aSupporting Information

for

[BMIM]OAc promoted One-Pot Synthesis of Pyrazolo[4',3':5,6]pyrido[2,3-*d*]pyrimidin-5-ones and their Antimicrobial Activity

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Contents

1. Experimental

1.1 General method

The chemicals necessary for the reactions were sourced from Sigma-Aldrich, TCI, and Sisco Research Laboratories Pvt. Ltd. in India. Since these chemicals were used as received, no additional purification was required. Reaction progress was monitored using thin-layer chromatography (TLC) on aluminum plates coated with F254 silica gel 60. Melting points of the synthesized compounds were determined using the open capillary tube method and the data were recorded a s observed. Nuclear magnetic resonance (NMR) spectra were collected using a 400 MHz Bruker spectrometer equipped with proton noise decoupling mode and a standard 5mm probe for structural conformation of prepared molecules. Samples were dissolved in deuterated DMSO, using d6 as a standard reference. The following abbreviations were used to describe the ^{1}H NMR signals: "s" for singlet, "d" for doublet, "t" for triplet, "q" for quartet, "dd" for double doublet, and "m" for Multiplet. Chemical shifts are reported in parts per million (ppm), and coupling constants (*J*) are given in Hertz (Hz).

2. Scanned copies of ^{1}H NMR,^{13}C NMR and MS spectra for all compounds **4(a-l)**

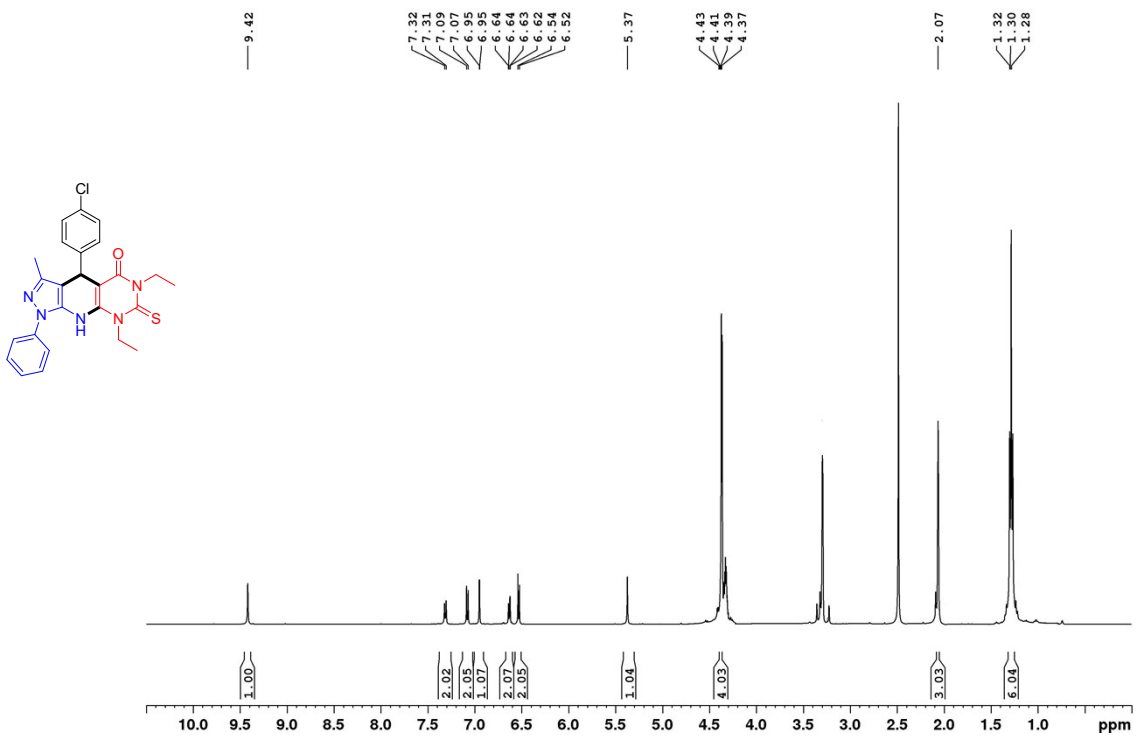

Fig S1: ^{1}H-NMR of 4-(4-chlorophenyl)-3,6,8-trimethyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4a)**

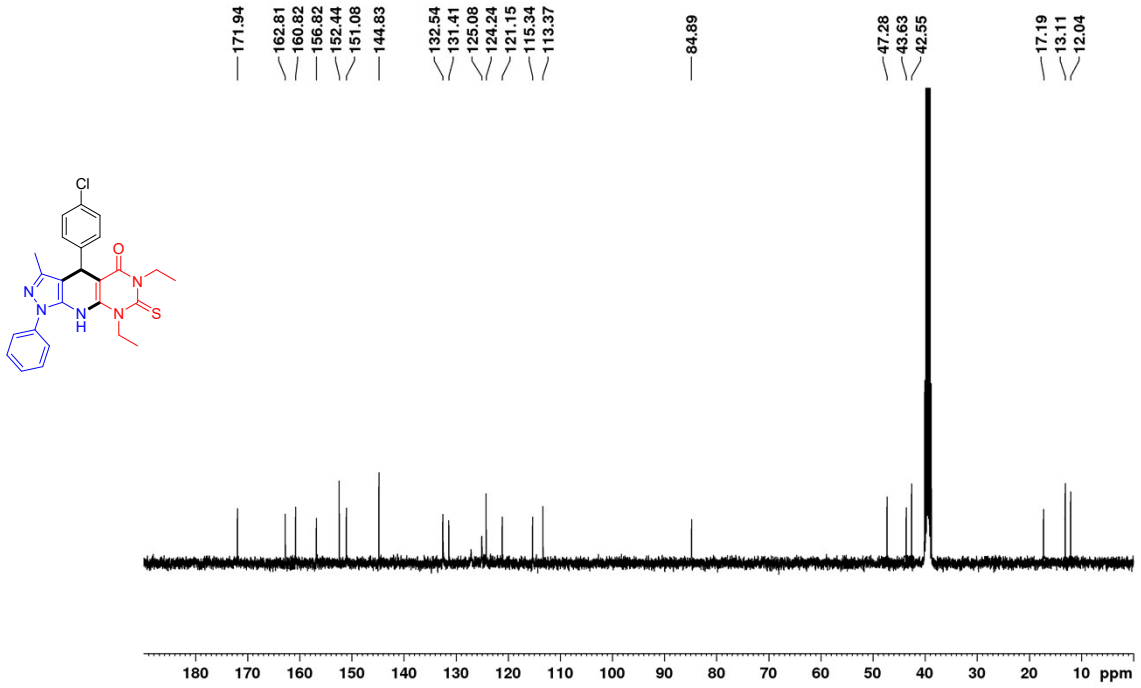

Fig S2: ^{13}C-NMR of 4-(4-chlorophenyl)-3,6,8-trimethyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4a)**

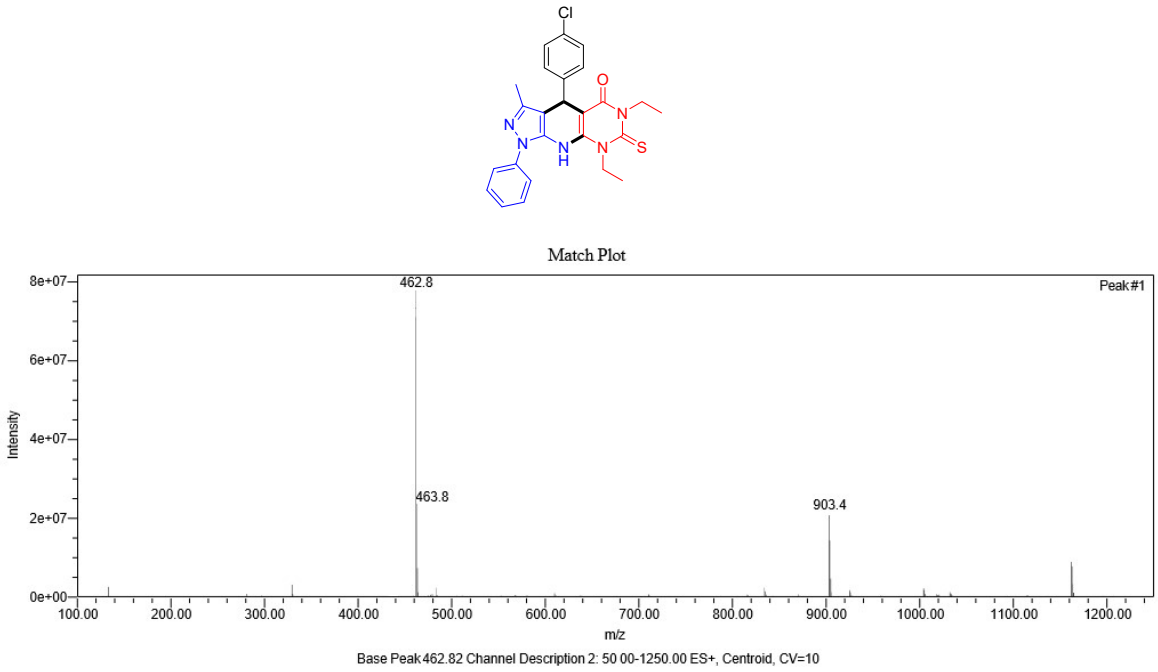

Fig S3: MS of 4-(4-chlorophenyl)-3,6,8-trimethyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4a)**

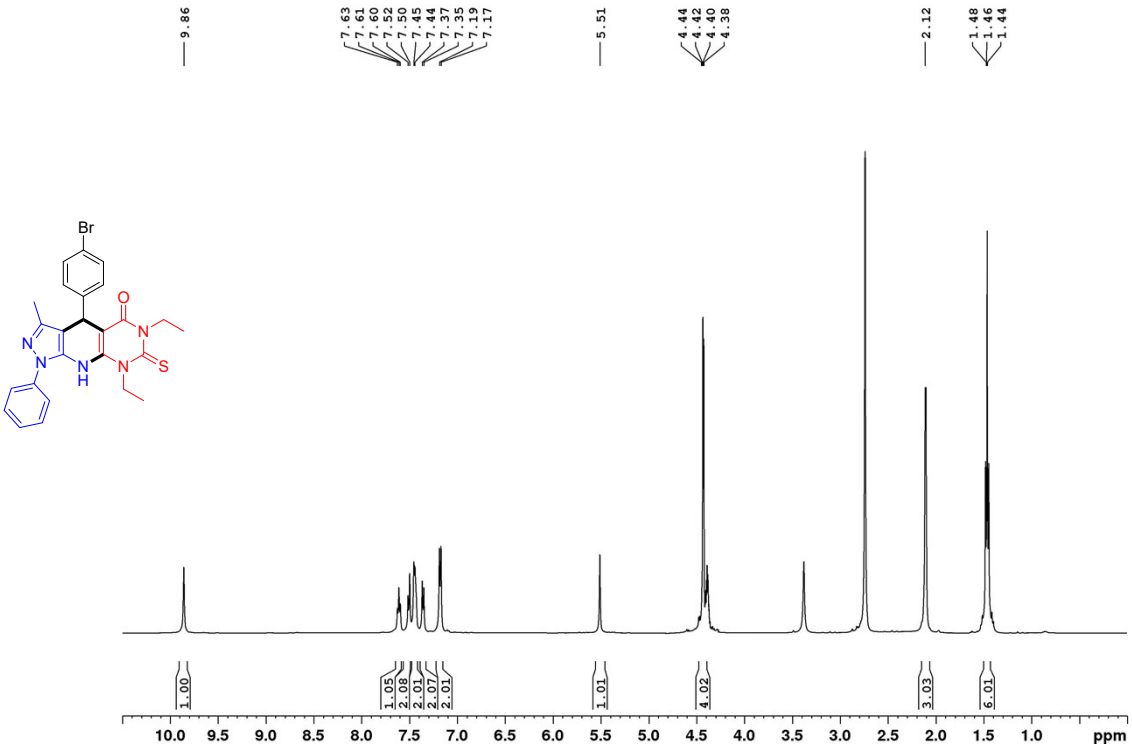

Fig S4: [1]H-NMR of 4-(4-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4b)**

