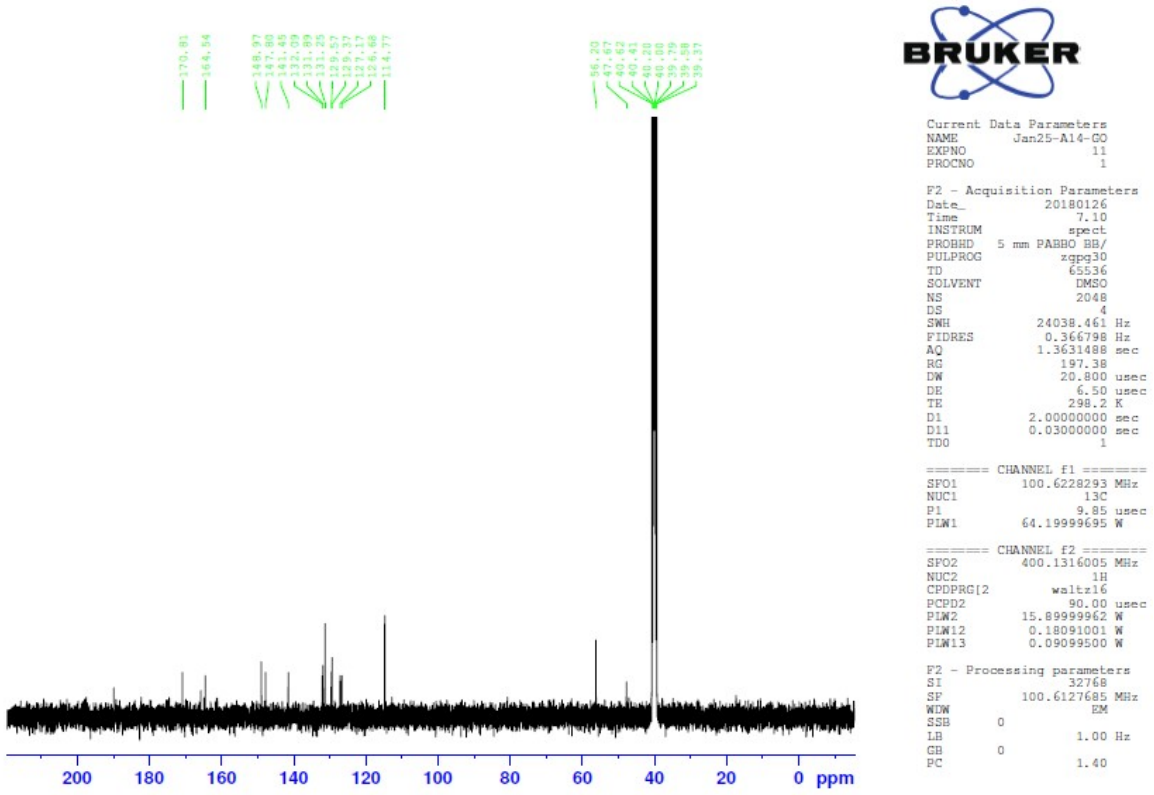
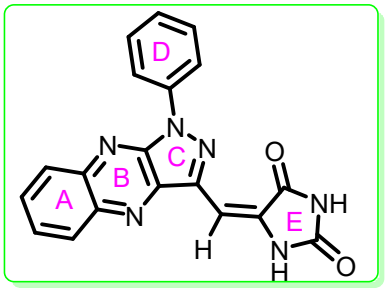


Fig S49. ^{13}CNMR Spectra. 3-(2)-4-methoxyphenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) thiazolidine-2,4-dione (**L6b)**



5-((1-phenyl-1*H*-pyrazolo[3,4-*b*]quinoxalin-3-yl)methylene)imidazolidine-2,4-dione (L1a); ^{1}HNMR (400 MHz, $CDCl_3$) δ (ppm): 8.56 (S, 1H, N_1H Imidazolidine), 8.27 (S, 1H, N_2H Imidazolidine), 7.84-7.89 (m, 2H, H-2 and H-6 ring D), 7.78-7.83 (m, 2H, H-5 and H8 Quinoxaline), 7.44-7.57 (m, 4H, H-6 and H-7 Quinoxaline, H-3 and H-5 ring D), 7.53 (S, 1H, H Arylidene), 7.47 (tt, 1H, H-4 ring D, J = 7.2 and 1.2 Hz). ^{13}C-NMR (400 MHz, $CDCl_3$) δ (ppm): 119.2, 122.3, 123.5 (Aromatic carbons ring D); 127.3, 129.1, 129.6, 130.5, 134.7, 139.6, 142.9, 152.8.

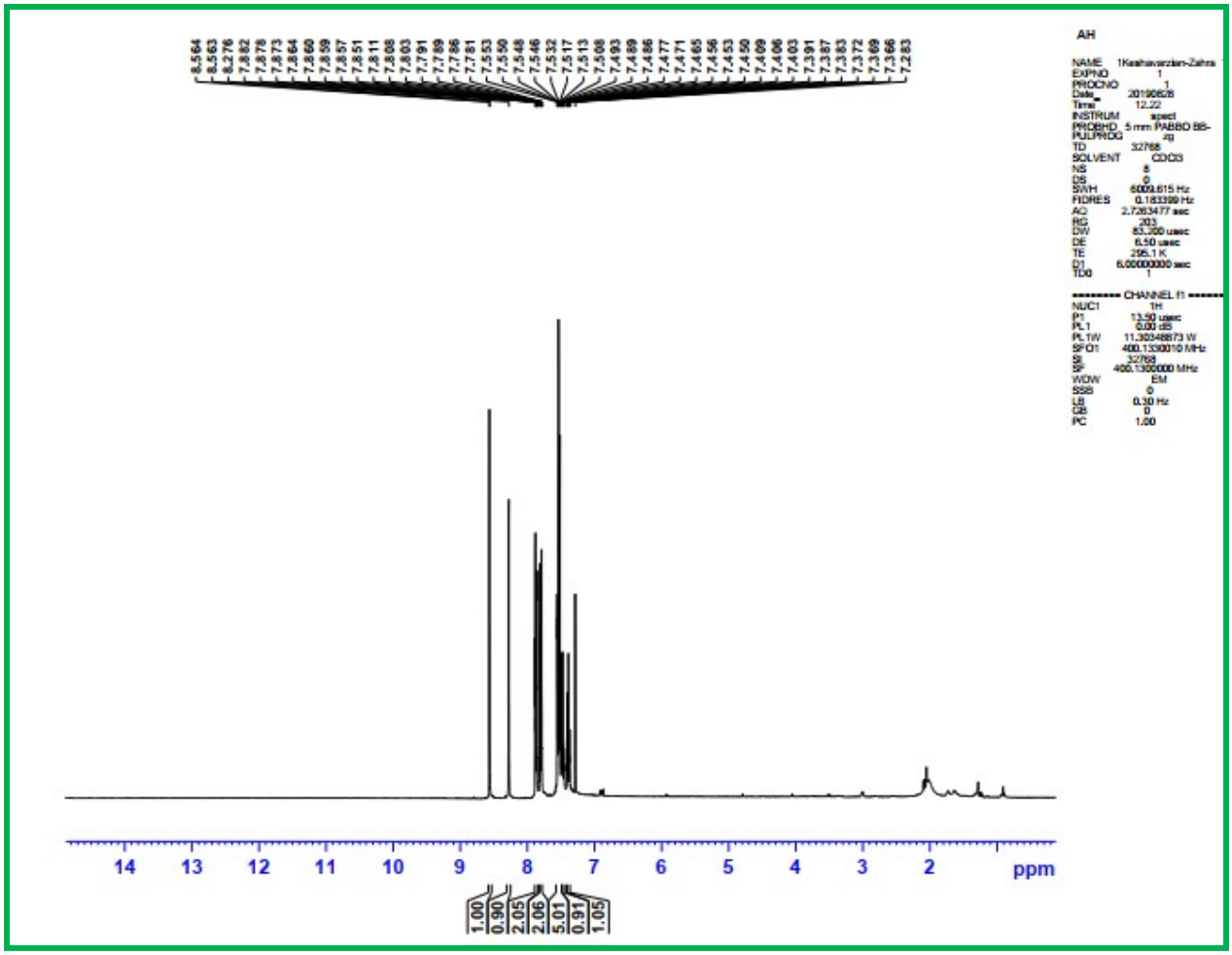


Fig S50. ^{1}HNMR Spectra. 5-((1-phenyl-1*H*-pyrazolo[3,4-*b*]quinoxalin-3 yl)methylene)imidazolidine-2,4-dione (**L1a)**

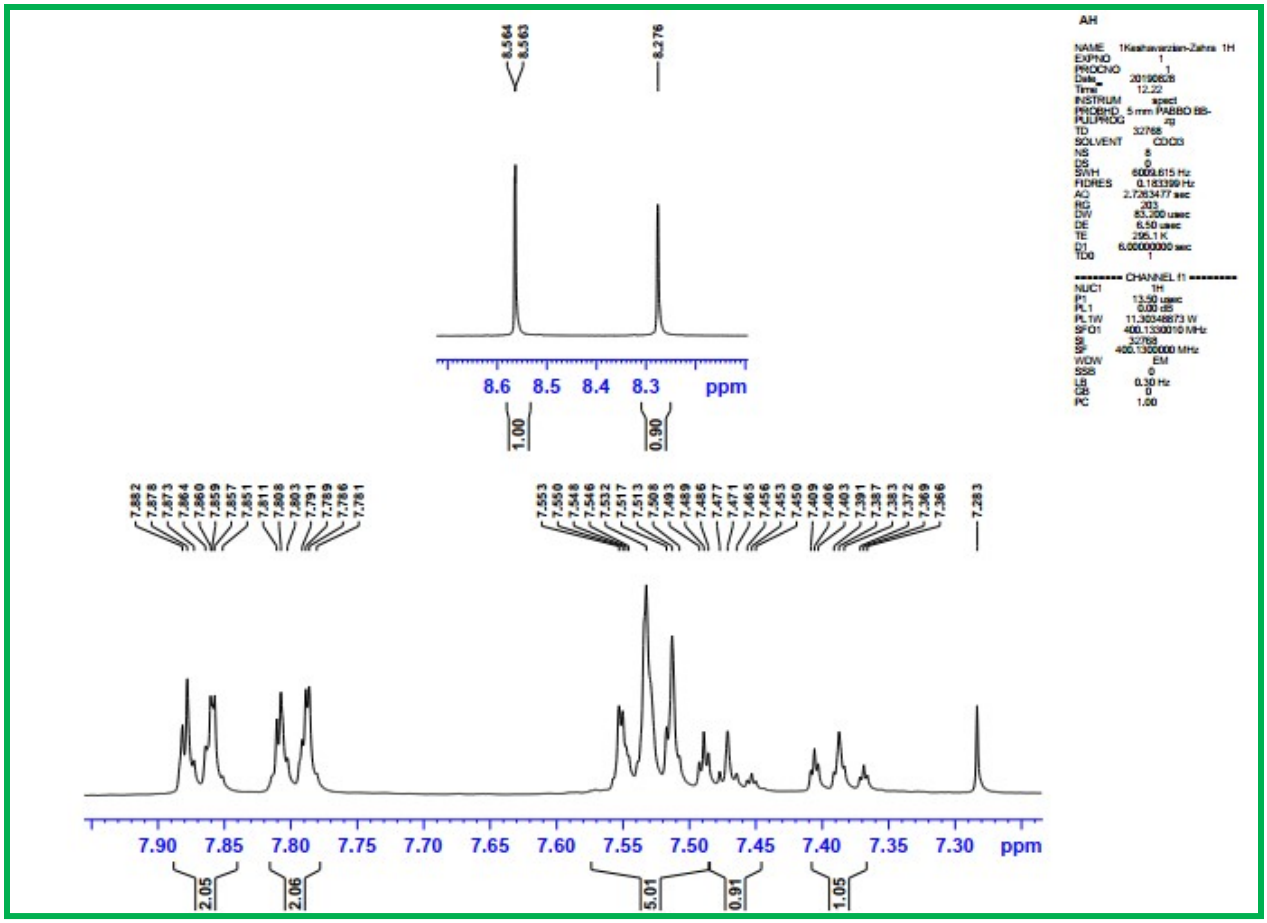


Fig S51. [1]HNMR expand spectra. 5-((1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxalin-3 yl) methylene) imidazolidine-2,4-dione (**L1a)**

