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Covalent Inhibition of Thioredoxin Reductase by Michael Acceptors: Rational Design, Synthesis, and Biological Evaluation of Oxazol-5(4H)-one Derivatives

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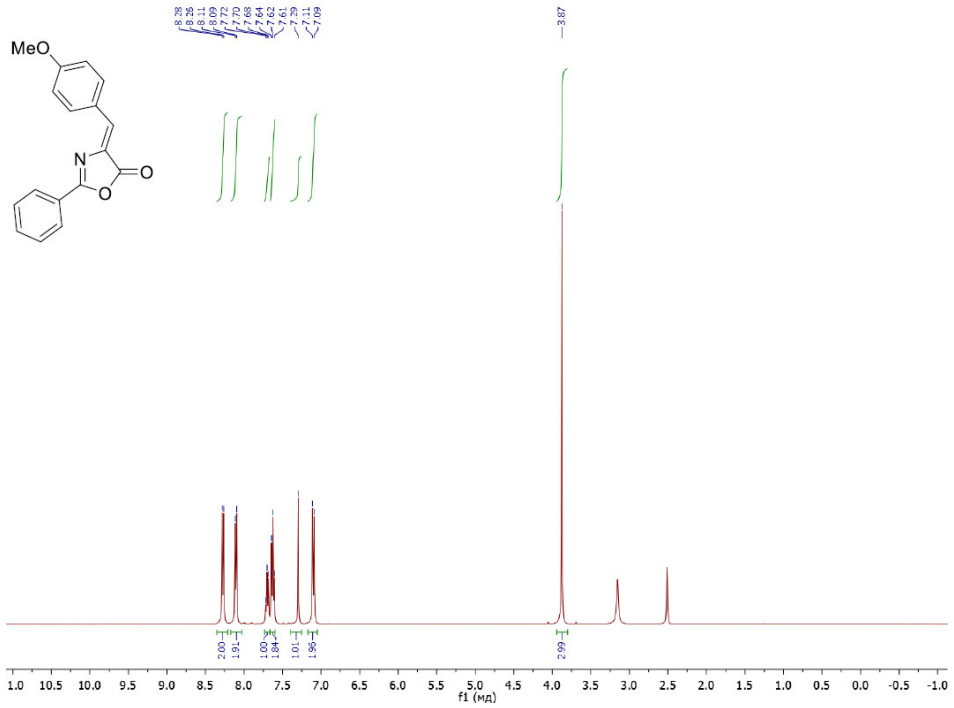

Fig. (S1). ^{1}H NMR spectrum of compound **1g** (DMSO-d_6, 400 MHz).

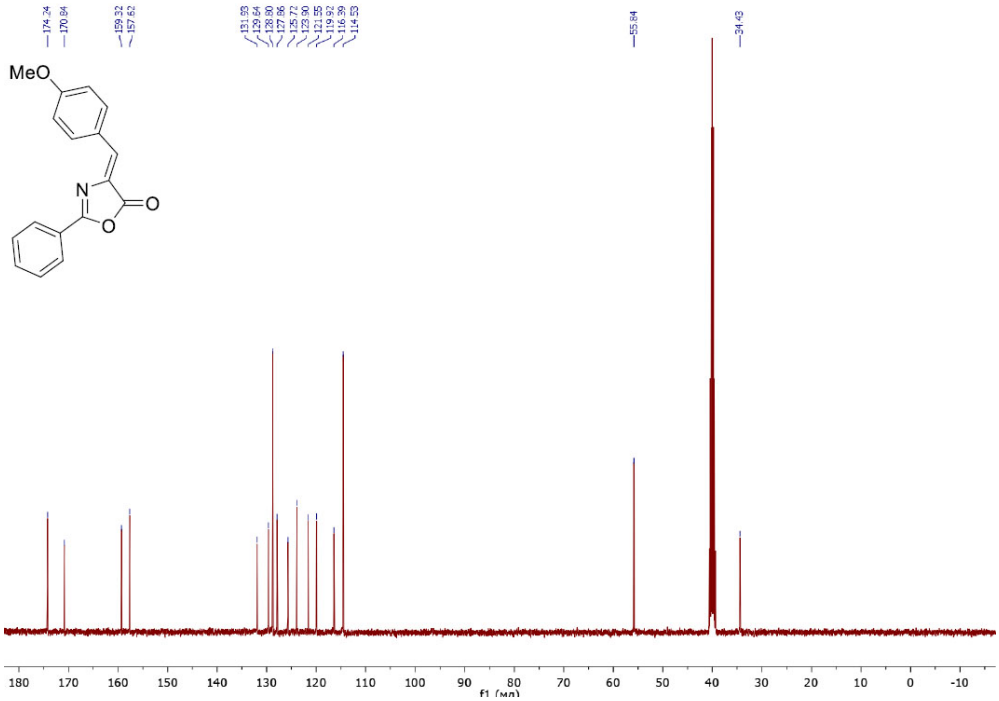

Fig. (S2). ^{13}C NMR spectrum of compound **1g** (DMSO-d_6, 101 MHz).