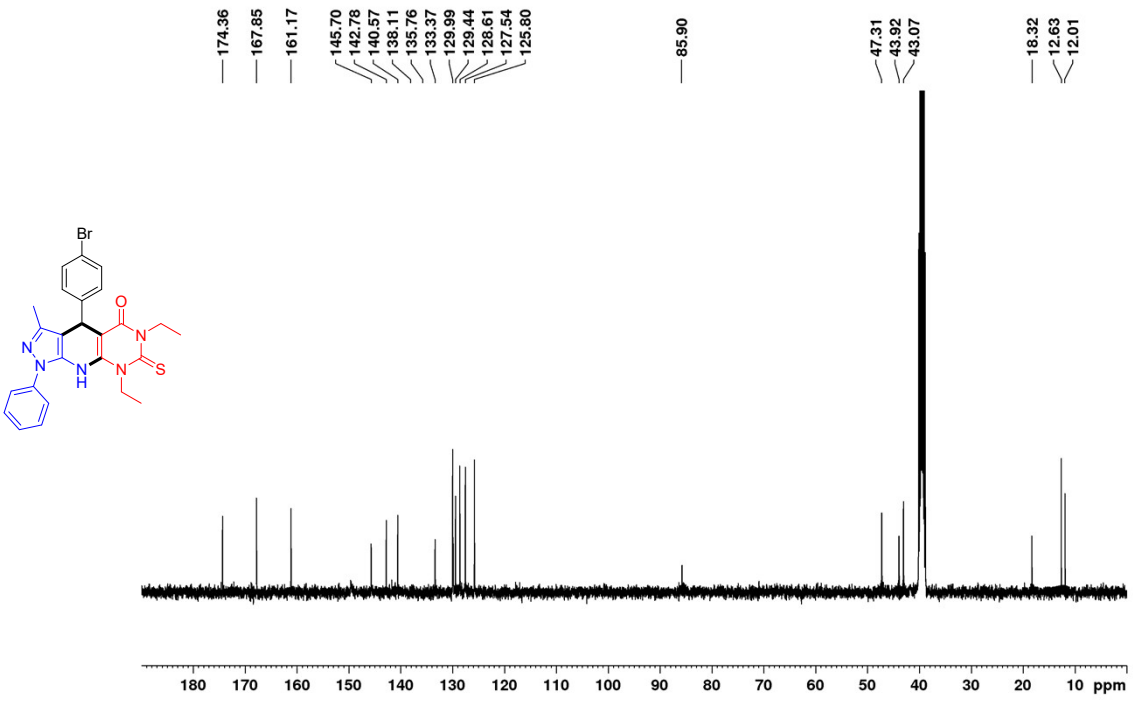

Fig S5: [13]C-NMR of 4-(4-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4b)**

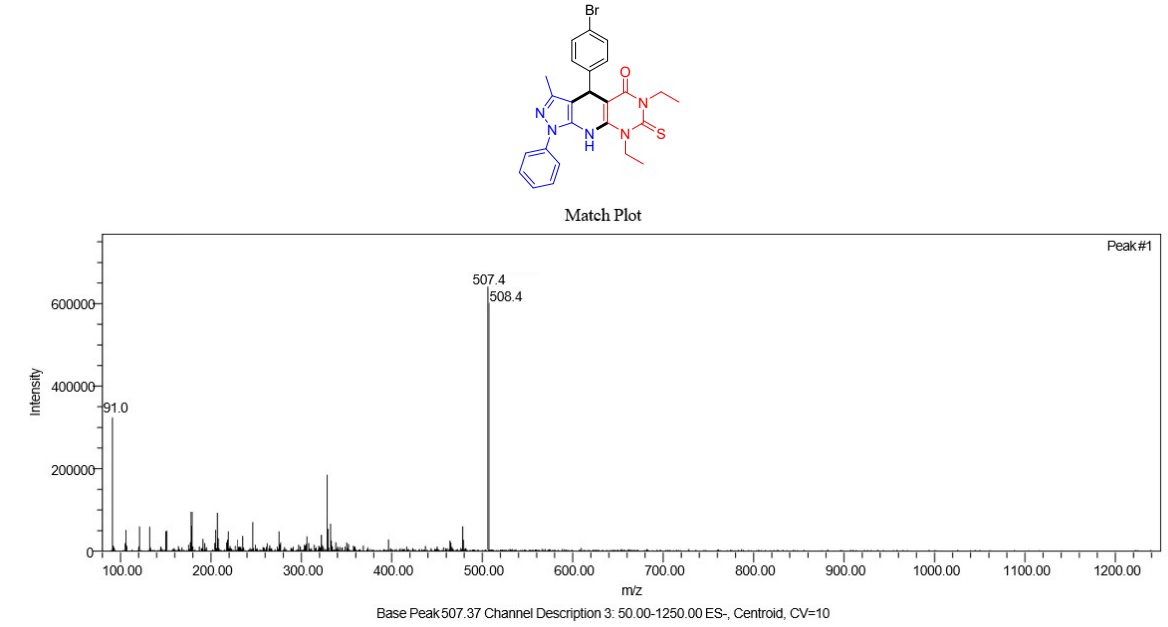

Fig S6: MS of 4-(4-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4b)**

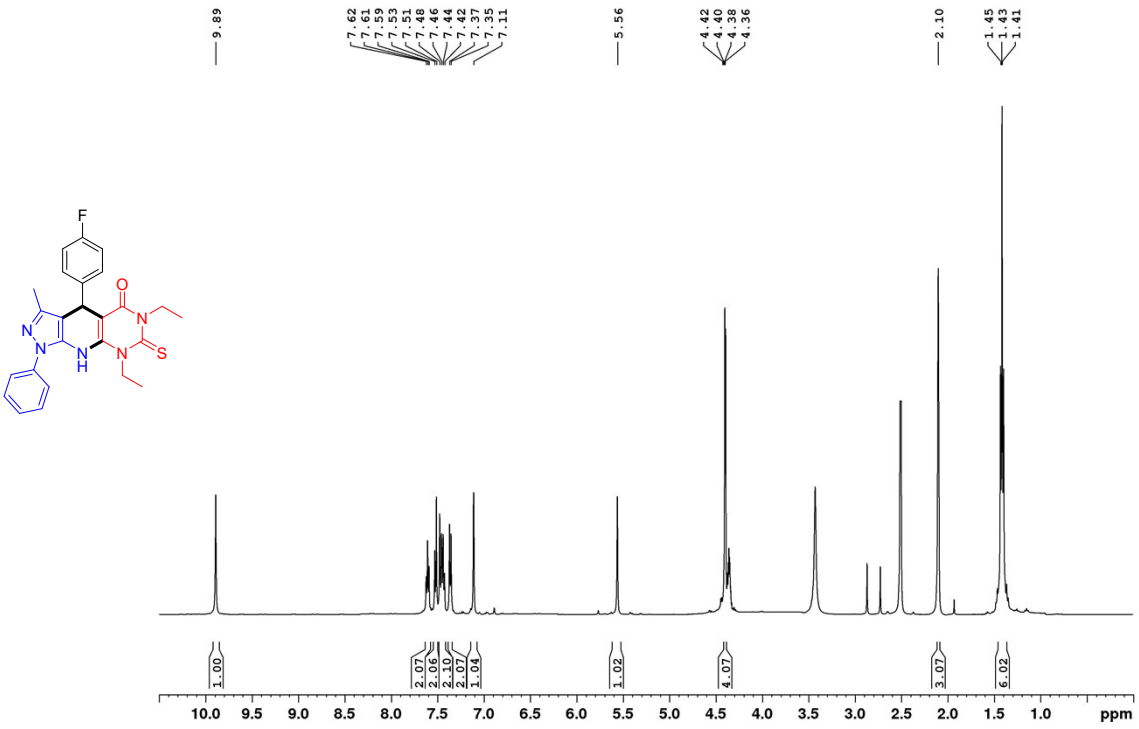

Fig S7: ^{1}H-NMR of 6,8-diethyl-4-(4-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4c)**

SSS

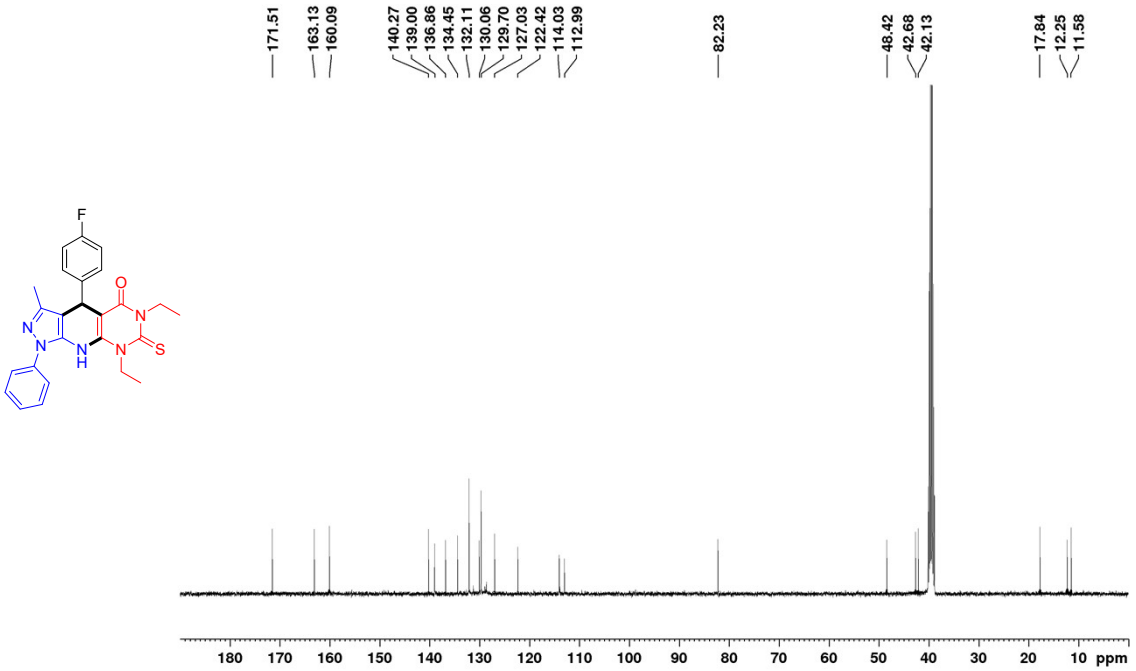

Fig S8: ^{13}C-NMR of 6,8-diethyl-4-(4-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4c)**

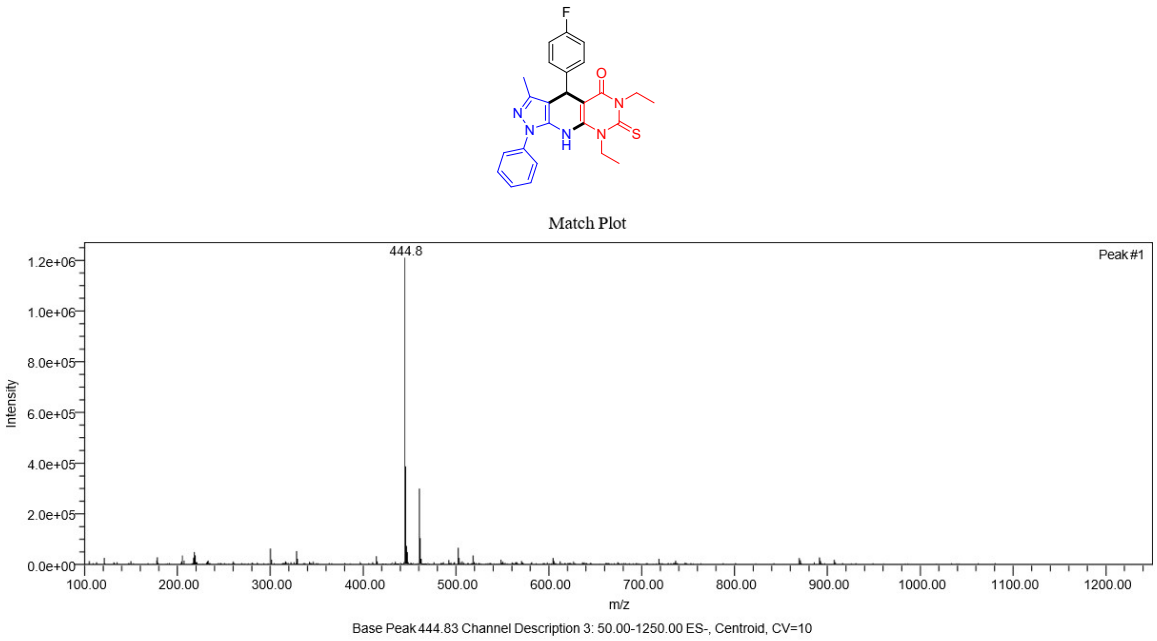

Fig S9: MS of 6,8-diethyl-4-(4-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4c)**