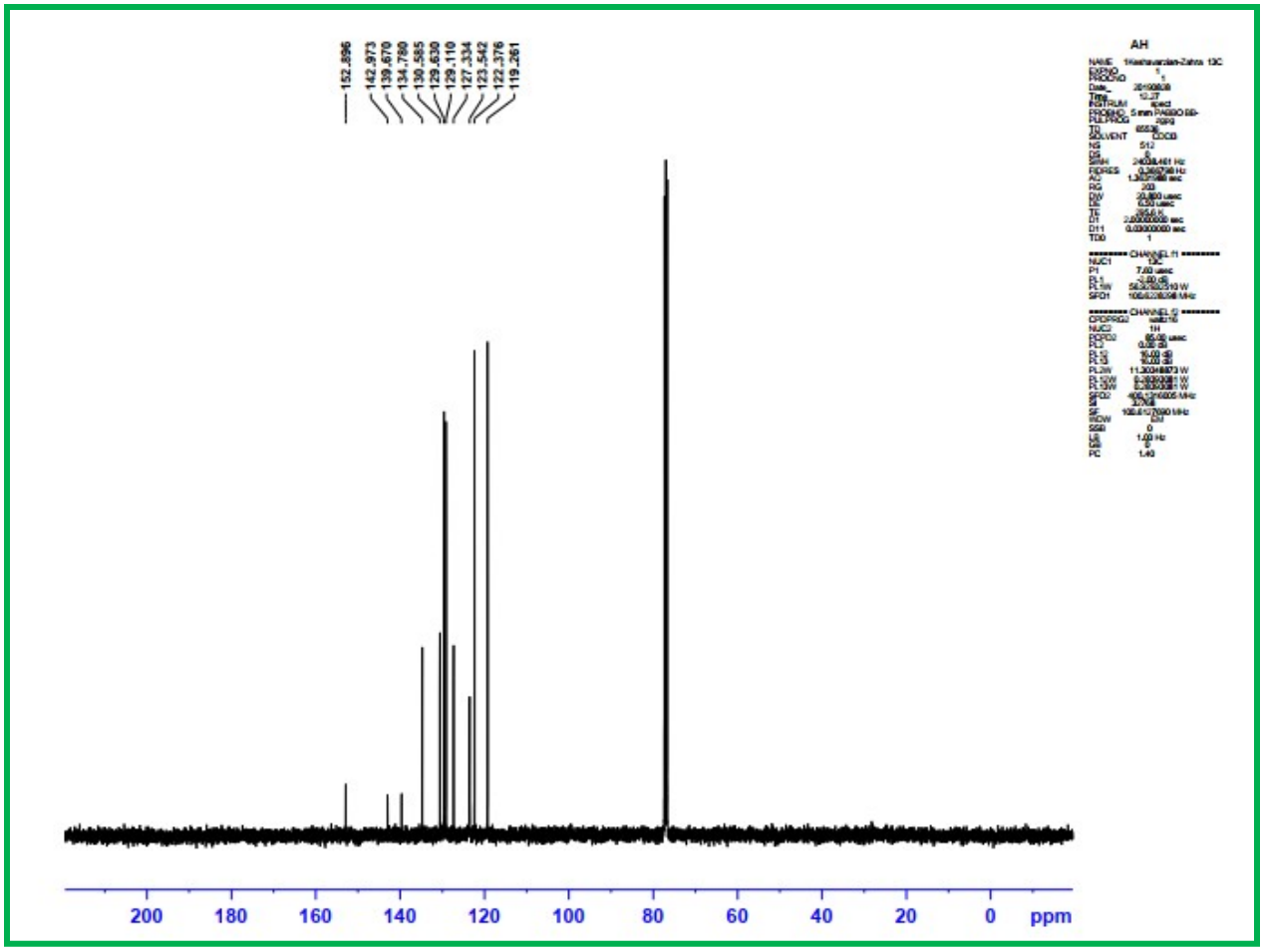


Fig S52. ^{13}CNMR spectra. 5-((1-phenyl-1*H*-pyrazolo[3,4-*b*] quinoxalin-3 yl) methylene) imidazolidine-2,4-dione (**L1a)**

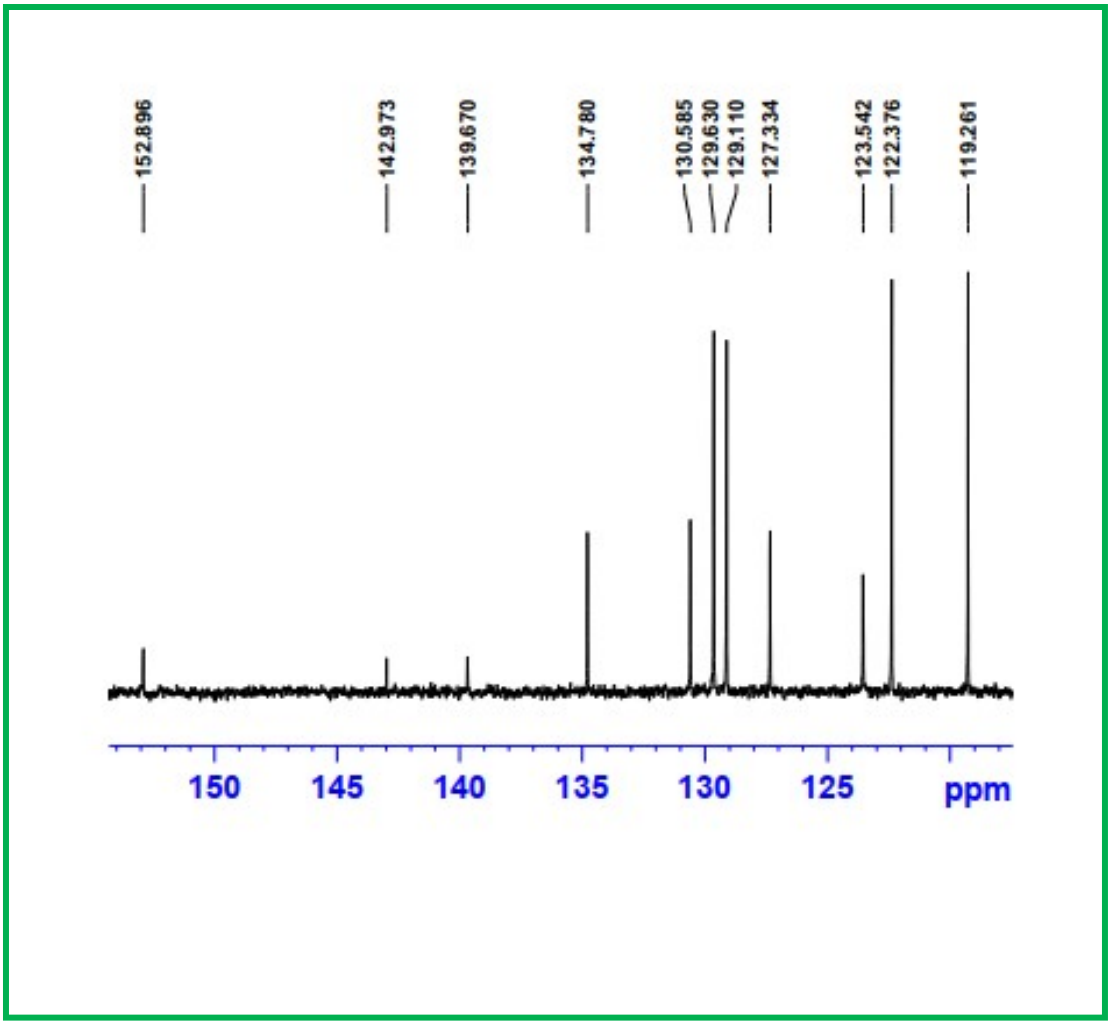


Fig S53. ^{13}CNMR expand spectra. 5-((1-phenyl-1*H*-pyrazolo[3,4-*b*]quinoxalin-3 yl)methylene)imidazolidine-2,4-dione (**L1a)**

3-(2-oxo-2-(thiophen-3-yl)ethyl)-5-(quinoxaline-2-yl methylene) thiazolidine 2,4 dione (L3c); ^{1}H-NMR (400MHz, DMSO); δ:9.37(s,1H, H-3 Quinoxaline),5.13(s,1H, H-Vinyl),8.15-8.22(m,1H,H-8 Quinoxaline), 8.05-8.11(m,1H,H-5 Quinoxaline) 8.11(d,d,1H,J=5Hz and J=1.2Hz, H-3 Thiophen) 7.87-7.92(m,2H,H-6 and H-7 quinoxaline) 7.30(AB Quartet,1H,J=4.8Hz and J=4Hz)5.23(s, 2H,CH_2); ^{13}C-NMR (100MHz, DMSO); δ:184.91,170.76,165.60 (C=O), 148.9, 147.7, 141.4, 136.9, 135.5, 132.1, 131.8, 129.6, 129.4,1 26.8, 48.0(CH_2).

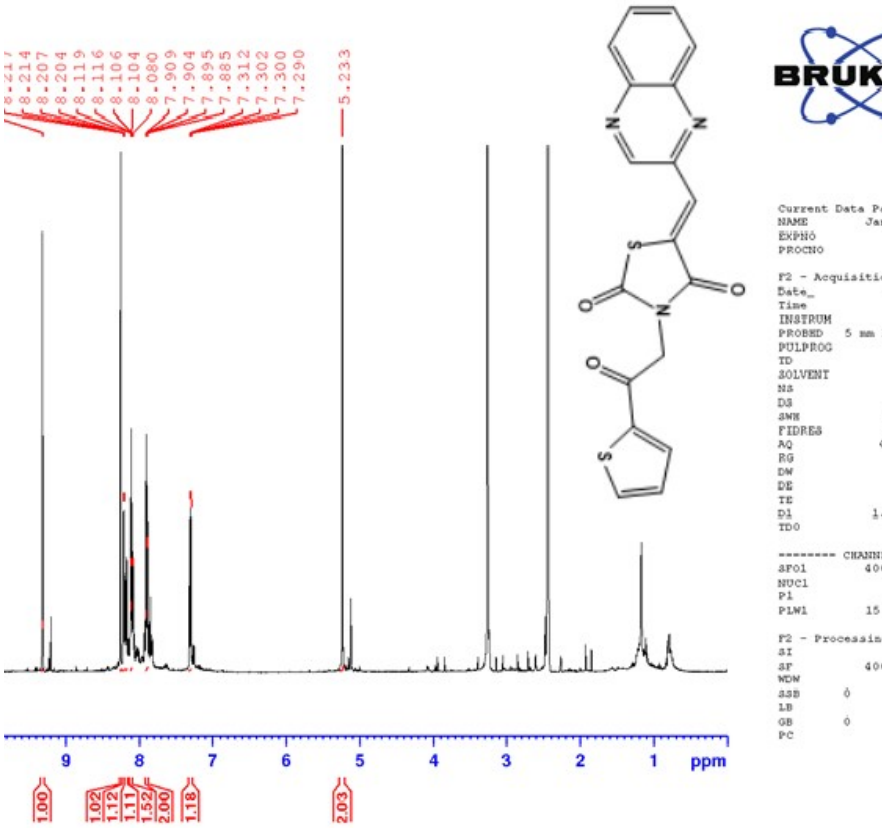


Fig S54. [1]HNMR Spectra. 3-(2-oxo-2-(thiophen-3-yl)ethyl)-5-(quinoxaline-2-yl methylene) thiazolidine 2,4 dione (**L3c**)