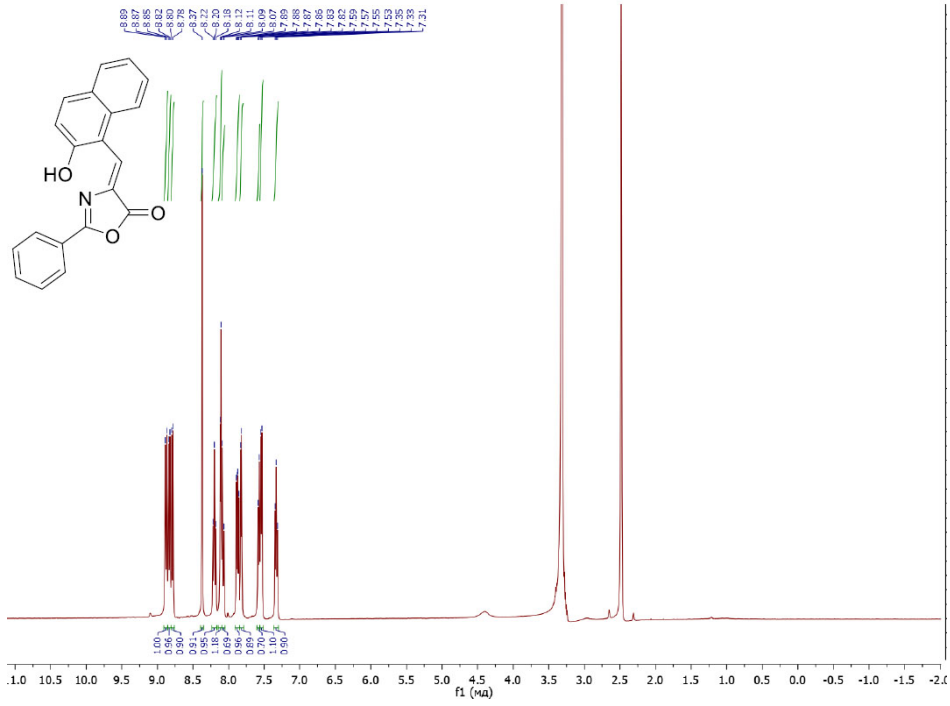

Fig. (S3). ^{1}H NMR spectrum of compound **1h** (DMSO-d_6, 400 MHz).