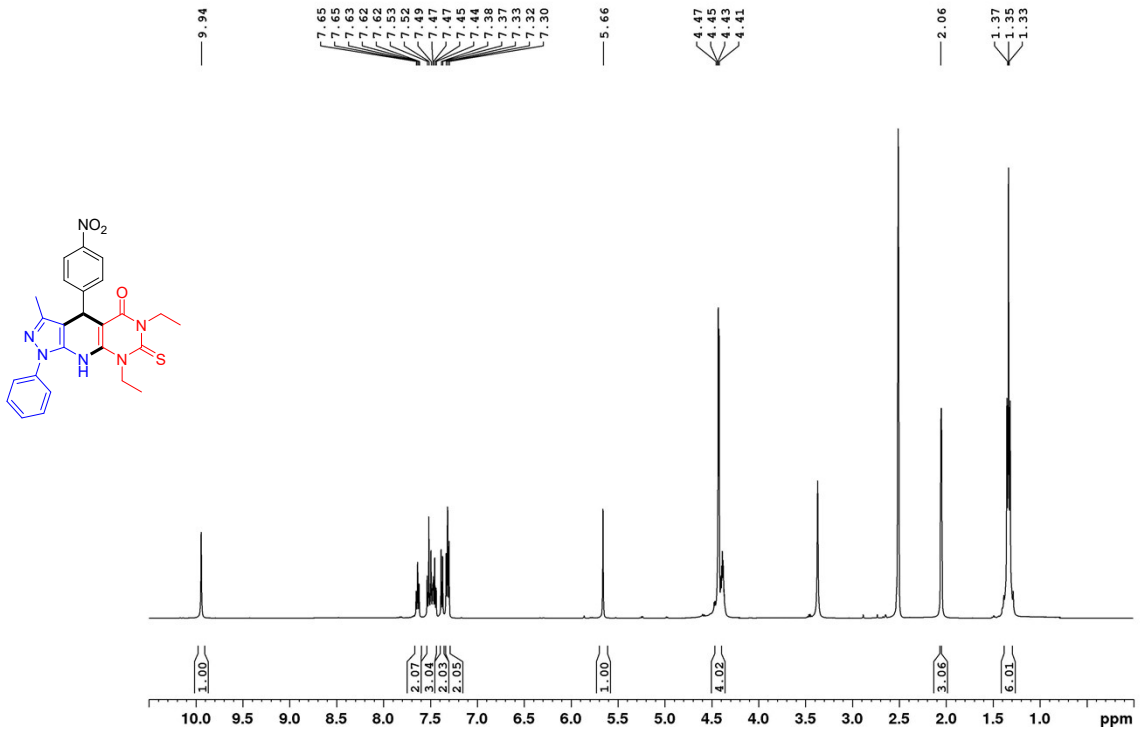

Fig S10: [1]H-NMR of 6,8-diethyl-3-methyl-4-(4-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4d)**

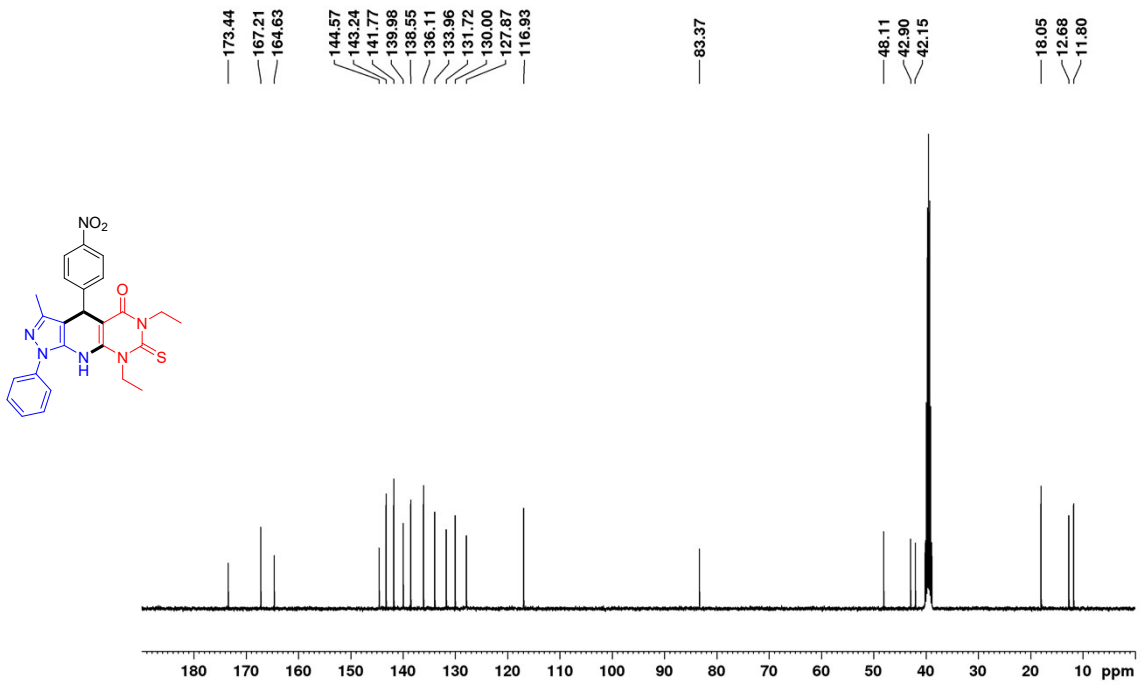

Fig S11: [13]C-NMR of 6,8-diethyl-3-methyl-4-(4-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4d)**

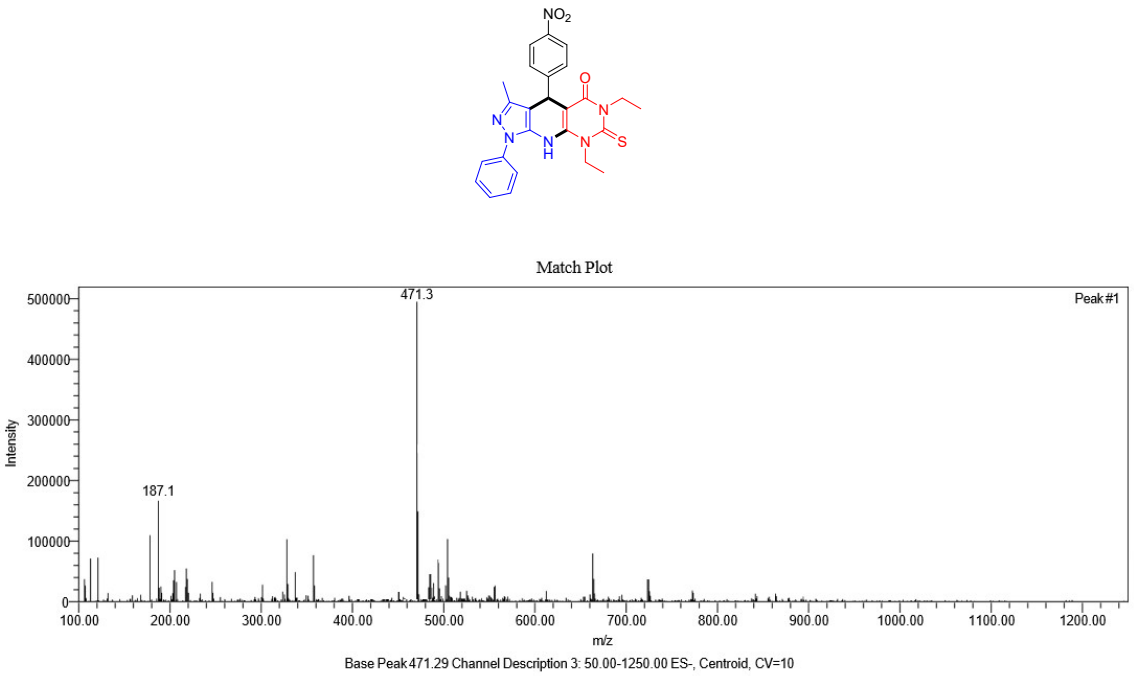

Fig S12: MS of 6,8-diethyl-3-methyl-4-(4-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4d)**

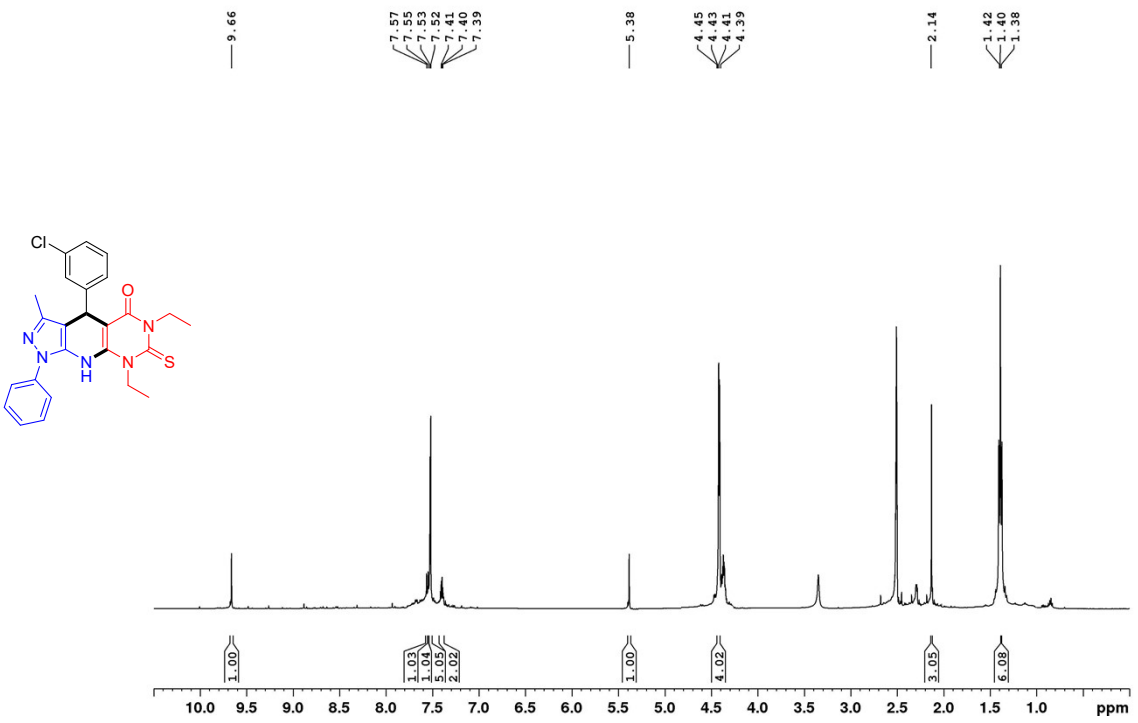

Fig S13: ^{1}H-NMR of 4-(3-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4e)**