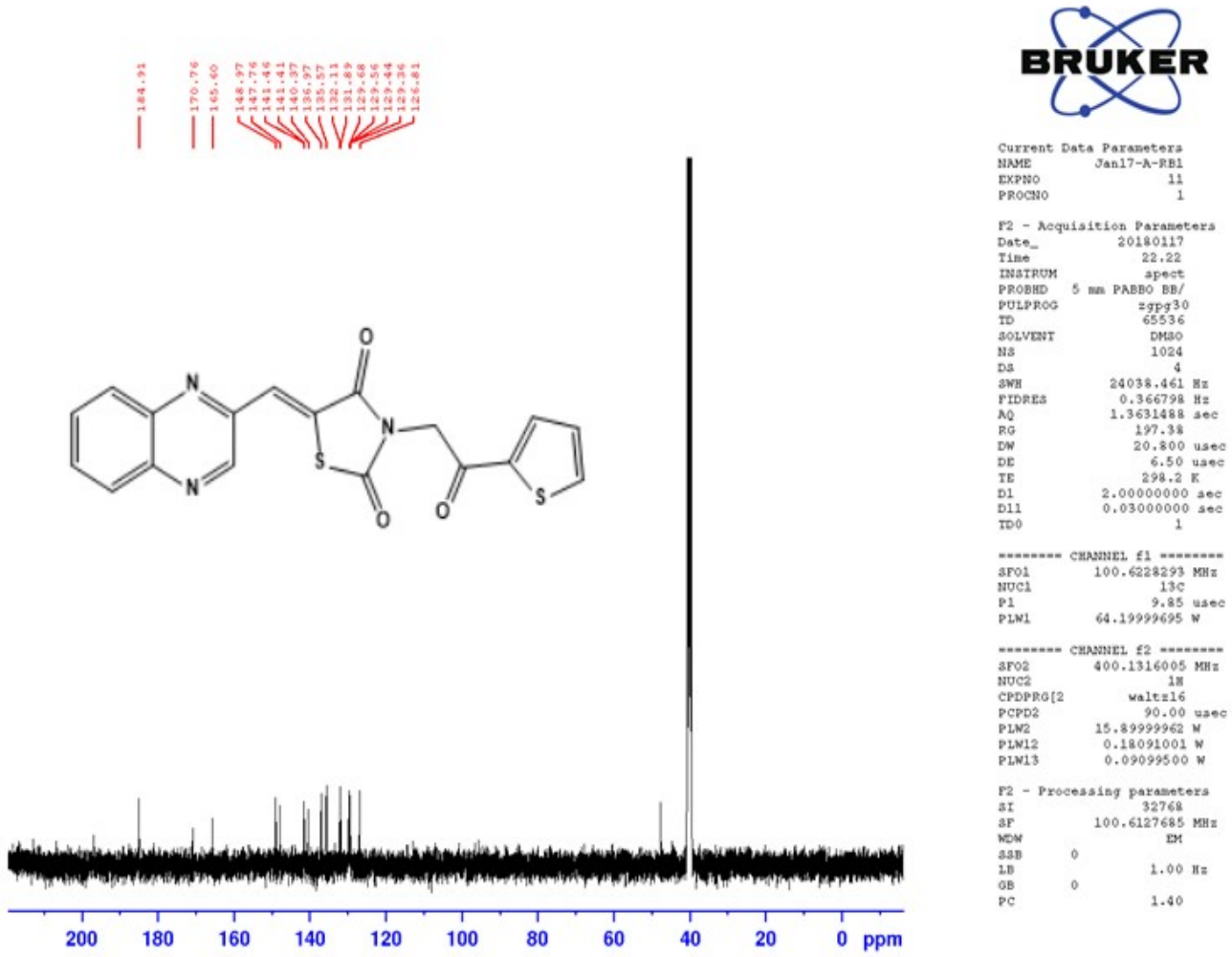


Fig S55. ^{13}CNMR Spectra. 3-(2-oxo-2-(thiophen-3-yl)ethyl)-5-(quinoxaline-2-yl methylene) thiazolidine 2,4 dione (**L3c**)

3-(2-oxo-2-phenyl ethyl)-5-)quinoxaline-2-yl methylene)thiazolidine 2,4 dione(L4b); IR (KBr, cm^{-1}) vmax:1695,1754cm^{-1}(C=O),1544cm^{-1}(C=N),1499cm^{-1}(C=C)1447cm^{-1}(C-N)^{1}H-NMR400) MHz, DMSO); δ:8/99(s,1H, H-3Quinoxaline), 4.42(s,1H, H Vinyl),5.17(s,2H,

$CH_2C=O$), 8.14-8.16(d, d,2H, Quinoxaline), 7.89-7.91(d, d,2H, Quinoxaline)7.78-7.80(m,2H, Acetophenone)7.53 7.55(m,2H, Acetophenone)7.48-7.50(m,1H, acetophenone); ^{13}C-NMR (100MHz, DMSO); 191.3, 172.4, 172.1, 146.0, 139.1, 133.1, 129.6, 129.4, 129.1, 127.6, 127.5, 48.0.

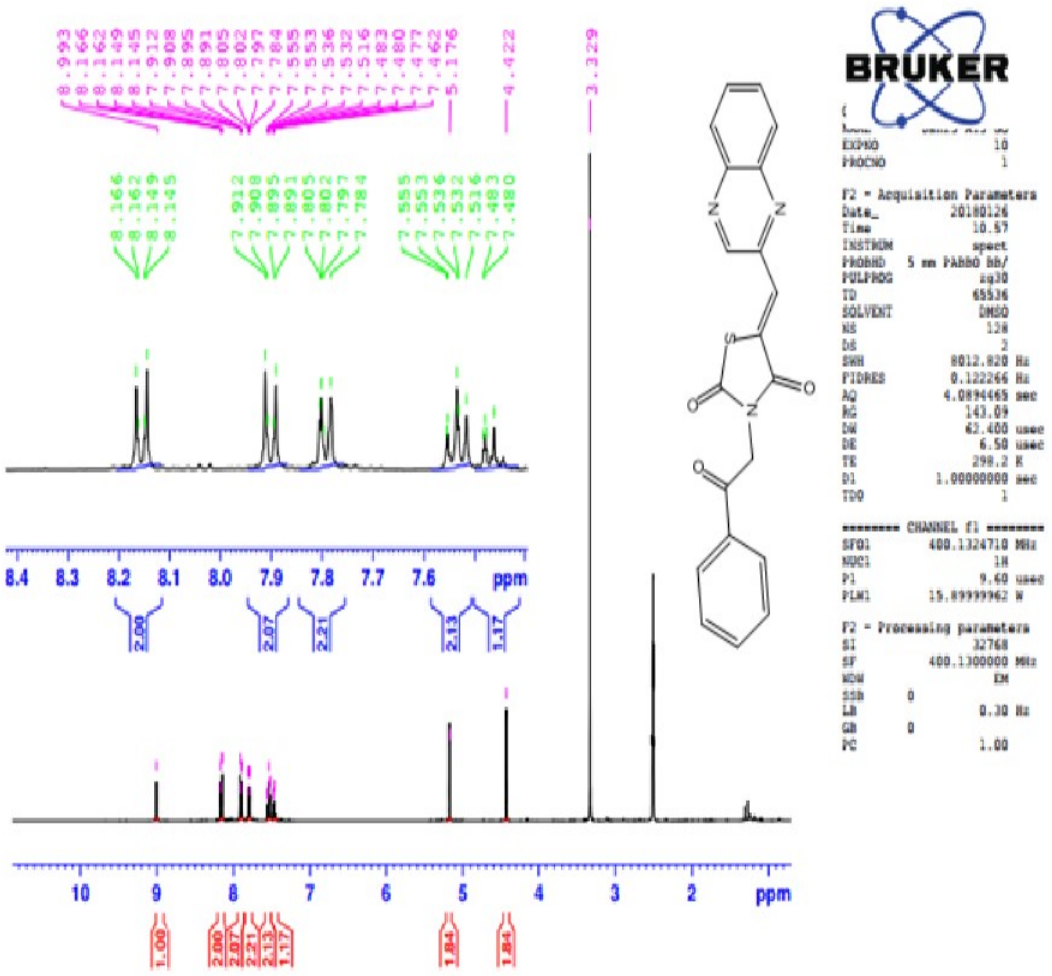
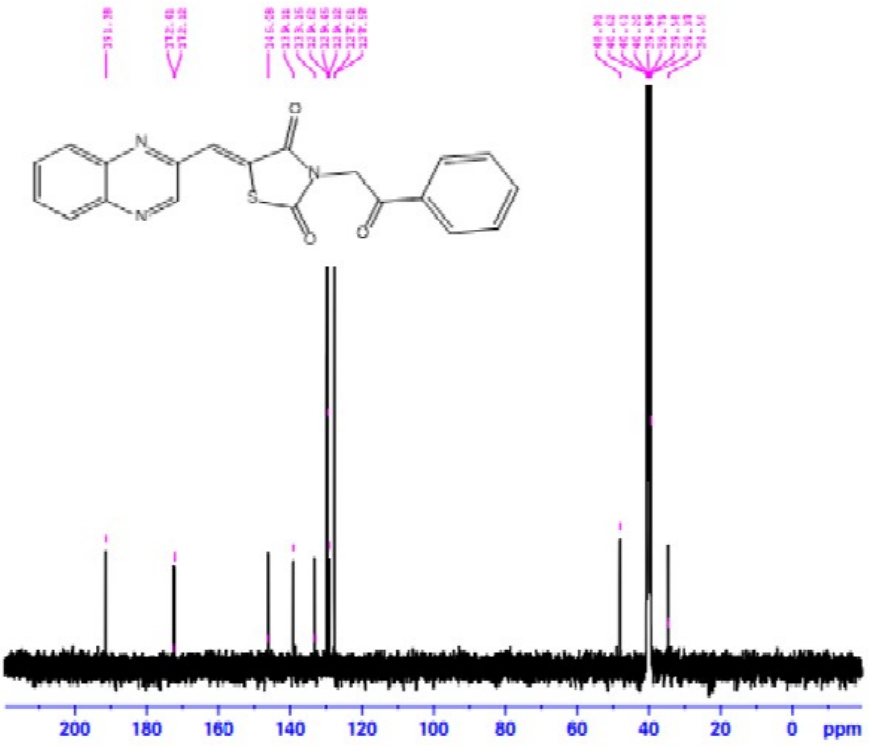


Fig S56. ^{1}HNMR Spectra. 3-(2-oxo-2-phenyl ethyl)-5-)quinoxaline-2-yl methylene)thiazolidine 2,4 dione **(L4b)**

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NS                  2048
DS                     4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                197.38
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DE                6.50 usec
TE              298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

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NUC1                 13C
P1                  9.85 usec
PL1          64.19999695 W

======== CHANNEL f2 ========
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NUC2                 1H
CPDPRG[2          waltz16
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PL2          15.89999962 W
PL12          0.18691801 W
PL13          0.99999500 W

F2 - Processing parameters
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Fig S57. ^{13}CNMR Spectra. 3-(2-oxo-2-phenyl ethyl)-5-)quinoxaline-2-yl methylene)thiazolidine 2,4 dione **(L4b)**