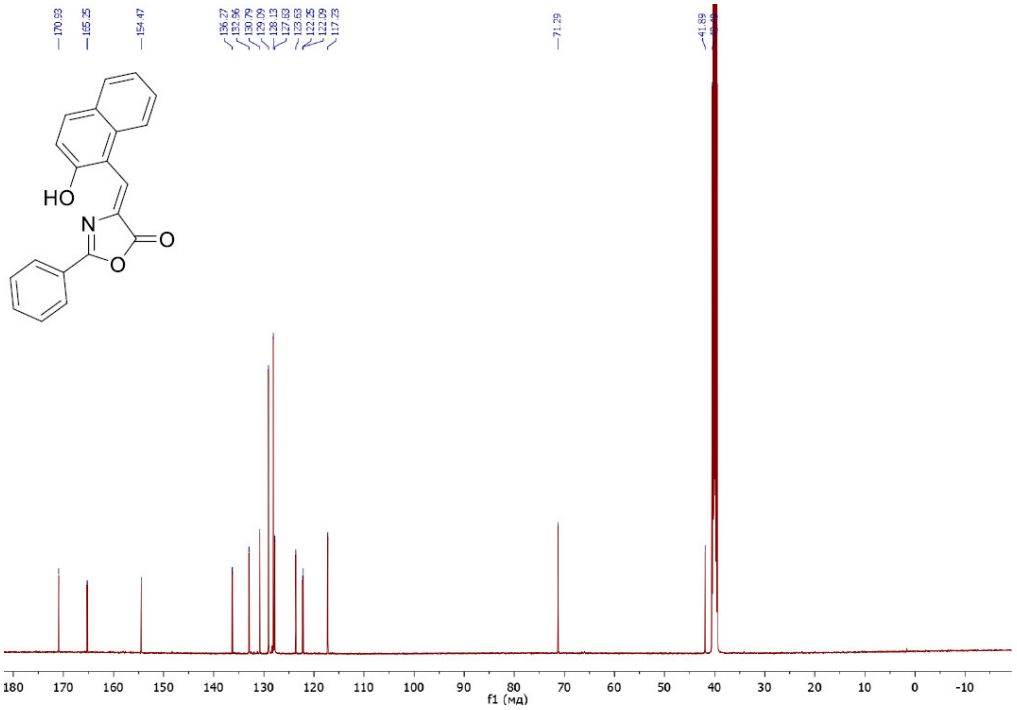

Fig. (S4). ^{13}C NMR spectrum of compound **1h** (DMSO-d_6, 126 MHz).

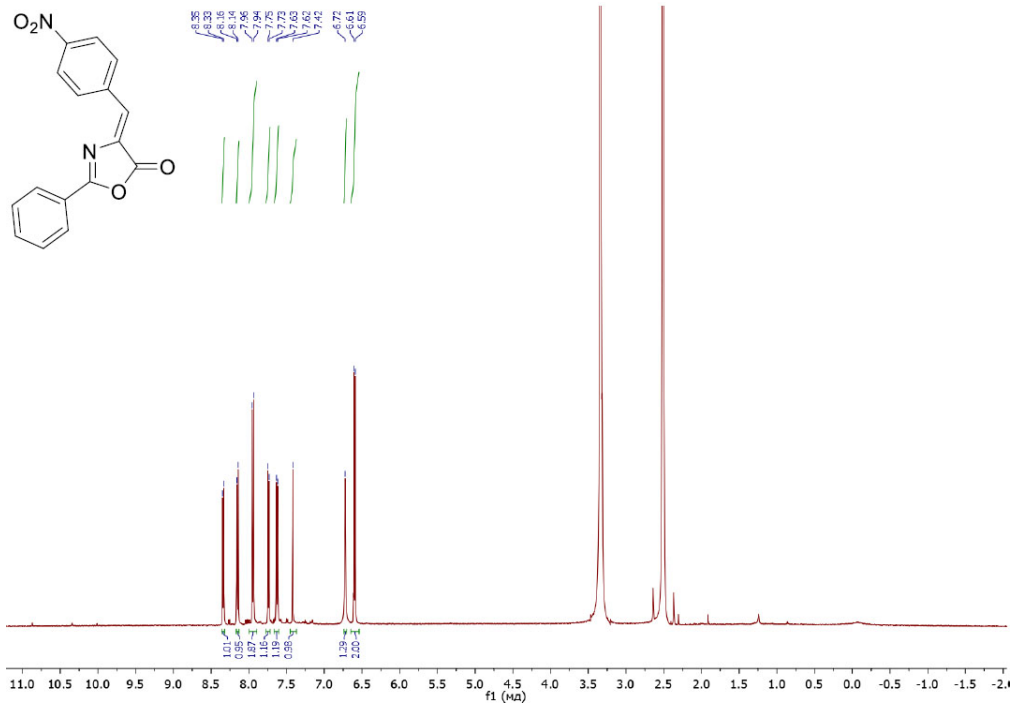

Fig. (S5). ^{1}H NMR spectrum of compound **1i** (DMSO-d_6, 500 MHz).