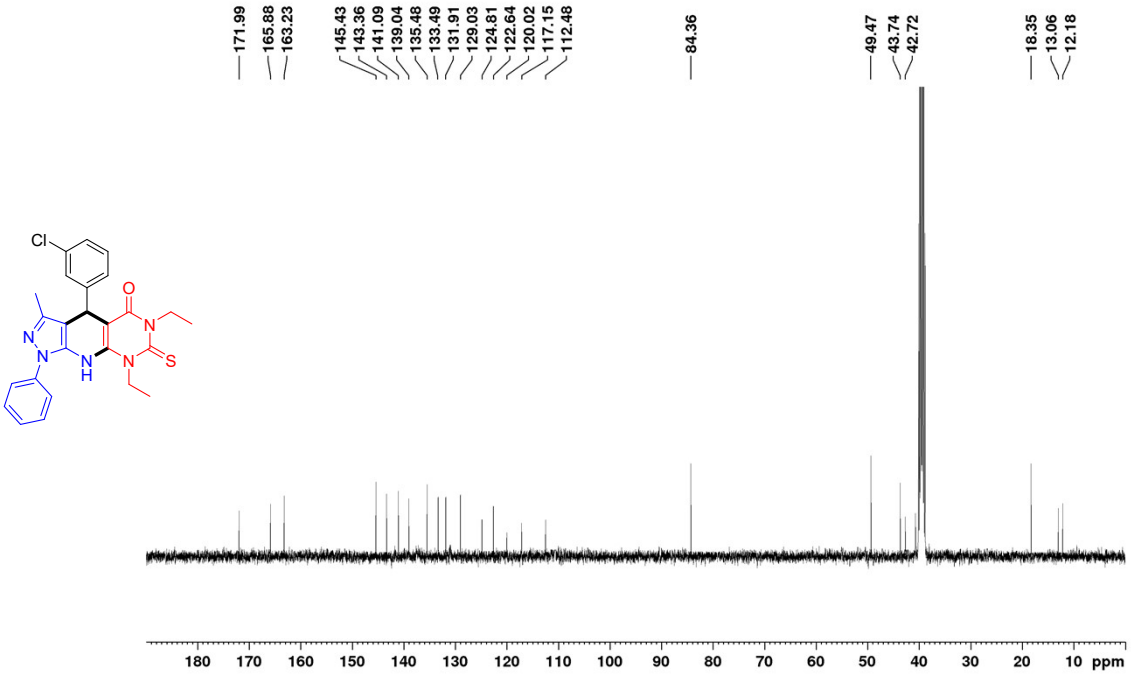

Fig S14: ^{13}C-NMR of 4-(3-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4e)**

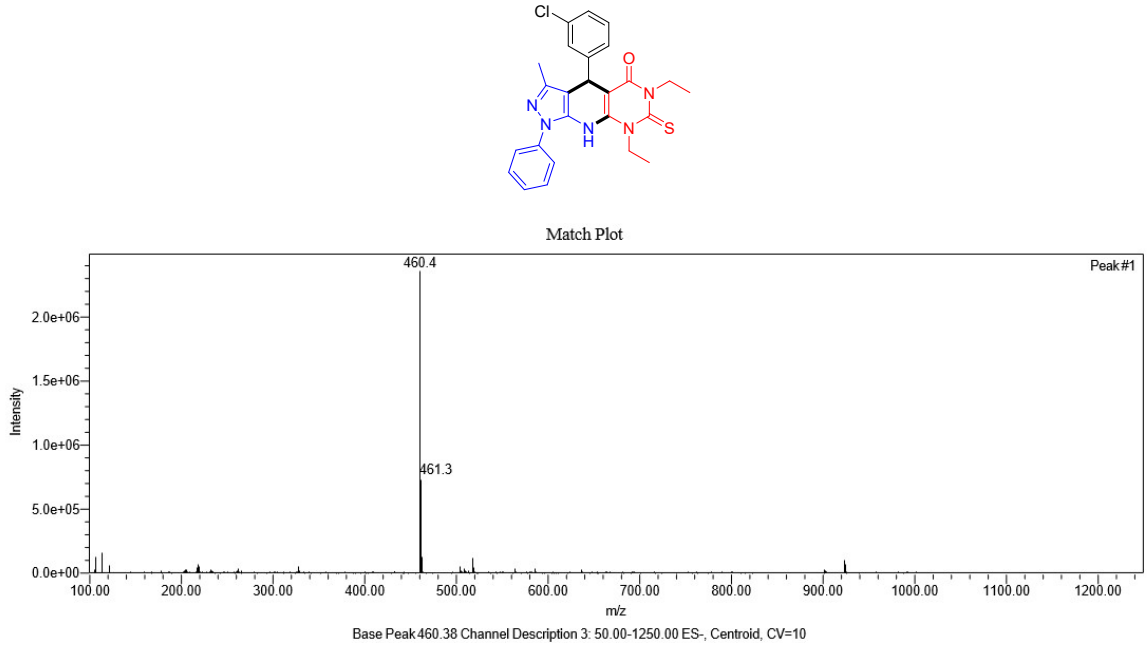

Fig S15: MS of 4-(3-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4e)**

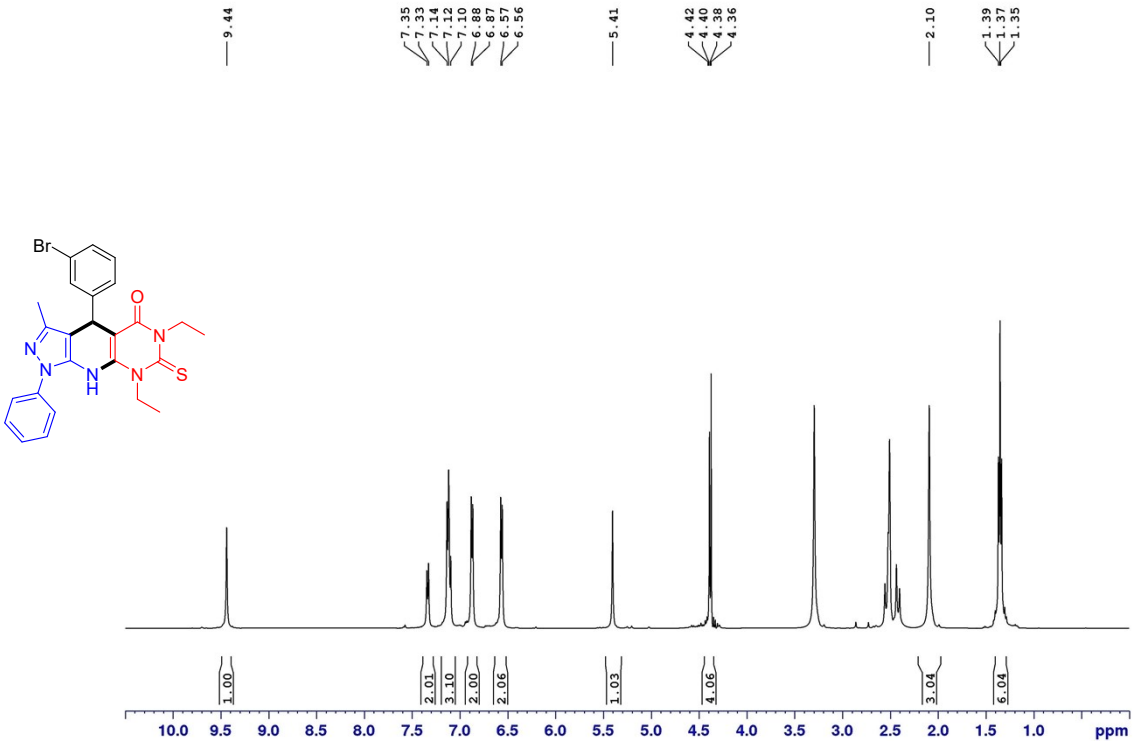

Fig S16: [1]H-NMR of 4-(3-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4f)**

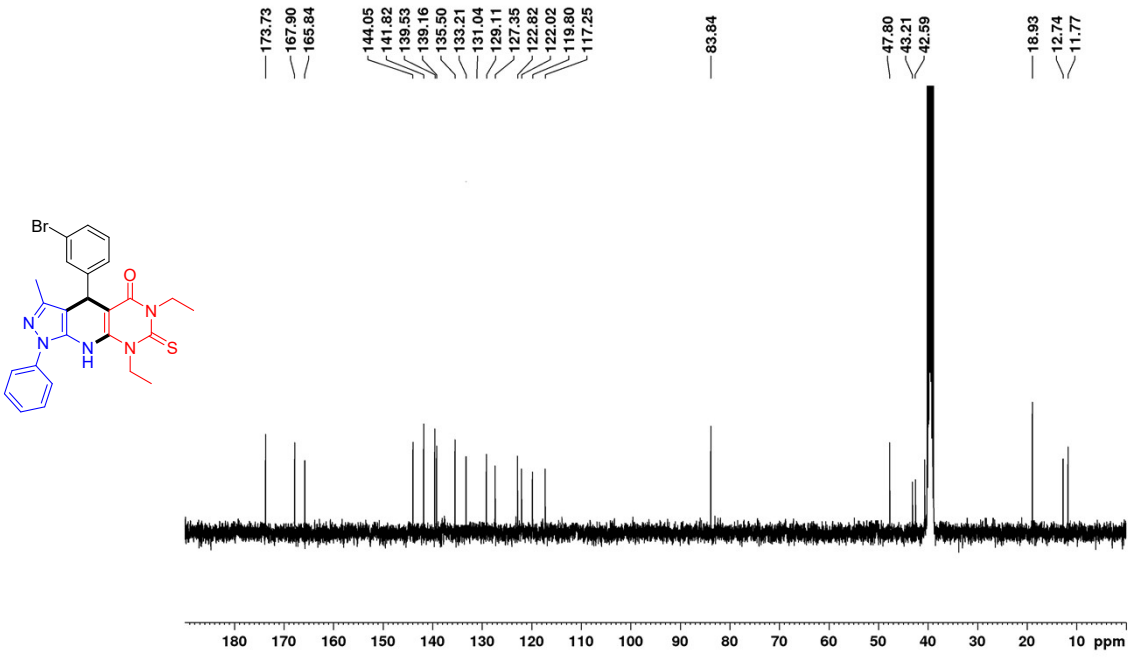

Fig S17: [13]C-NMR of 4-(3-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4f)**