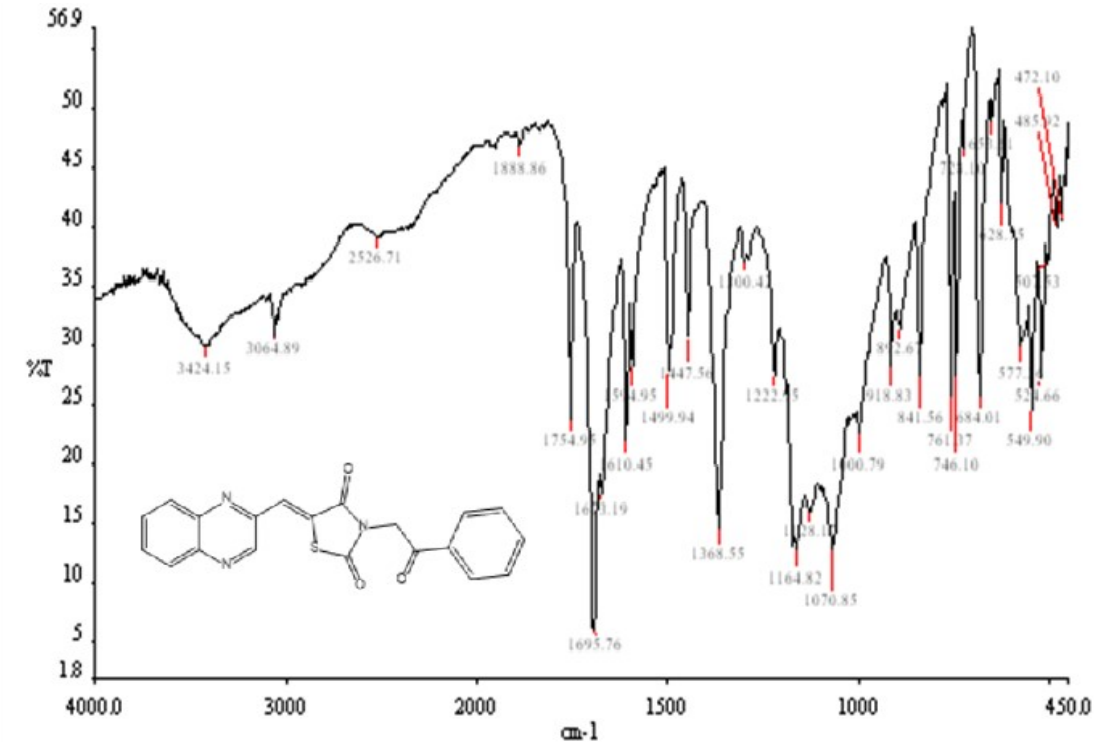


Fig S58. FTIR Spectra. 3-(2-oxo-2-phenyl ethyl)-5-) quinoxaline-2-yl methylene) thiazolidine 2,4 dione **(L4b)**

(Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one(L5a); IR (KBr, cm^{-1}) *v*: 2922(C-H aromatic), 1706(C=O), 1474(C=N), 1299(C=C).^{1}HNMR (400 MHz, DMSO d_6) δ: 9.04(S, 1H, H-3 Quinoxaline), 7.85(S, 1H, $H_{c=c}$), 8.02(d, 1H,J=9.2 Hz, H-8 Quinoxaline), 8.14(d, 1H,J=2.4, Hz H-5 Quinoxaline), 8.08 (d,J=9.2 Hz1H, H-7 Quinoxaline), 3.59(s, 3H, CH_3) ppm;^{13}C NMR (100 MHz, DMSO-d6) δ: 29.70 (C-Me), 123.05,127.97, 128.38, 130.42, 132.35, 132.68, 137.38, 141.54, 147.96, 178.82, 203.01.

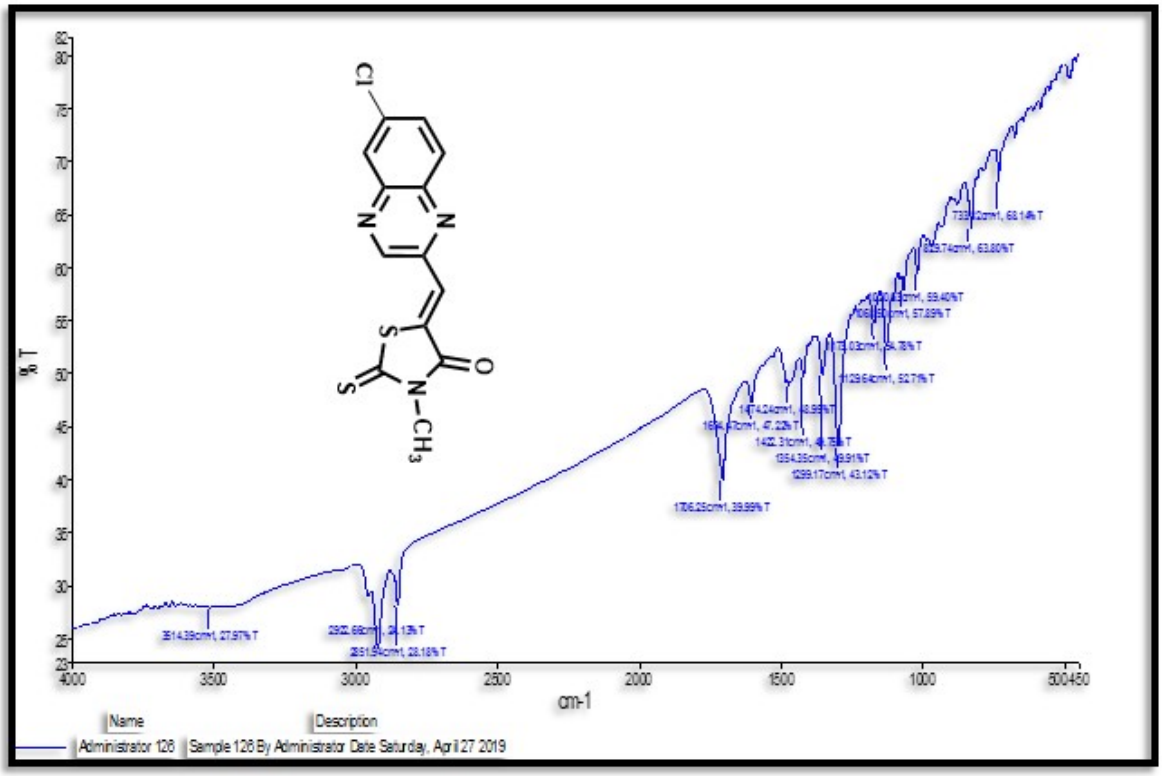


Fig S59. FTIR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one **(L5a)**

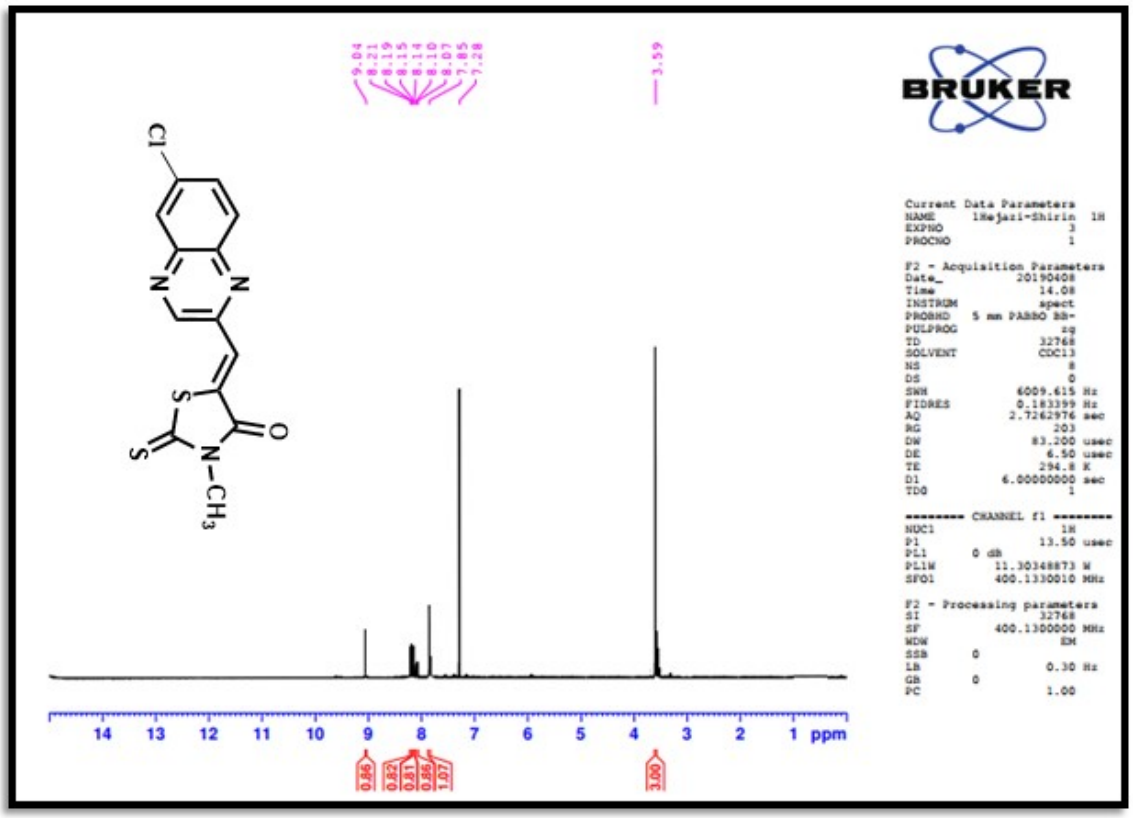


Fig S60. ^{1}HNMR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one **(L5a)**