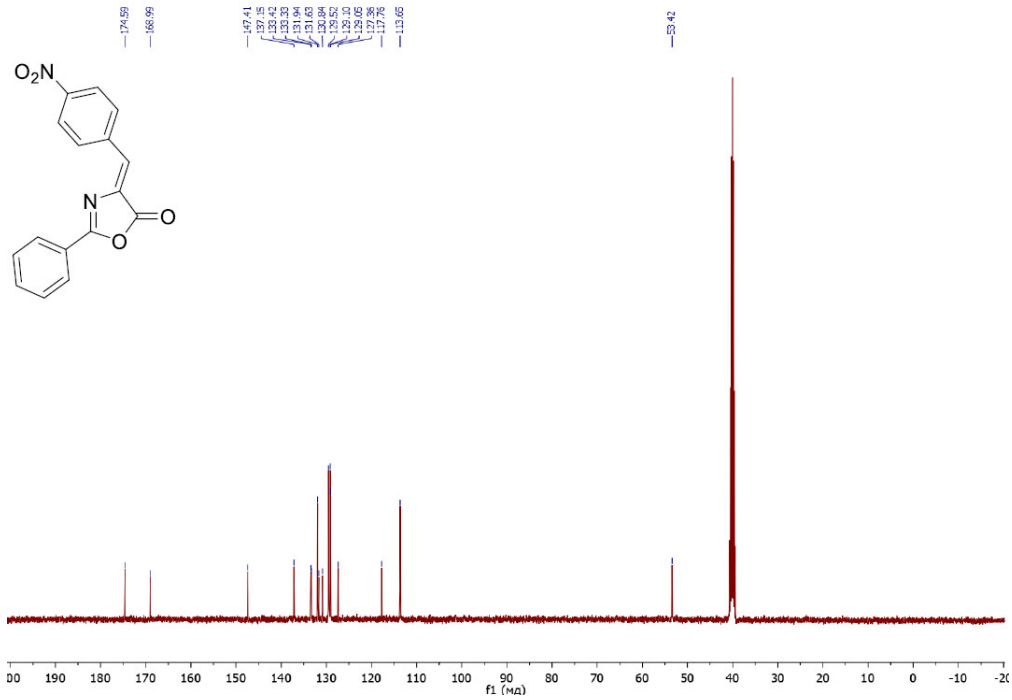

Fig. (S6). ^{13}C NMR spectrum of compound **1i** (DMSO-d_6, 101 MHz).

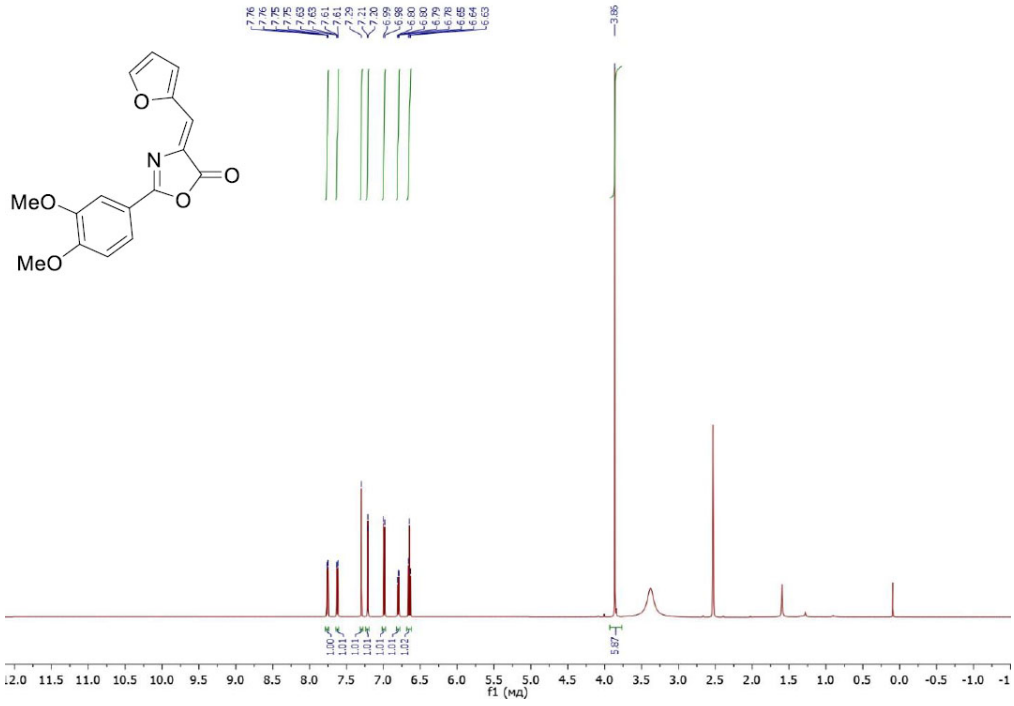

Fig. (S7). ^{1}H NMR spectrum of compound **1j** (DMSO-d_6, 400 MHz).