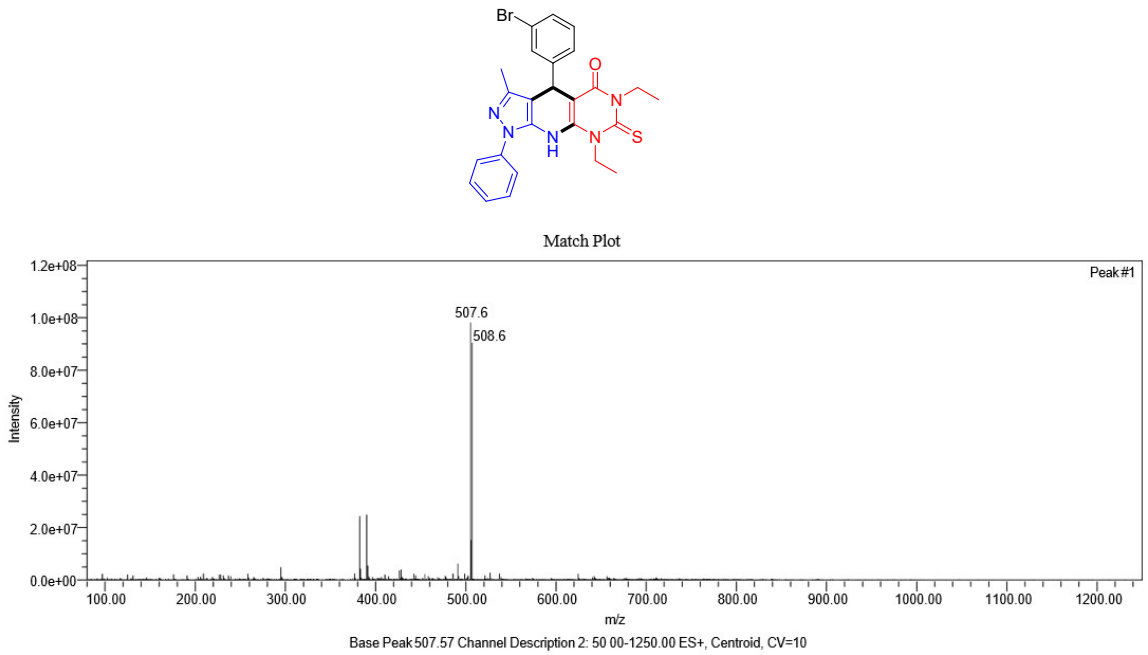

Fig S18: MS of 4-(3-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4f)**

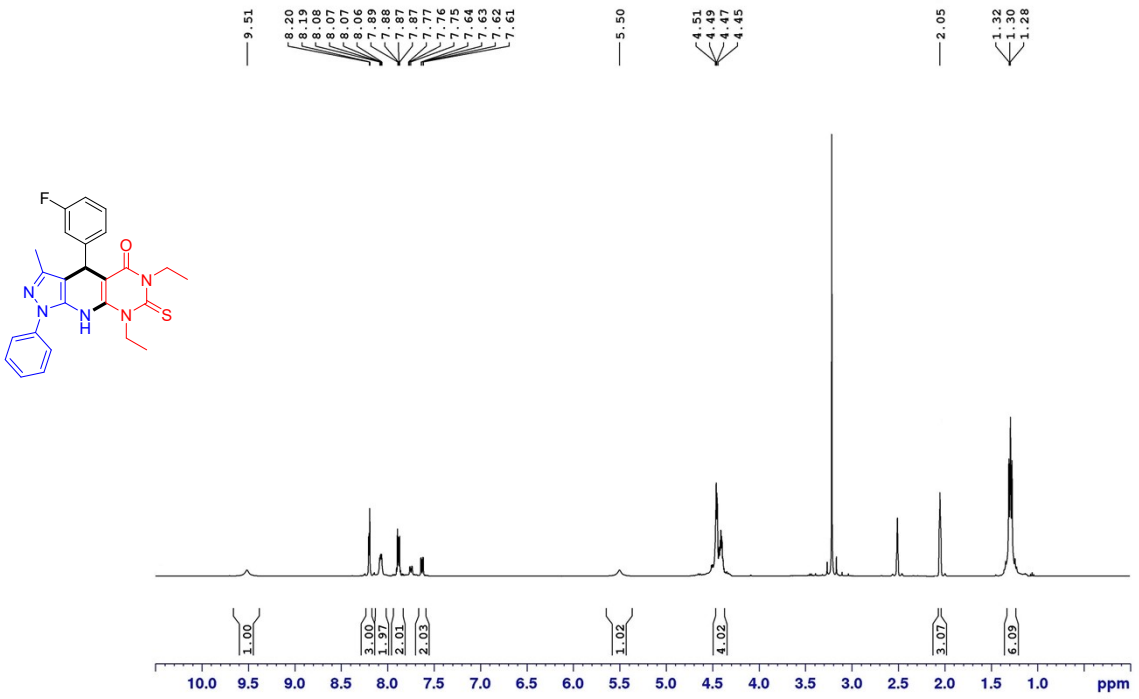

Fig S19: ^{1}H-NMR of 6,8-diethyl-4-(3-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4g)**

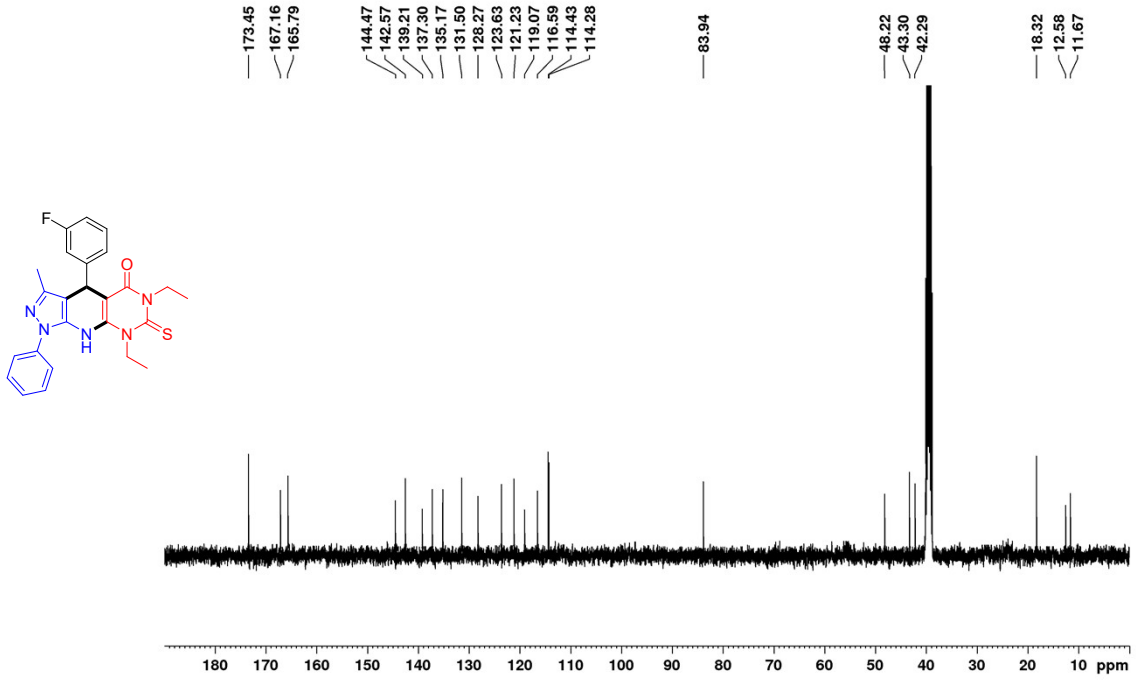

Fig S20: ^{13}C-NMR of 6,8-diethyl-4-(3-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4g)**

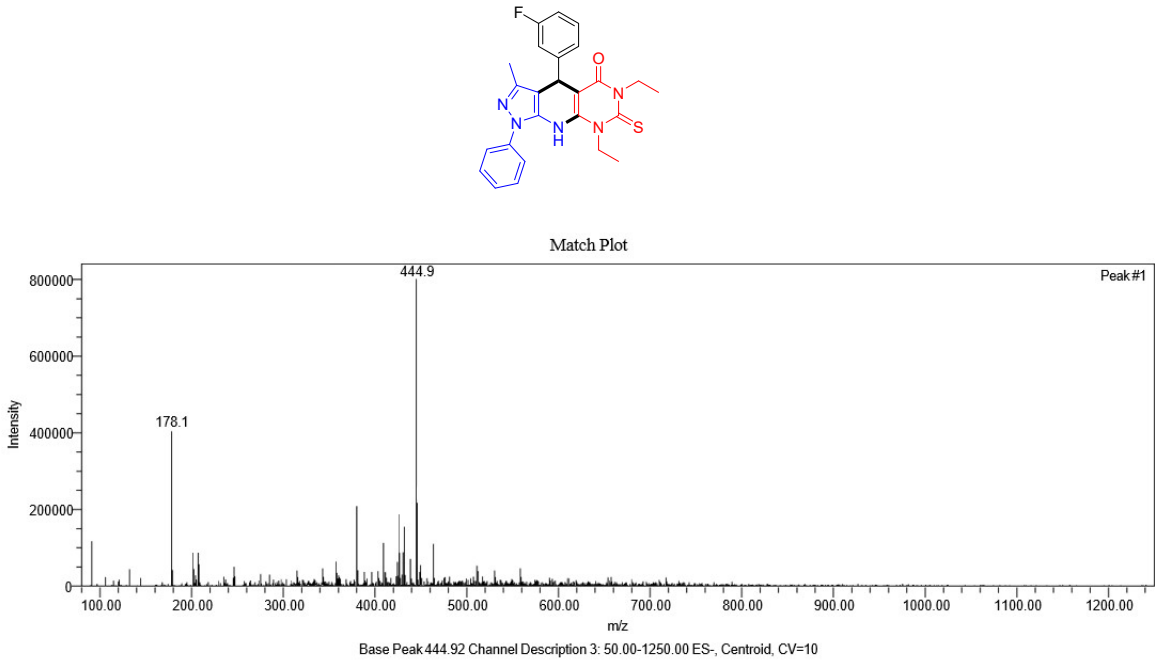

Fig S21: MS of 6,8-diethyl-4-(3-fluorophenyl)-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4g)**

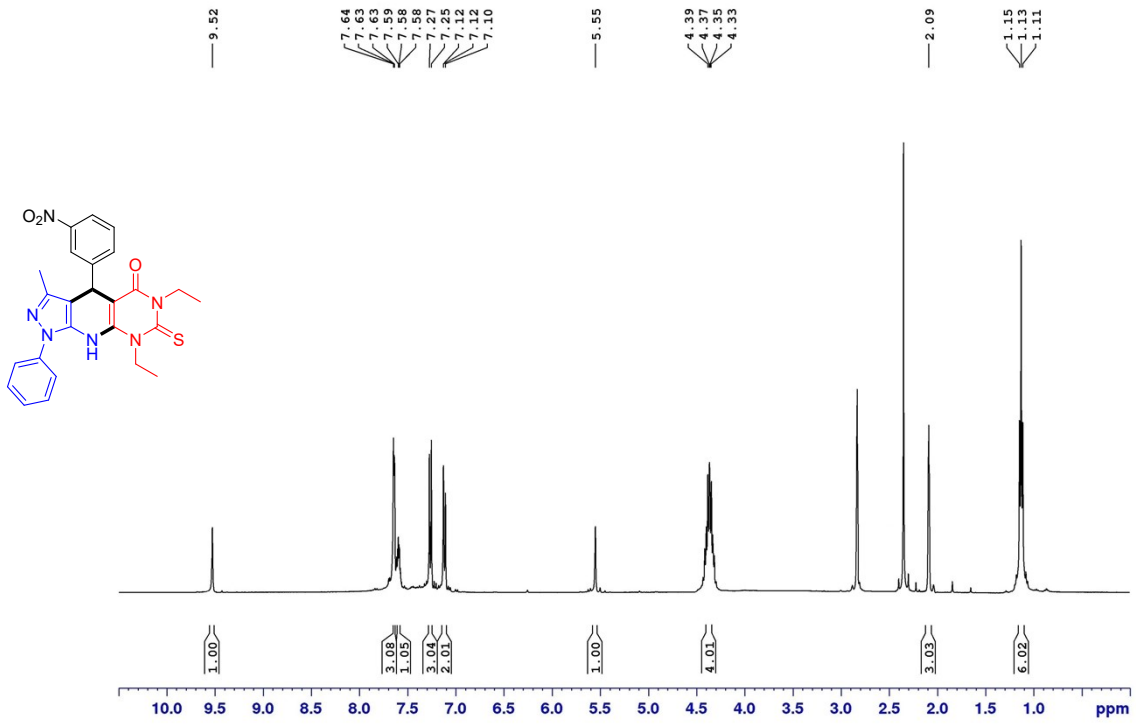

Fig S22: [1]H-NMR of 6,8-diethyl-3-methyl-4-(3-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4h)**