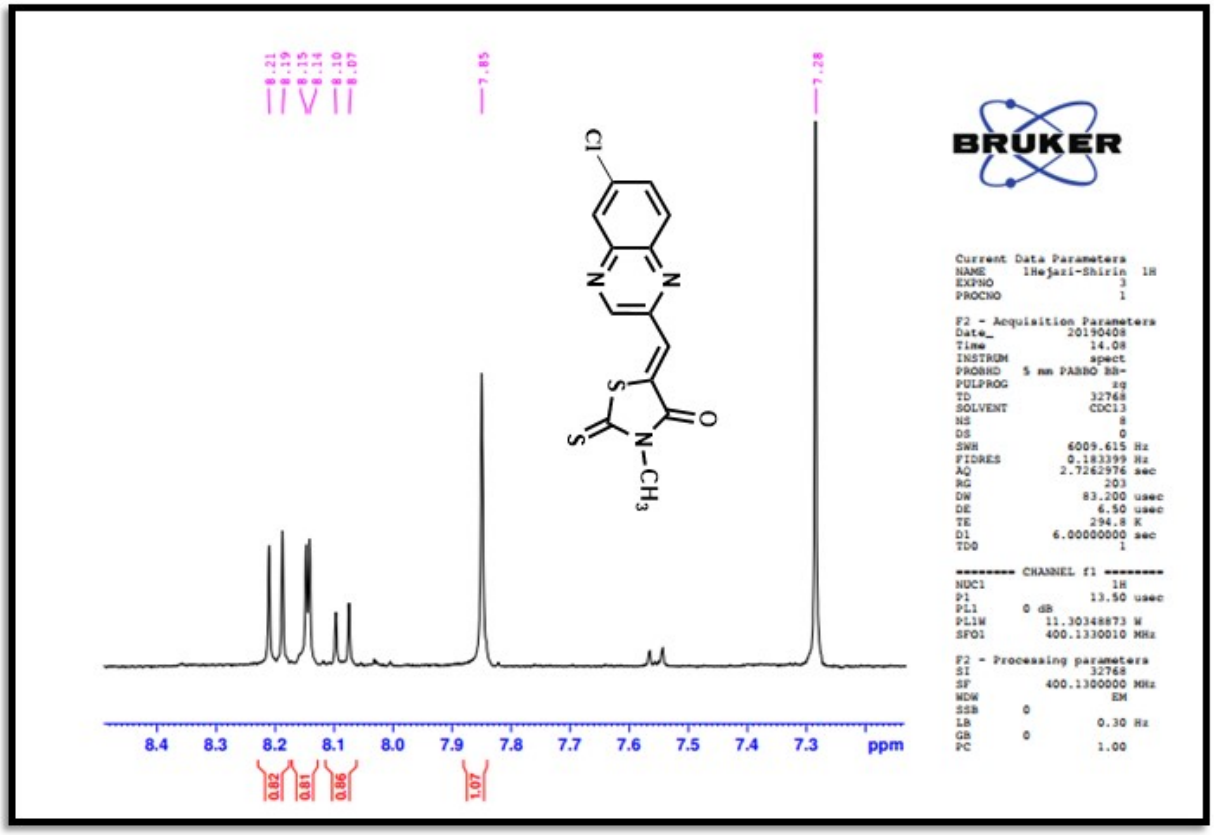


Fig S61. [1]HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one **(L5a)**

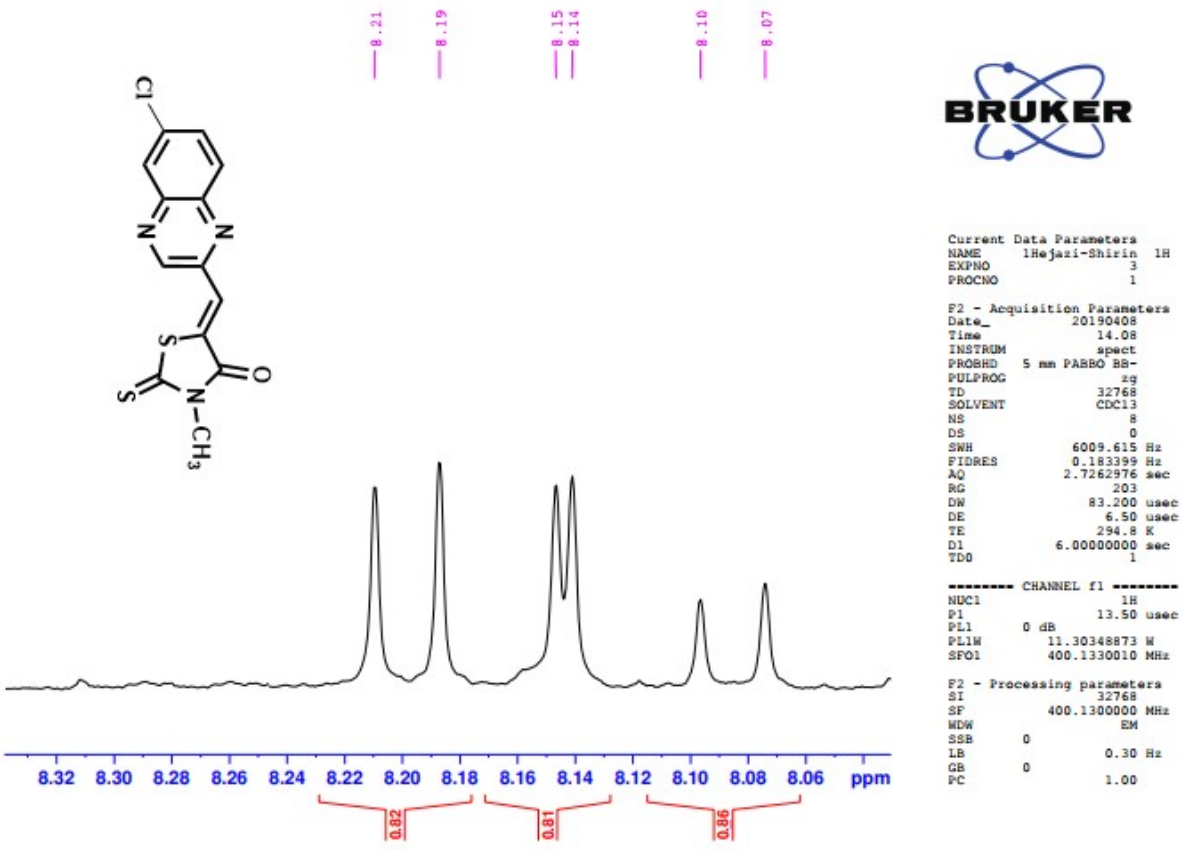


Fig S62. ^{1}HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one **(L5a)**

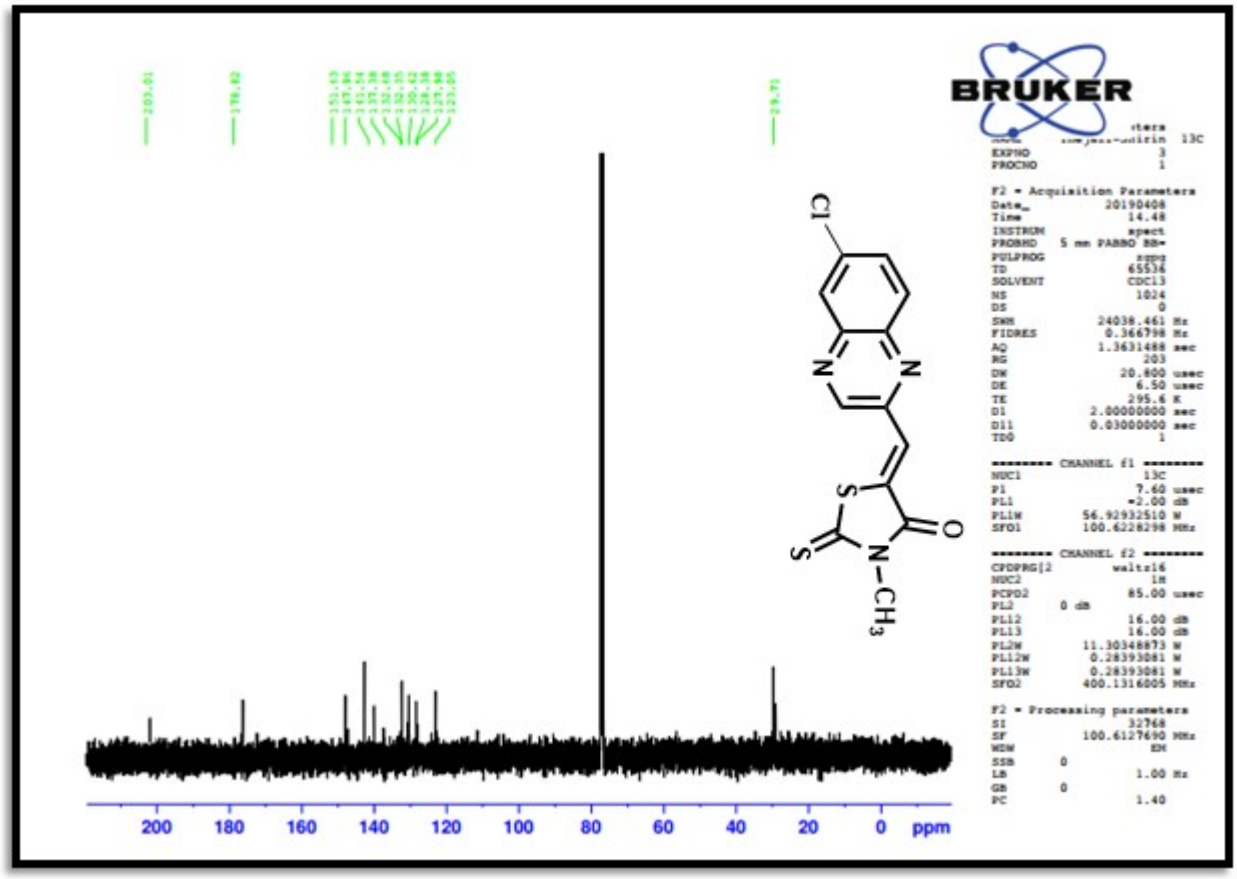
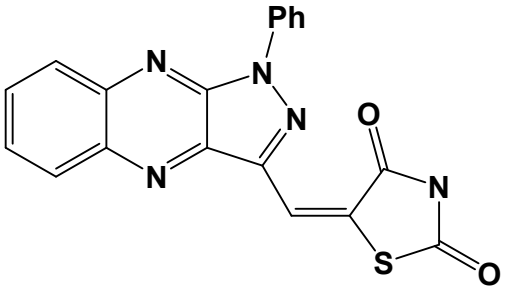


Fig S63. ^{13}**CNMR expand Spectra.** (Z)-5-((6-chloroquinoxalin-2-yl) methylene)-3-methyl-2-thioxothiazolidin-4-one **(L5a)**



5-((1-phenyl-1H-pyrazolo[3,4-b] quinoxalin-3-yl) methylene) thiazolidine-2,4-dione(L3a) ;IR (KBr, cm^{-1}) v_{max}:3334.32cm^{-1}(NH),1509.99cm^{-1}(C=O),1424.17cm^{-1}(C=S);^{1}H-NMR (500MHz, DMSO); δ:9.36(s,1H, NH),8.28(s,1H, H-Vinyl),7.98(d,2H, j=8, H-2′and H-5′),7.81(d,2H, j=8, H-3′and H-4′),7.52-7.59(m,4H, H-2, H-3, H-5 and H-6),7.39(t,1H, j=14.5, H-4); ^{13}C-NMR (125MHz, DMSO); δ:119.5,122.4,126.6,130.1 (Aromatic carbons ring D),127.6,129.8 (Aromatic carbons ring A),142.9,143.8,152.7 (Ring B),139.5 (Ring C),131.2 (C Vinyl),133.7 (C_5),168.7 (C=O),183.6(C=S).

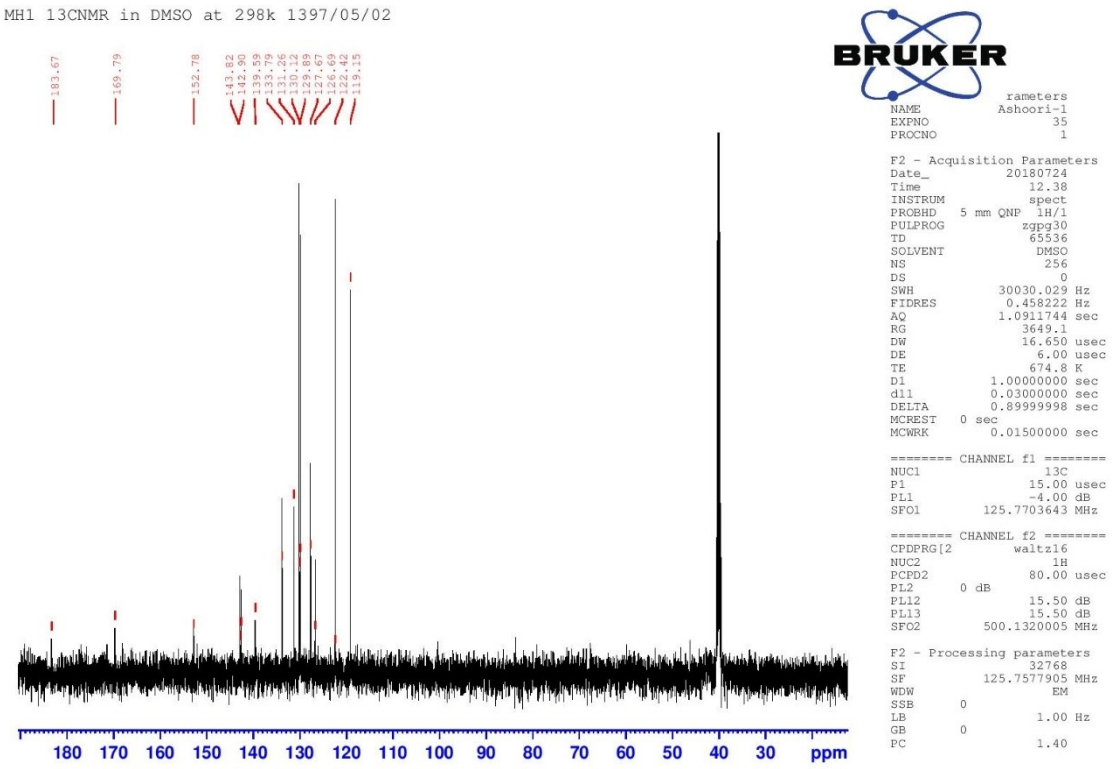


Fig S68. ^{13}CNMR Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b] quinoxalin-3-yl) methylene) thiazolidine-2,4-dione **(L3a)**