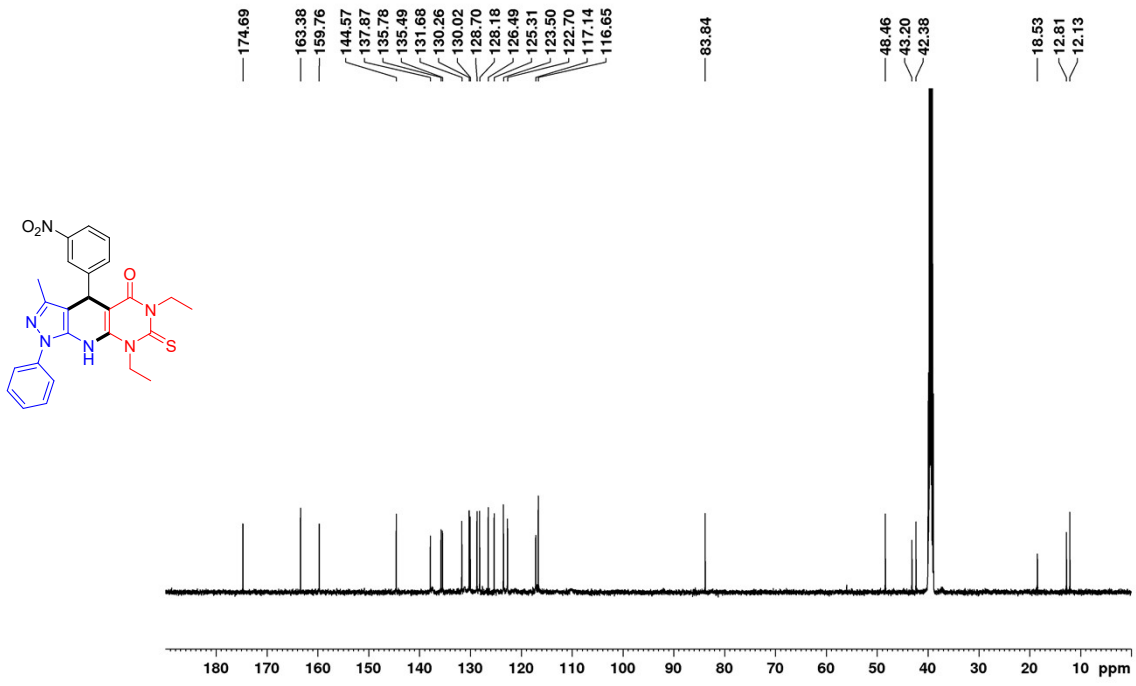

Fig S23: [13]C-NMR of 6,8-diethyl-3-methyl-4-(3-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4h)**

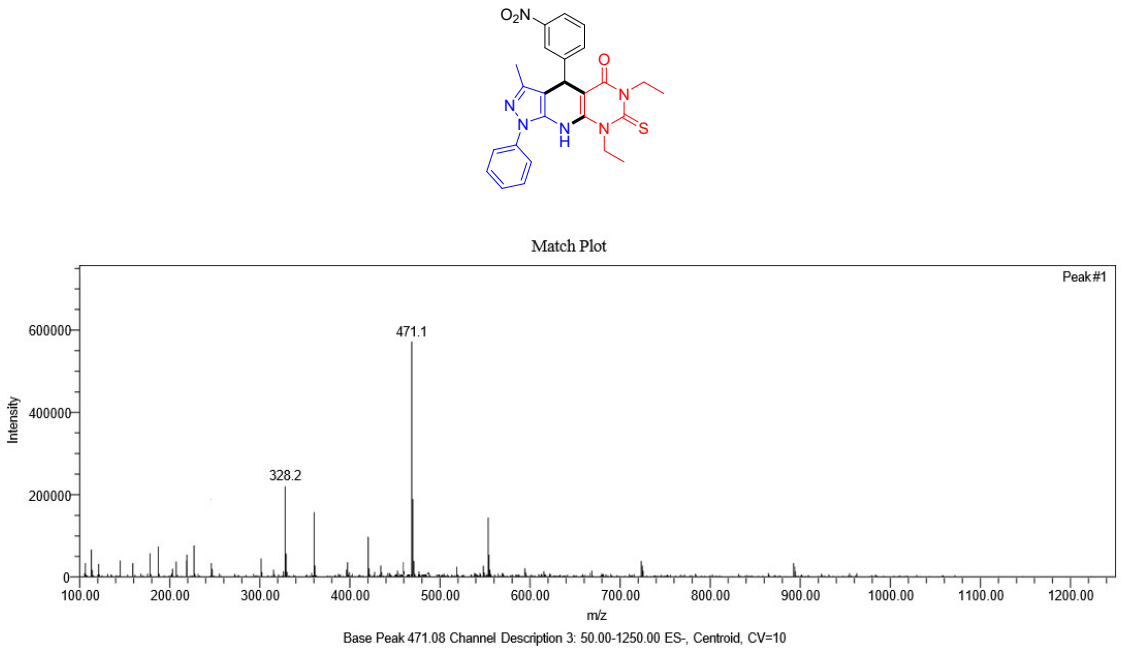

Fig S24: MS of 6,8-diethyl-3-methyl-4-(3-nitrophenyl)-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4h)**

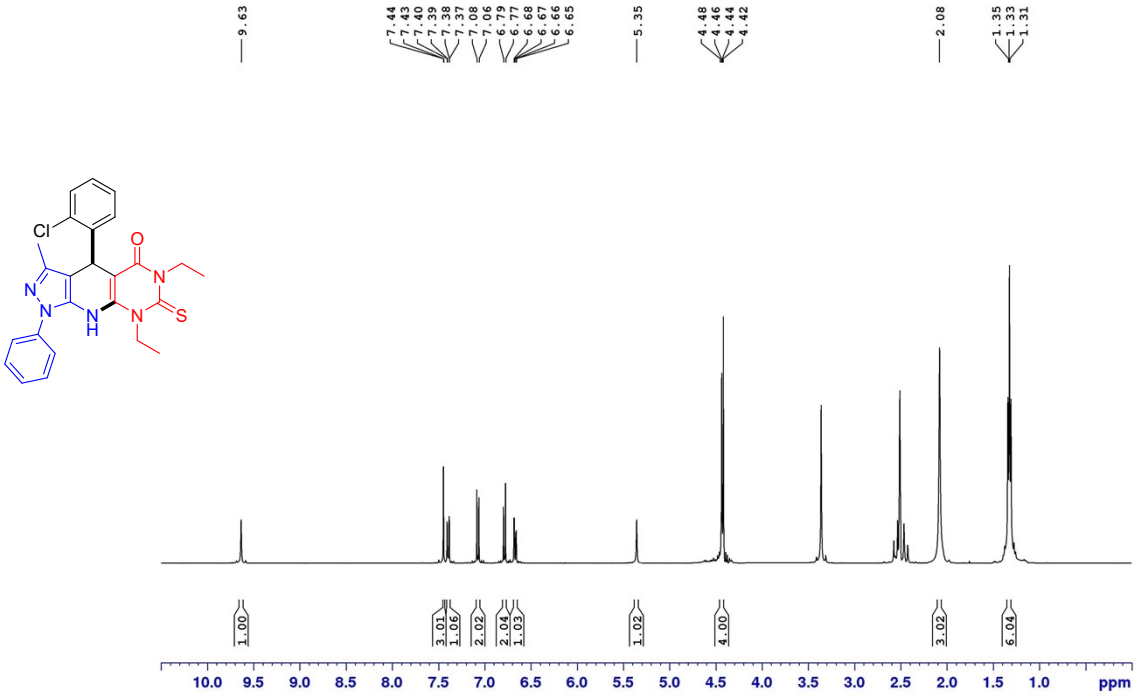

Fig S25: [1]H-NMR of 4-(2-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4i)**

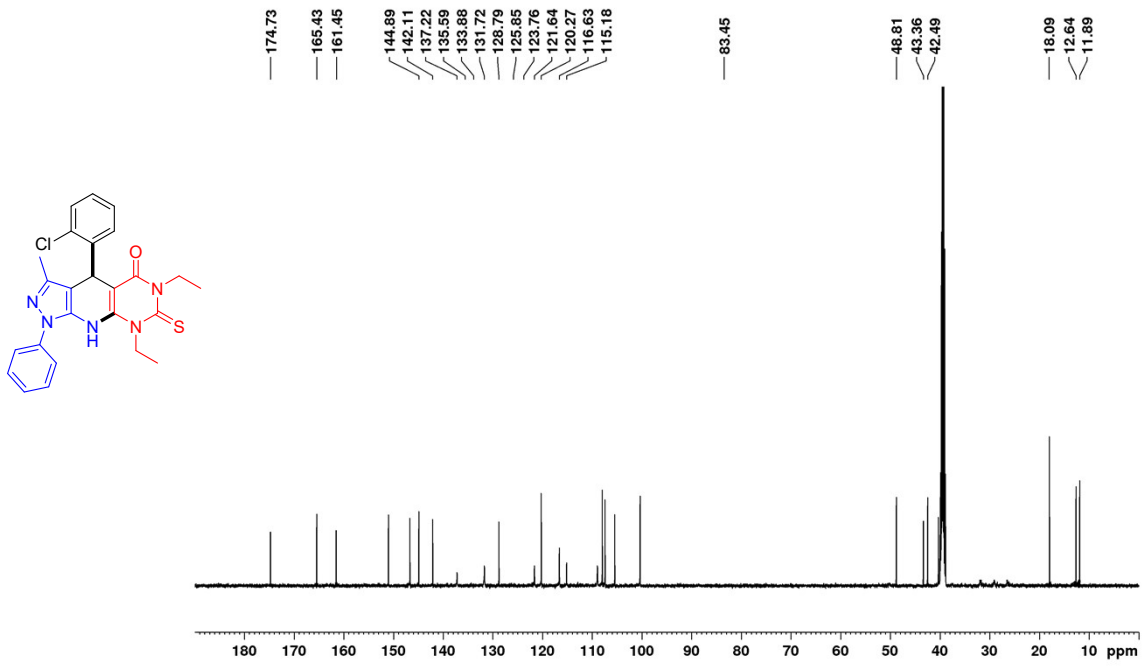

Fig S26: ^{13}C-NMR of 4-(2-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4i)**

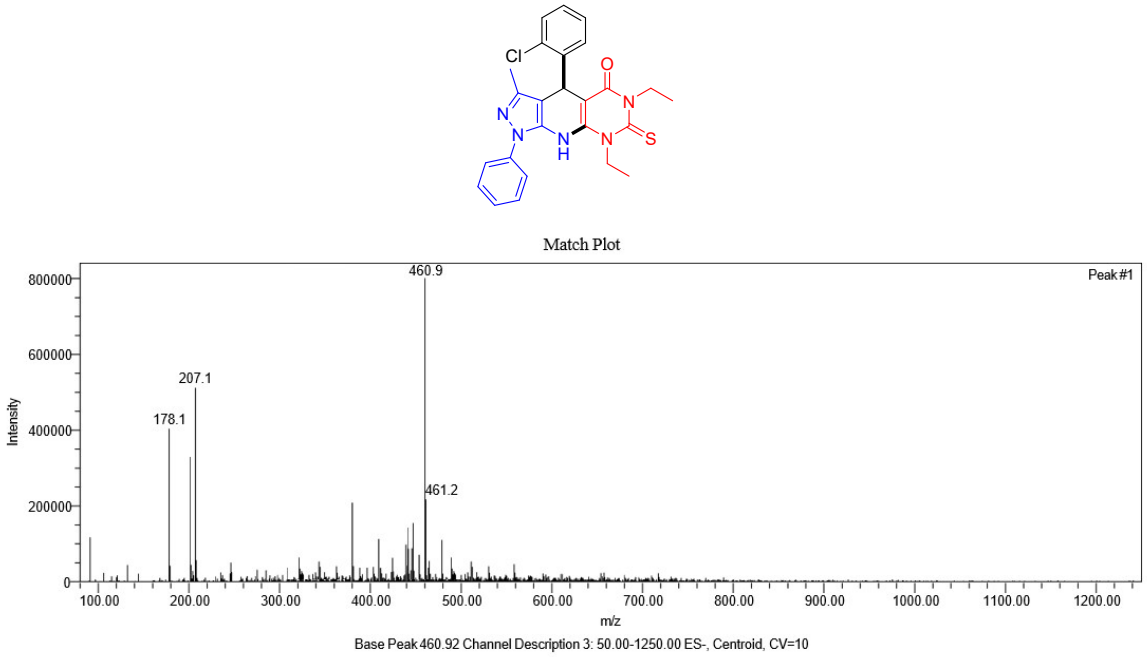

Fig S27: MS of 4-(2-chlorophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4i)**

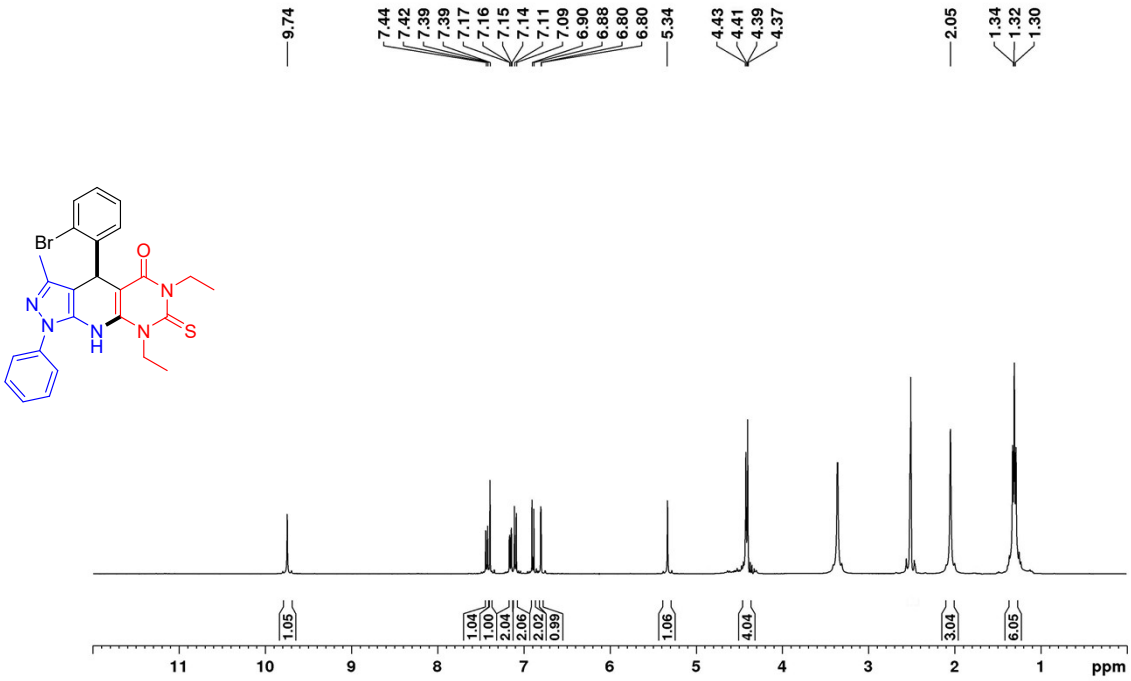

Fig S28: [1]H-NMR of 4-(2-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4j)**

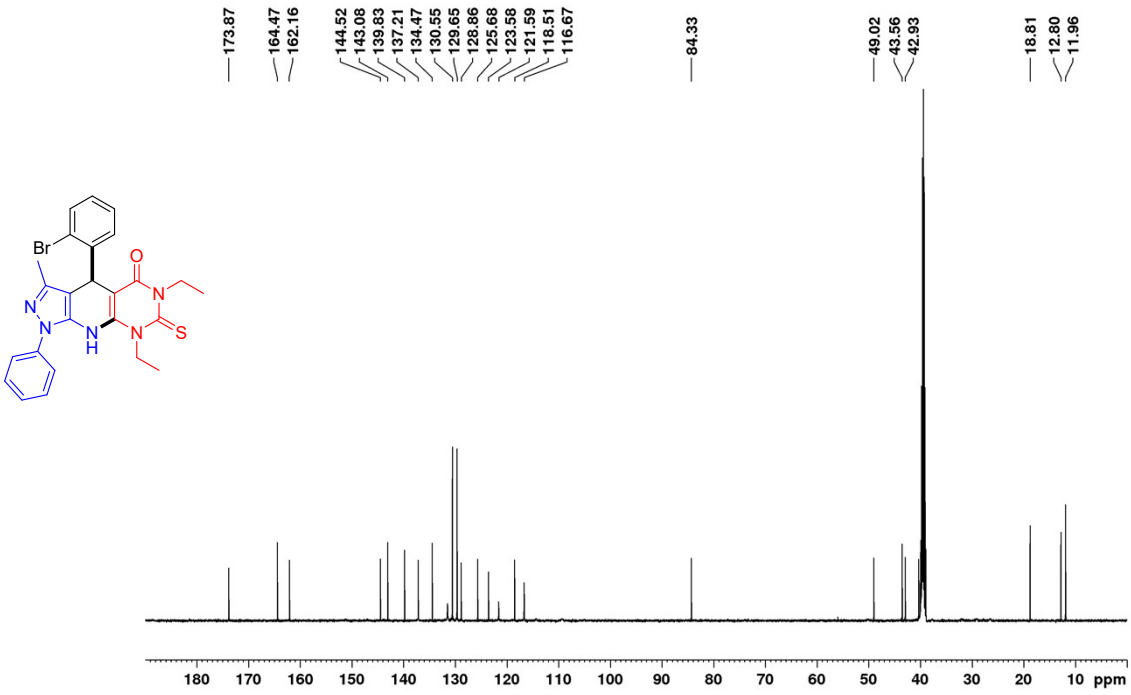

Fig S29: [13]C-NMR of 4-(2-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4j)**

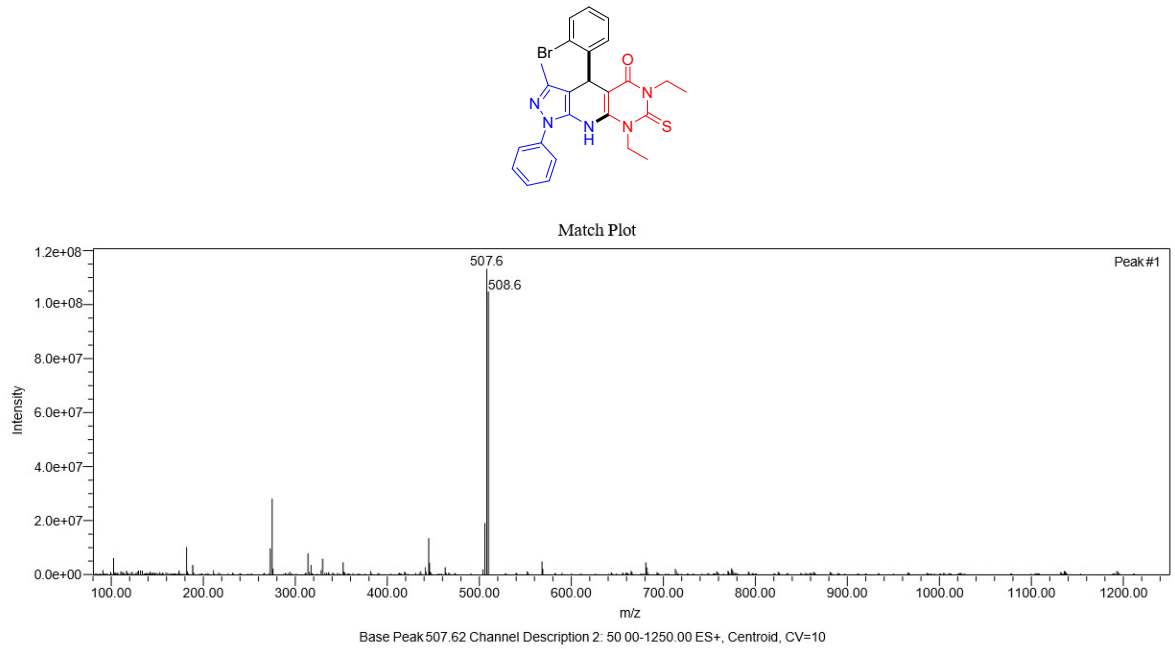

Fig S30: MS of 4-(2-bromophenyl)-6,8-diethyl-3-methyl-1-phenyl-7-thioxo-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4j)**

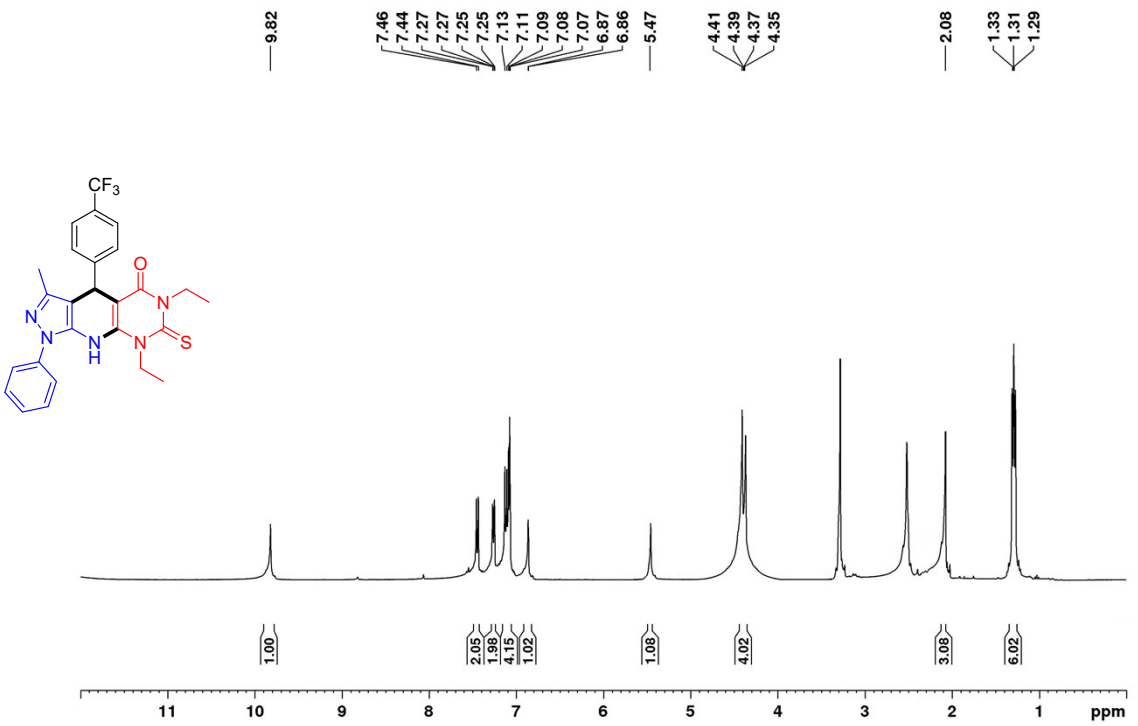

Fig S31: ^{1}H-NMR of 6,8-diethyl-3-methyl-1-phenyl-7-thioxo-4-(4-(trifluoromethyl)phenyl)-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4k)**

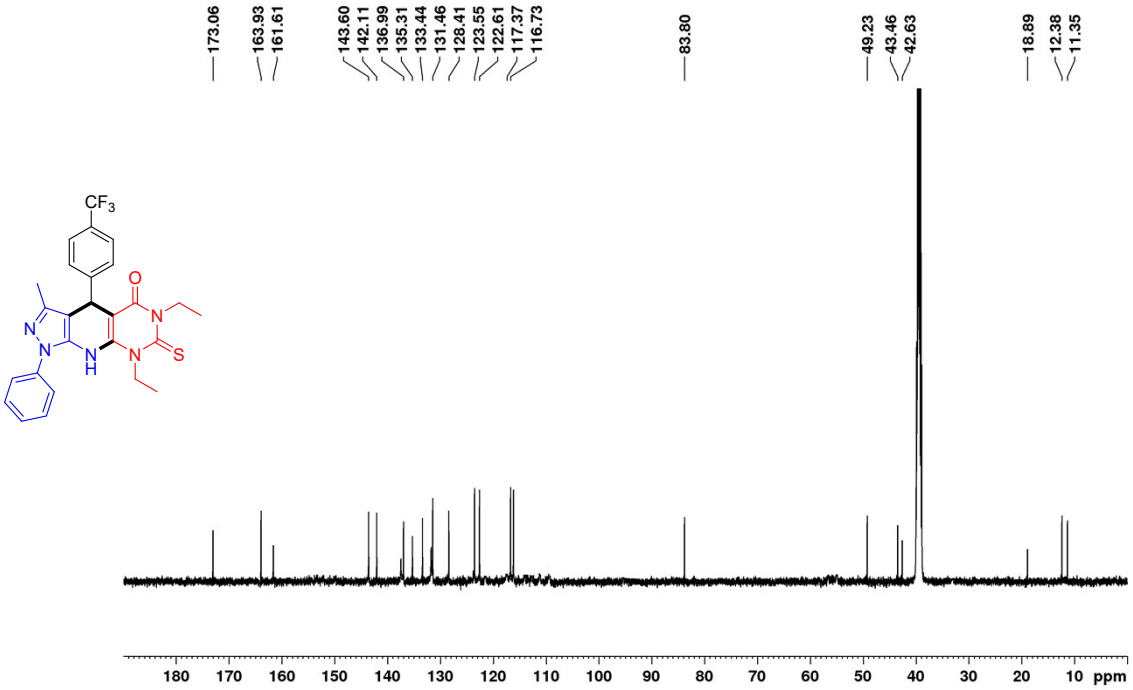

Fig S32: ^{13}C-NMR of 6,8-diethyl-3-methyl-1-phenyl-7-thioxo-4-(4-(trifluoromethyl)phenyl)-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4k)**