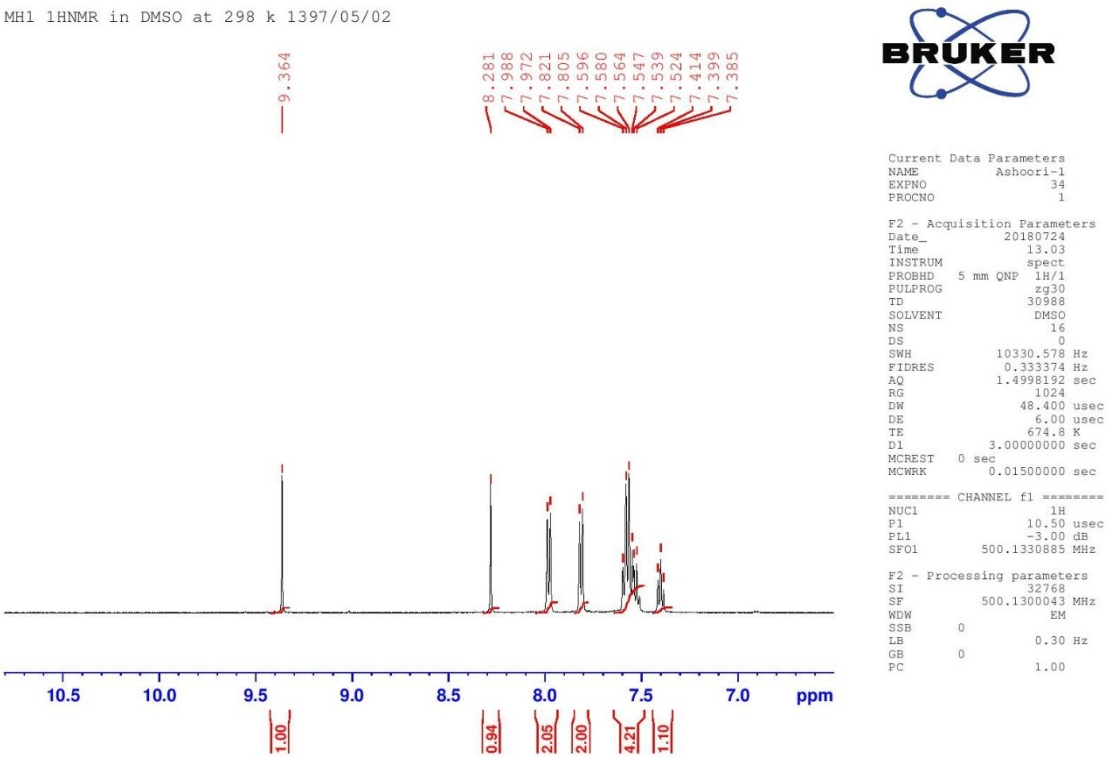


Fig S69. ^{1}HNMR expand Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b] quinoxalin-3-yl) methylene) thiazolidine-2,4-dione **(L3a)**

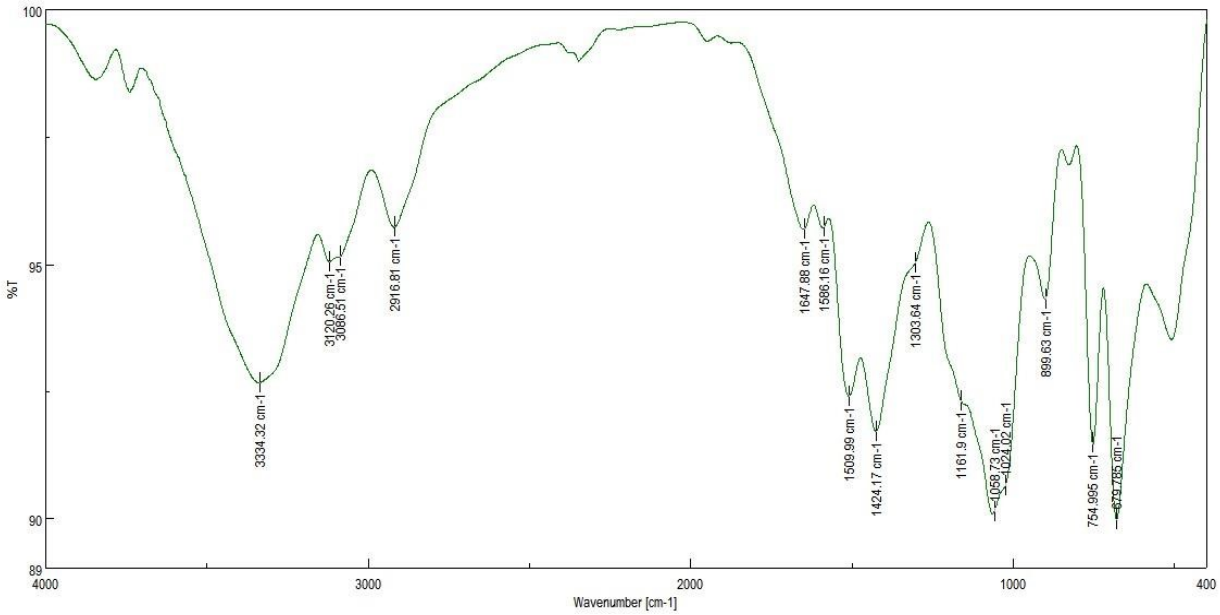


Fig S70. FTIR Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b] quinoxalin-3-yl) methylene) thiazolidine-2,4-dione **(L3a)**

(Z)-3-(2-(4-Bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene)imidazolidine-2,4-dione; IR (KBr): ν_{max} = 3433 (NH), 2863 (CH aldehyde), 1728, 1700, 1694 (3 C=O), 1690-1647 (CH aromatic&olefinic, C=N), 1324 (C-N), 665 (C-Br) cm^{-1};^{1}H NMR (400 MHz, DMSO): δ4.07 (s, 2H, CH_2), 5.56 (s, 1H, NH), 7.19-7.54 (m, 4H, Ar-H), 7.72 (s, 1H, CH), 7.79 (d, 2H, J = 8.4 Hz, Ar-H), 7.98 (d, 2H, J = 8.4 Hz, Ar-H), 8.25 (s, 1H, NCH) ppm.

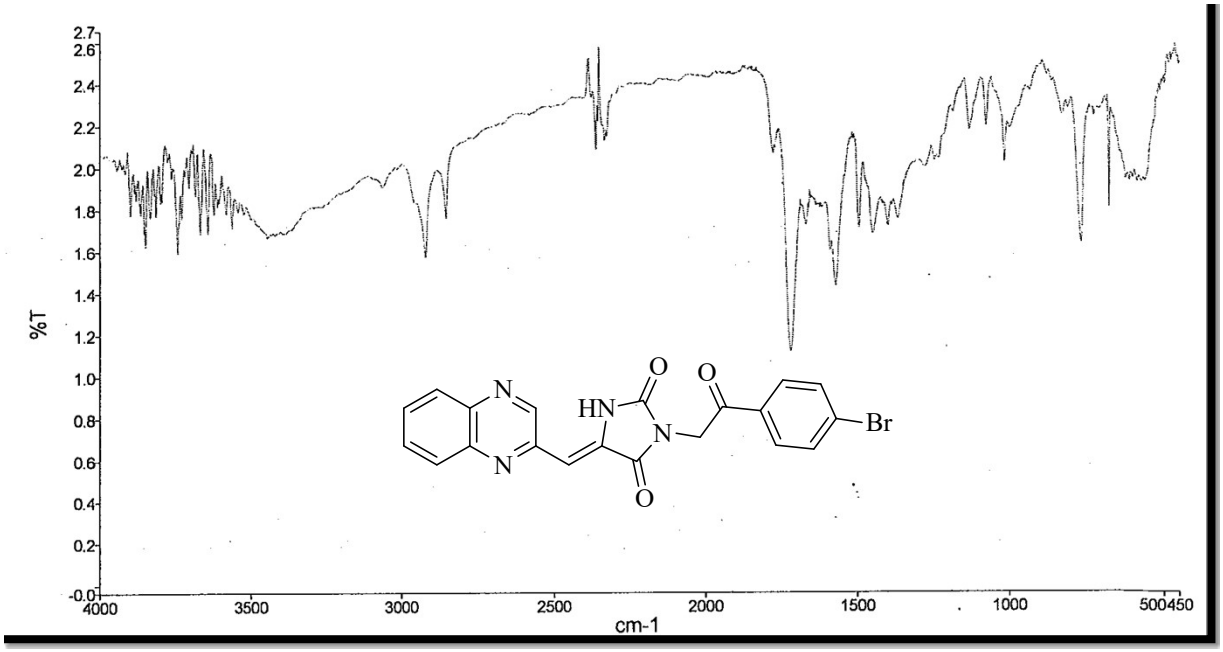


Fig S71. FTIR Spectra. (Z)-3-(2-(4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) imidazolidine-2,4-dione (**L3b)**

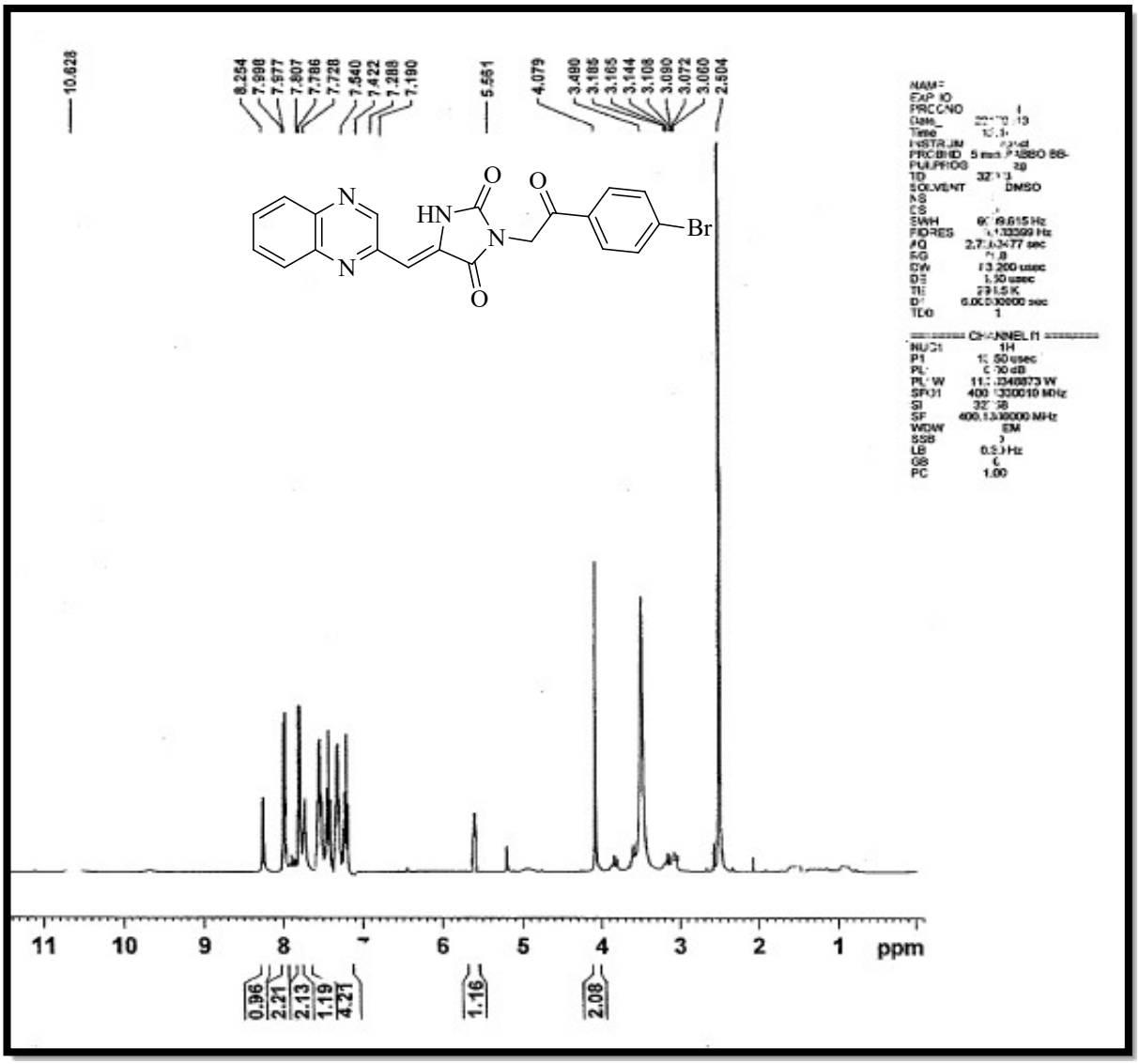


Fig S72. ^{1}HNMR Spectra. (Z)-3-(2-(4-bromophenyl)-2-oxoethyl)-5-(quinoxalin-2-ylmethylene) imidazolidine-2,4-dione **(L3b)**

3-(2)- (E)-3-(2-(naphthalen-2-yl)-2-oxoethyl)-5-(quinoxalin-2 ylmethylene) imidazolidine-2,4-dione; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 5,19(s, 1H, CH_2) 6.90 (s, 1H, H_{vinyl}), 7.59 (M, 2H, H- Phenyl), 7.73 (M, 3H, H- Phenyl), 7.80 (M, 2H, H- Phenyl) 8.04 (d, 1H, J = 8.8 Hz, 6 or 7-H Quinoxaline), 8.49 (d, 1H, J = 8.8 Hz, 5-H Quinoxaline), 8.22 (s, 1H, 8-H Quinoxaline), 9.13 (s, 1H, 3-H Quinoxaline), 9.25 (s, 1H, H_{NH}).