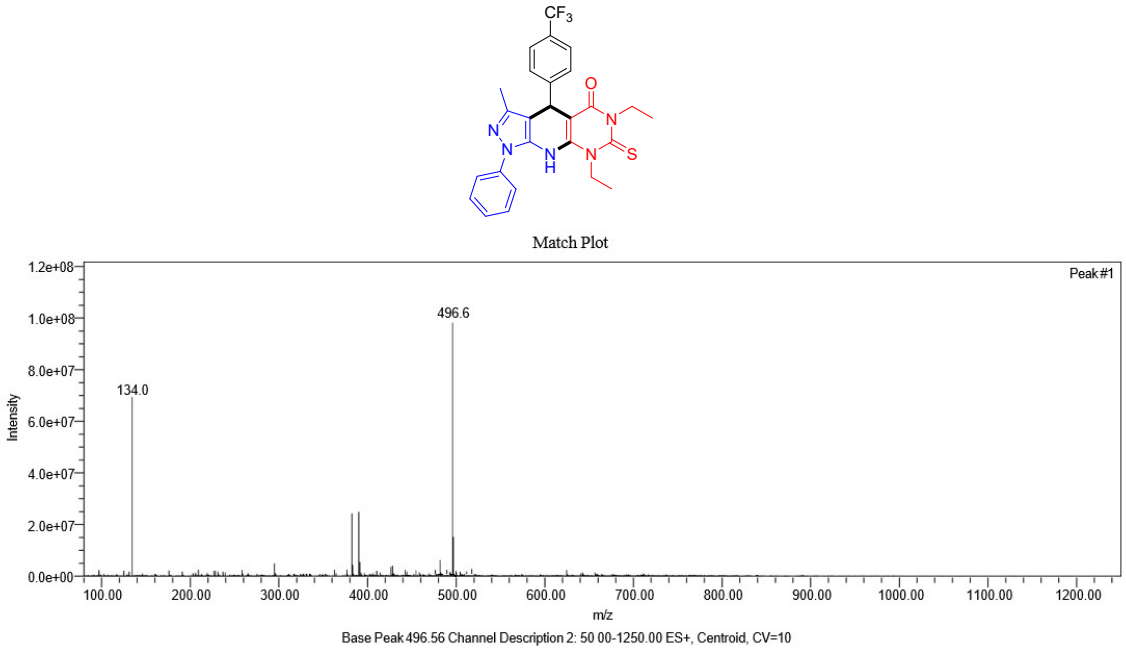

Fig S33: MS of 6,8-diethyl-3-methyl-1-phenyl-7-thioxo-4-(4-(trifluoromethyl)phenyl)-1,4,6,7,8,9-hexahydro-5H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-5-one **(4k)**

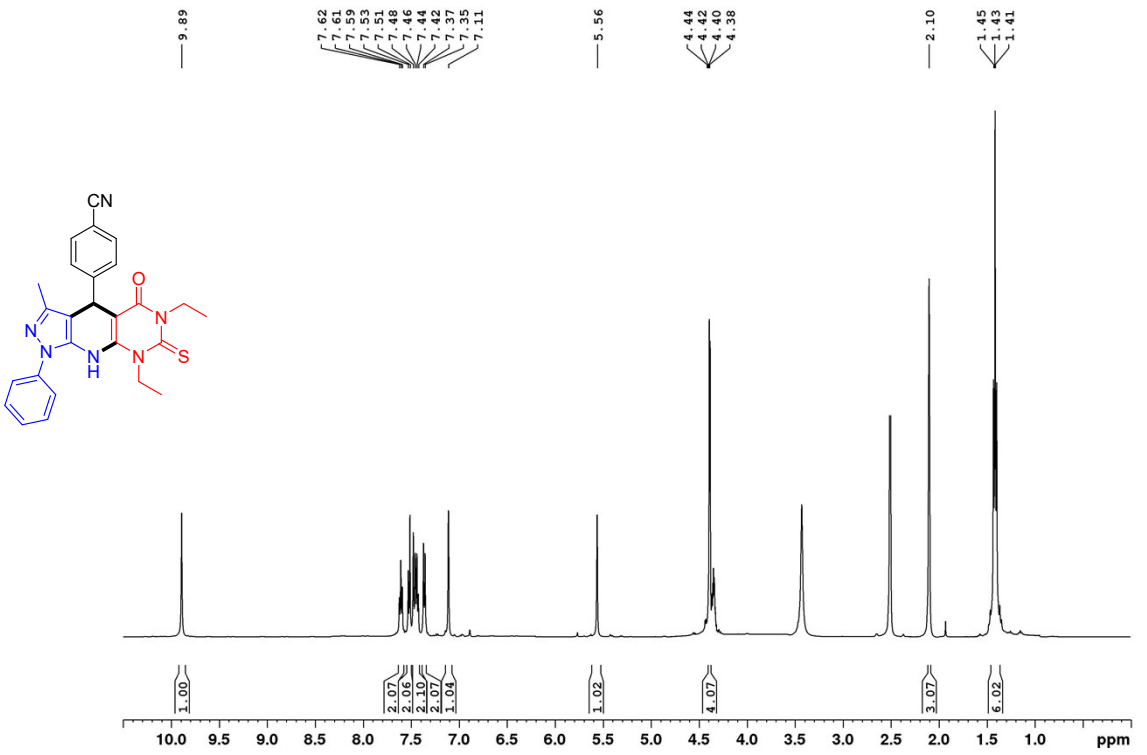

Fig S34: [1]H-NMR of 4-(6,8-diethyl-3-methyl-5-oxo-1-phenyl-7-thioxo-4,5,6,7,8,9-hexahydro-1H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-4-yl)benzonitrile **(4l)**

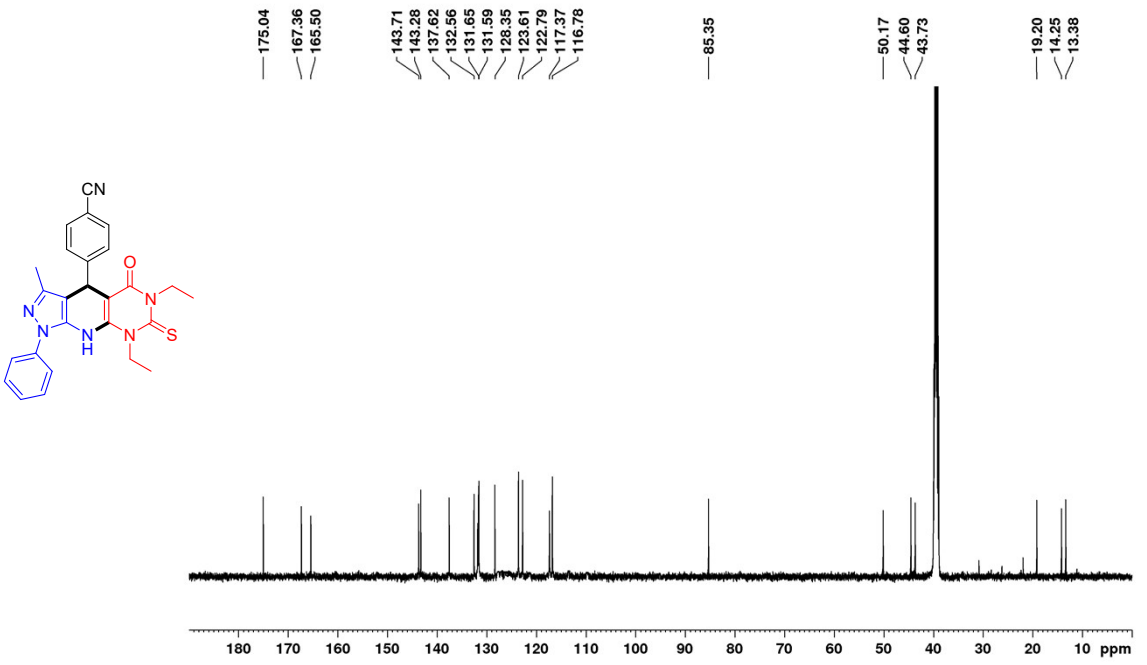

Fig S35: [13]C-NMR of 4-(6,8-diethyl-3-methyl-5-oxo-1-phenyl-7-thioxo-4,5,6,7,8,9-hexahydro-1H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-4-yl)benzonitrile **(4l)**

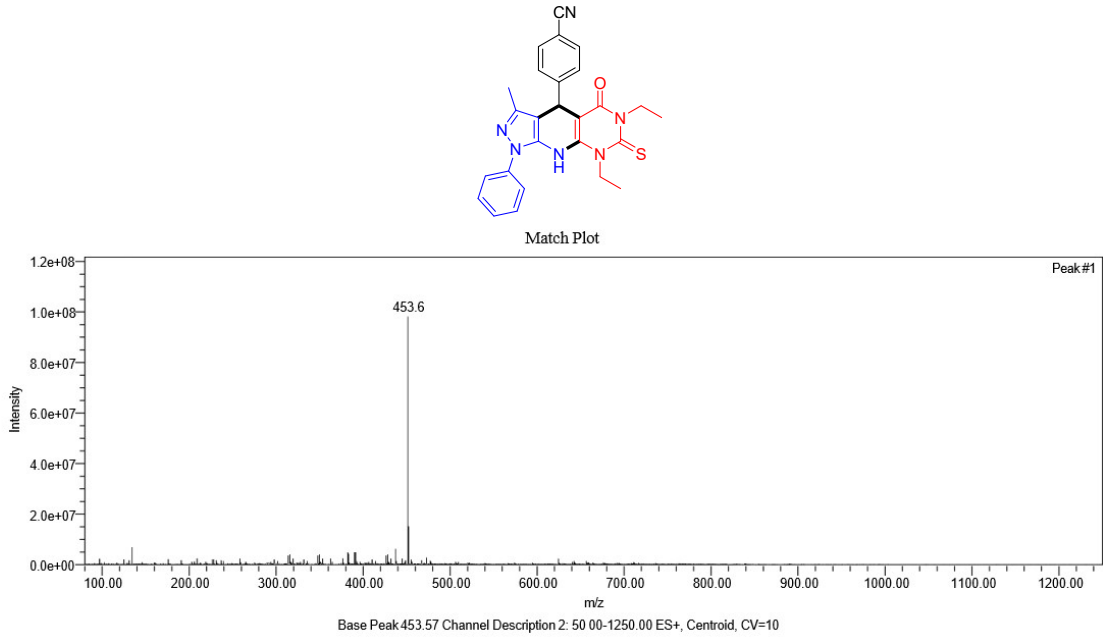

Fig S36: MS of 4-(6,8-diethyl-3-methyl-5-oxo-1-phenyl-7-thioxo-4,5,6,7,8,9-hexahydro-1H-pyrazolo[4',3':5,6]pyrido[2,3-d]pyrimidin-4-yl)benzonitrile **(4l)**