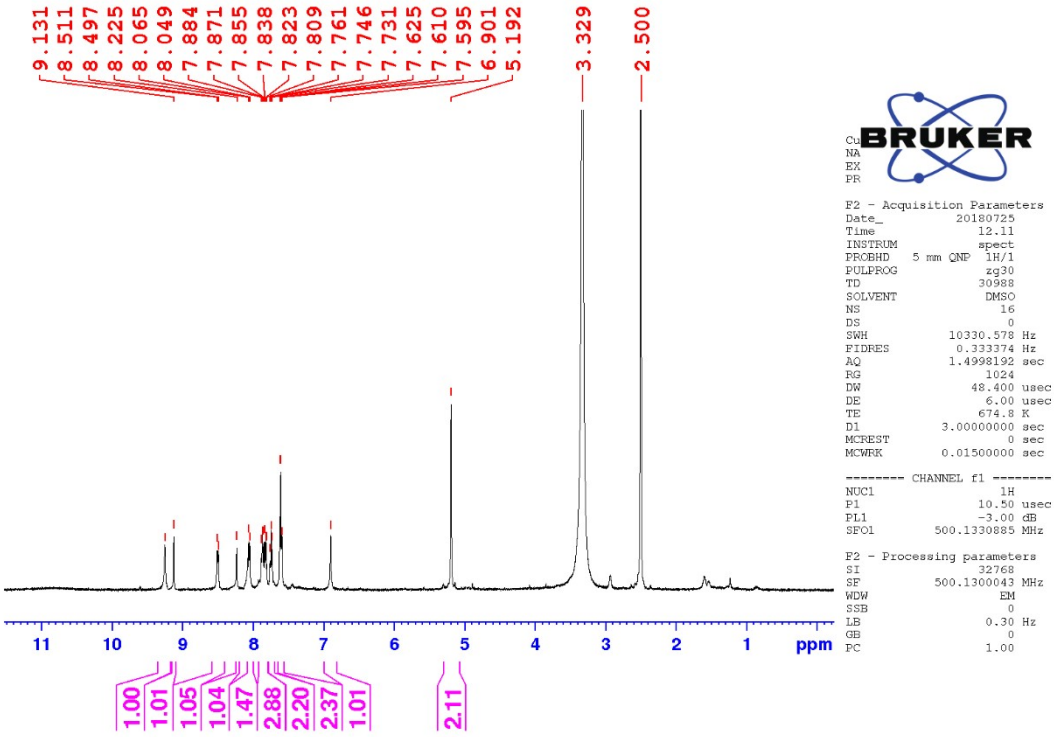


Fig S78. ^{1}HNMR Spectra. 3-(2)- (E)-3-(2-(naphthalen-2-yl)-2-oxoethyl)-5-(quinoxalin-2 ylmethylene) imidazolidine-2,4-dione(**L8c**)

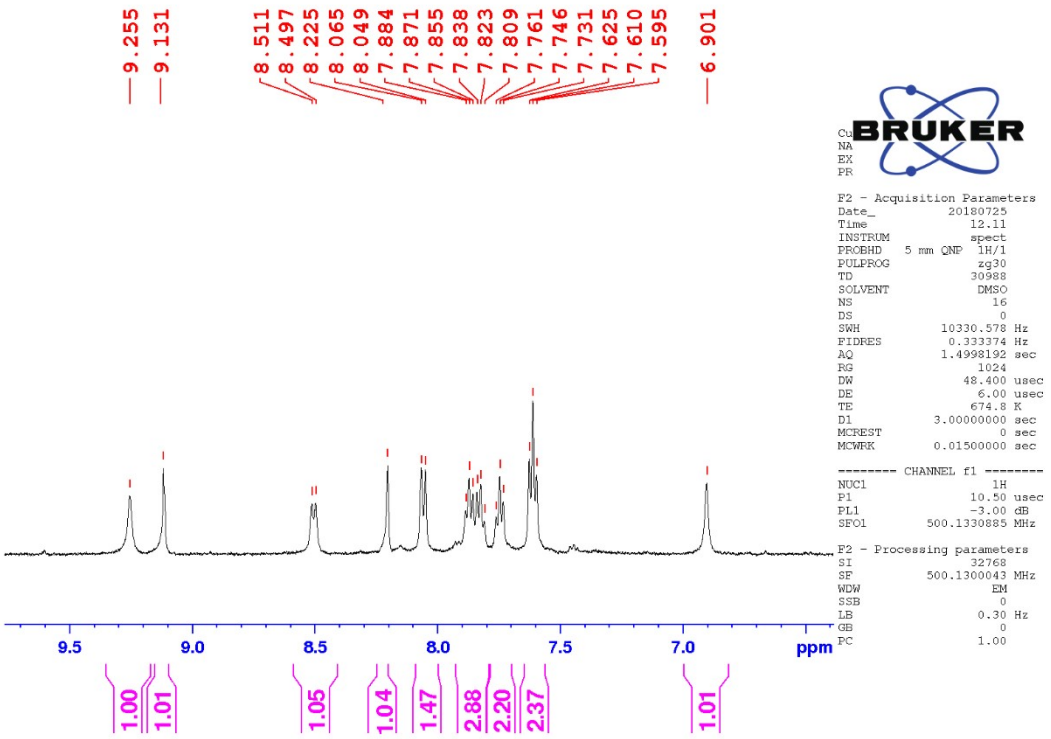


Fig S79. [1]HNMR expand Spectra. 3-(2)- (E)-3-(2-(naphthalen-2-yl)-2-oxoethyl)-5-(quinoxalin-2 ylmethylene) imidazolidine-2,4-dione (**L8c**)

(Z)-5-((6-chloroquinoxalin-2-yl)methylene)-3-ethyl-2-thioxothiazolidin-4-one; IR (KBr, cm^{-1}) *ν* :2922(C-H aromatic), 1718(C=O), 1630(C=N),1289(C=C).[1]HNMR (400 MHz, DMSO d_6) δ (ppm): 9.04(S, 1H, H-3 Quinoxaline), 8.02(d, 1H, J=8.8 Hz H-8 Quinoxaline), 8.14(d, 1H, J=2.4 Hz H-5 Quinoxaline), 7.85(S. 1H, $H_{c=c}$), 8.08(d, 1H, J=8.8 Hz H-7 Quinoxaline), 4.28(q, 2H, J=7.2 Hz, CH_2), 0.93(t,3H, J=7.2 Hz, CH_3). [13]C NMR (100 MHz, DMSO-d6) δ: 14.13, 47.39, 124.46, 128.94, 132.20, 132.32, 136.17, 143.40, 147.07, 147.17, 147.94, 176.07, 207.03.

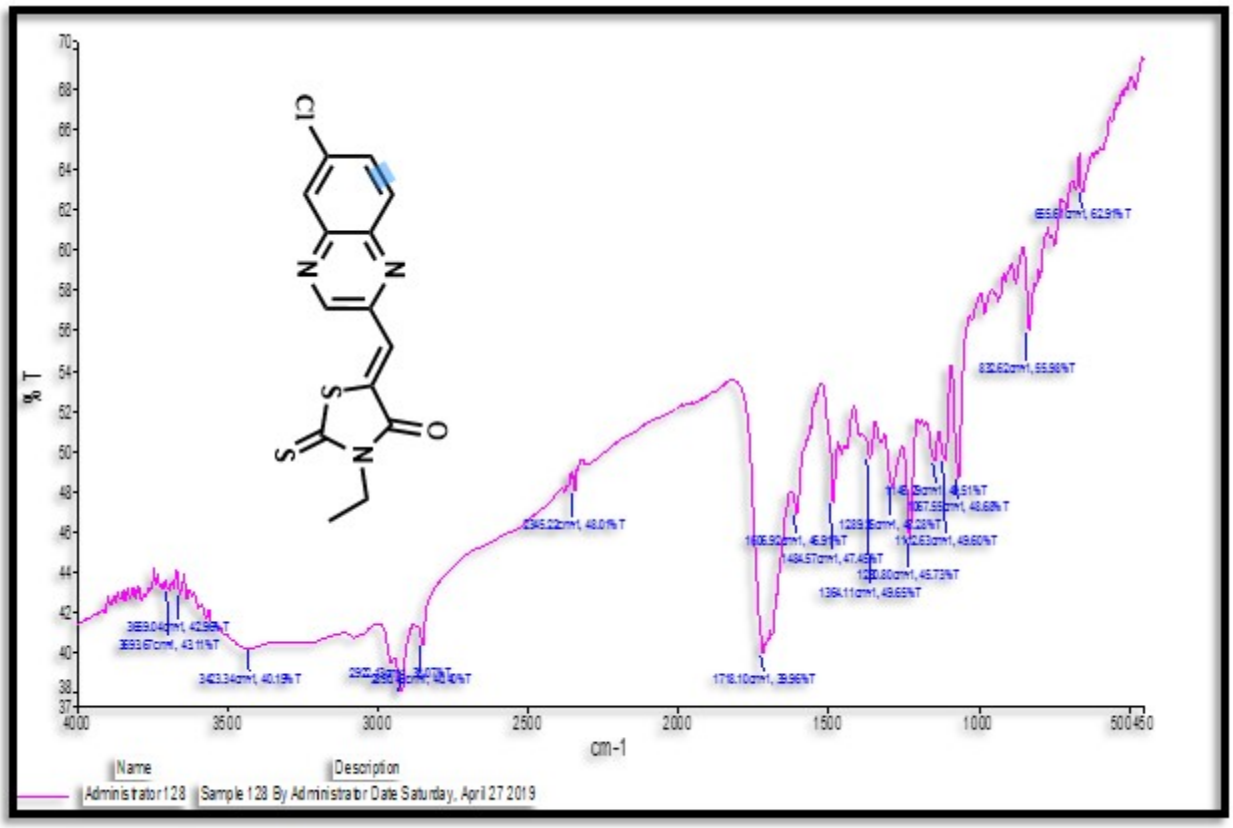


Fig S80. FTIR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl)methylene)-3-ethyl-2-thioxothiazolidin-4-one (**L7c**)

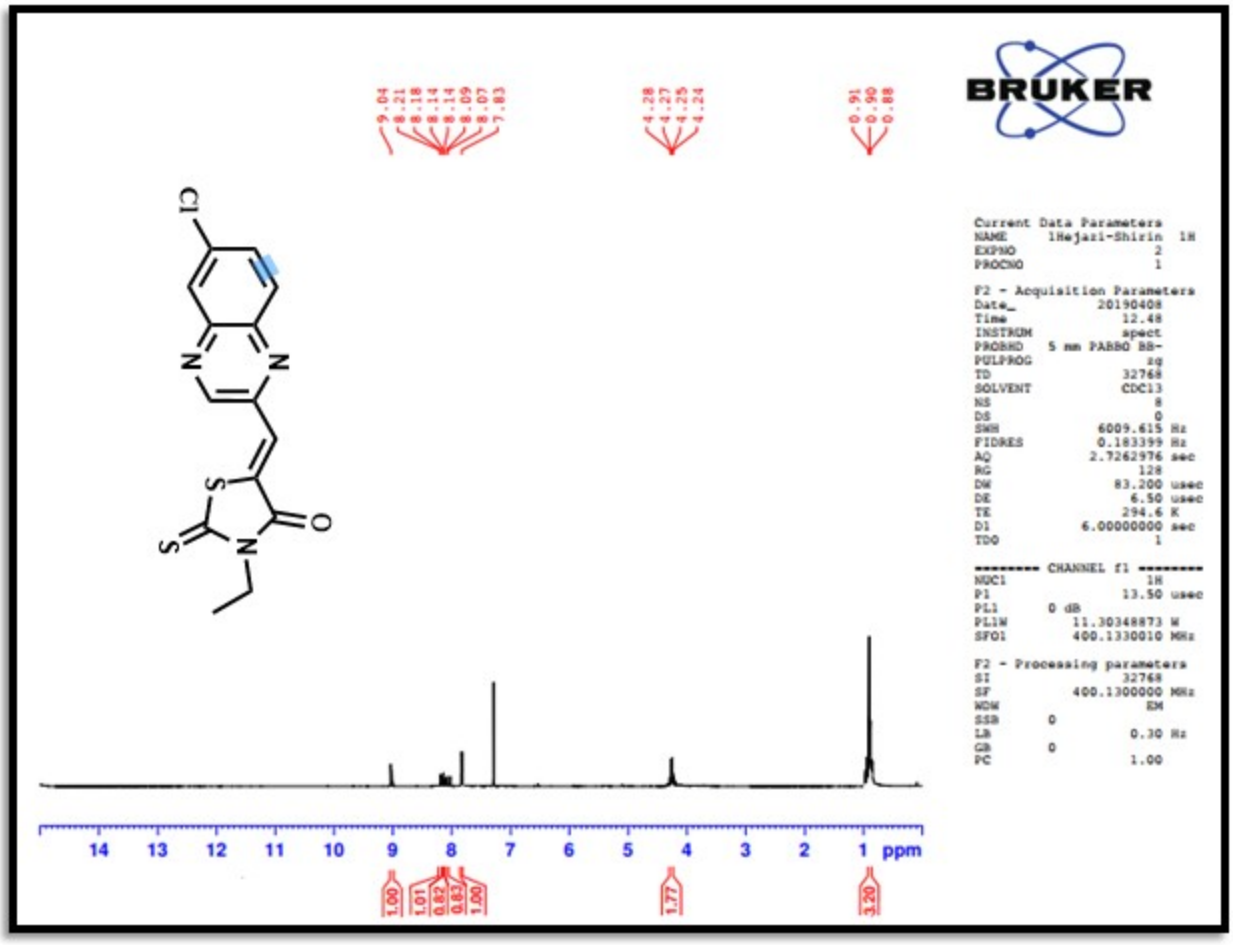


Fig S81. ^{1}HNMR Spectra. (Z)-5-((6-chloroquinoxalin-2-yl)methylene)-3-ethyl-2-thioxothiazolidin-4-one (**L7c**)

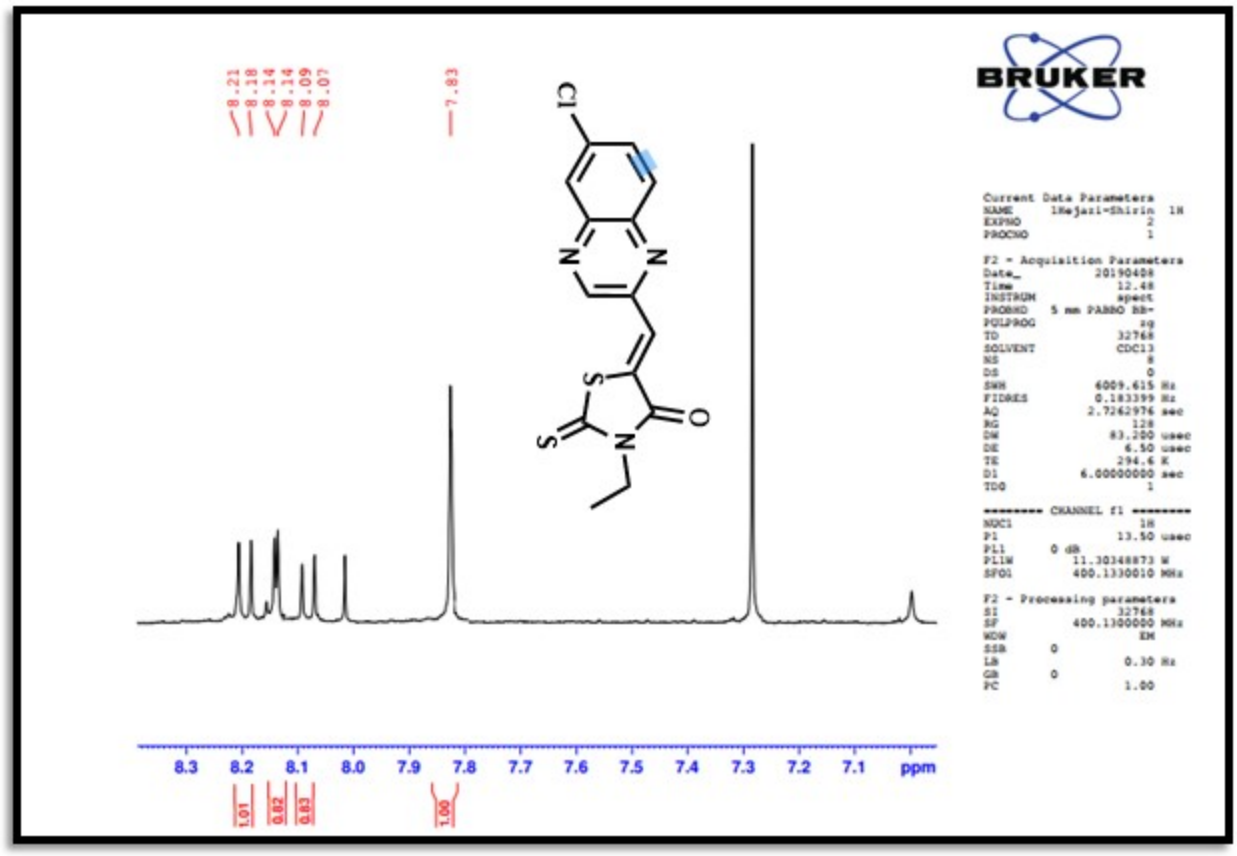


Fig S82. ^{1}HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl)methylene)-3-ethyl-2-thioxothiazolidin-4-one (**L7c**)

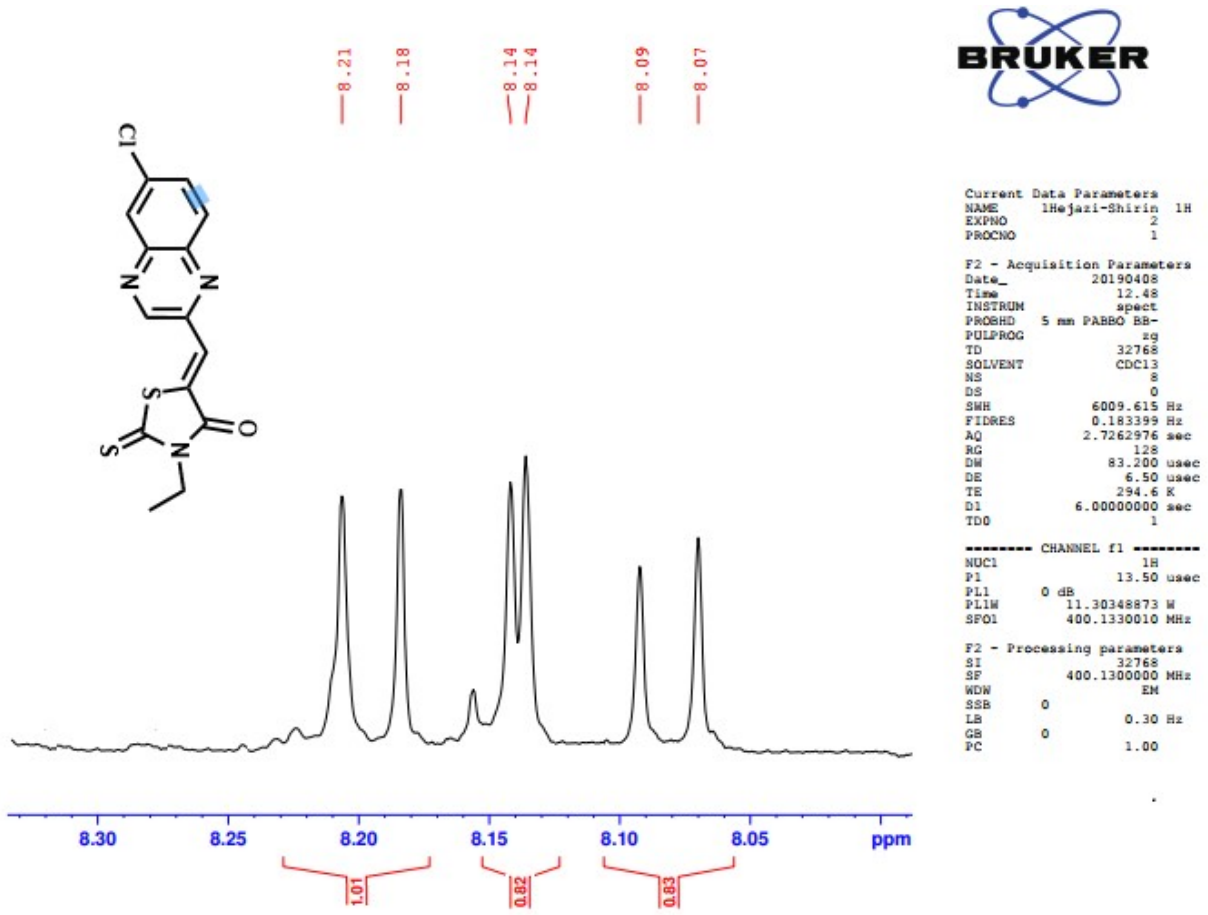
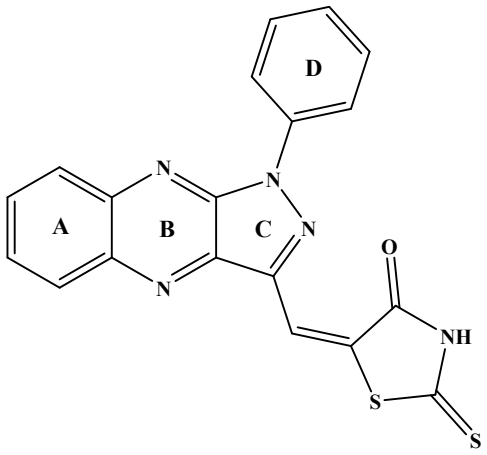


Fig S83. ^{1}HNMR expand Spectra. (Z)-5-((6-chloroquinoxalin-2-yl)methylene)-3-ethyl-2-thioxothiazolidin-4-one (**L7c**)



5-((1-phenyl-1H-pyrazolo[3,4-b]quinoxalin-3-yl)methylene)-2-thioxothiazolidin-4-one(2a); IR(KBr, cm^{-1})ν_{max}:3334.32cm^{-1}(NH),1509.99cm^{-1}(C=O),1424.17cm^{-1}(C=S); ^{1}H-NMR (500MHz,DMSO); δ:9.36(s,1H,NH),8.28 (s,1H,H-Vinyl),7.98(d, 2H, j=8,H-2′and H- 5′), 7.81(d,2H, j=8, H-3′and H-4′),7.52-7.59(m,4H, H-2, H-3, H-5 and H-6),7.39 (t,1H, j=14.5, H-4); ^{13}C-NMR (125MHz, DMSO); δ:119.15, 122.42, 126.69, 127.67(Aromatic carbons ring D), 129.89, 130.12(Aromatic carbons ring A), 131.26,133.79(Ring B), 139.59, 142.90, 143.82 (Ring C),152.76 (Vinyl), 152.78(C=C), 169.79(C=O), 183.67(C=S).

Fig S84. FTIR Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b]quinoxalin-3-yl)methylene)-2-thioxothiazolidin-4-one **(2a)**

Fig 86 ^{13}CNMR Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b]quinoxalin-3-yl)methylene)-2-thioxothiazolidin-4-one**(2a)**

Fig S87. ^{1}HNMR expand Spectra. 5-((1-phenyl-1H-pyrazolo[3,4-b]quinoxalin-3-yl)methylene)-2-thioxothiazolidin-4-one **(2a)**