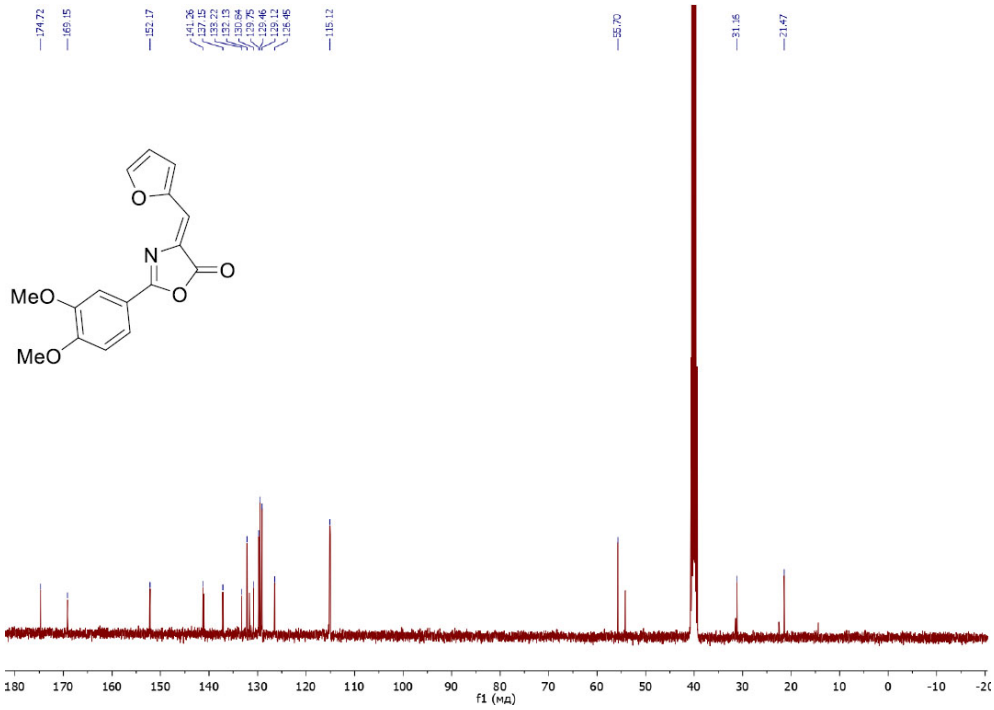

Fig. (S8). ^{13}C NMR spectrum of compound **1j** (DMSO-d_6, 101 MHz).

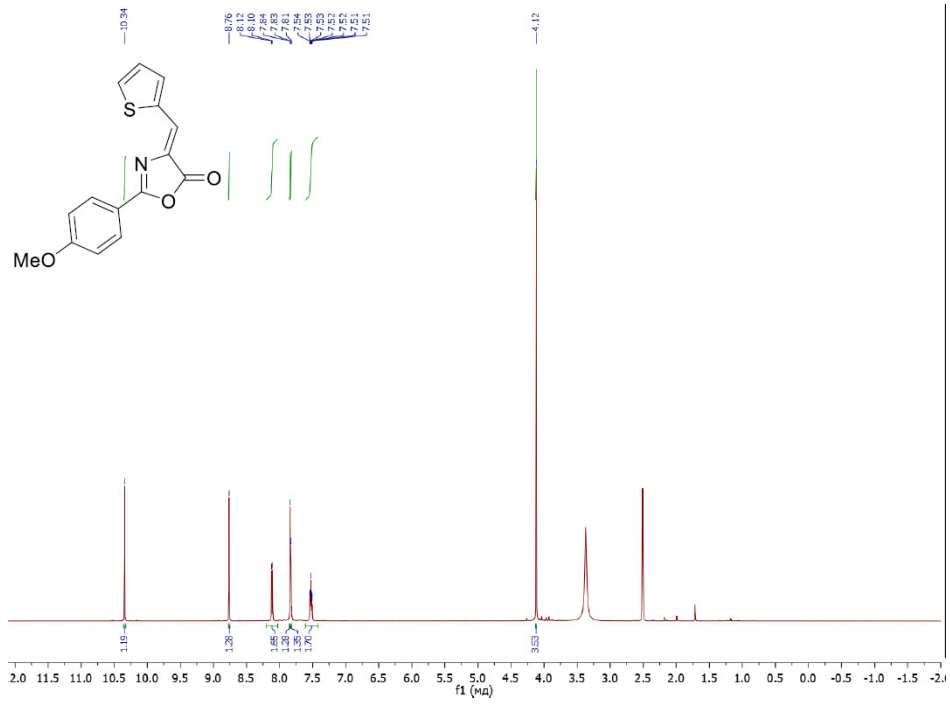

Fig. (S9). ^{1}H NMR spectrum of compound **1k** (DMSO-d_6, 500 MHz).

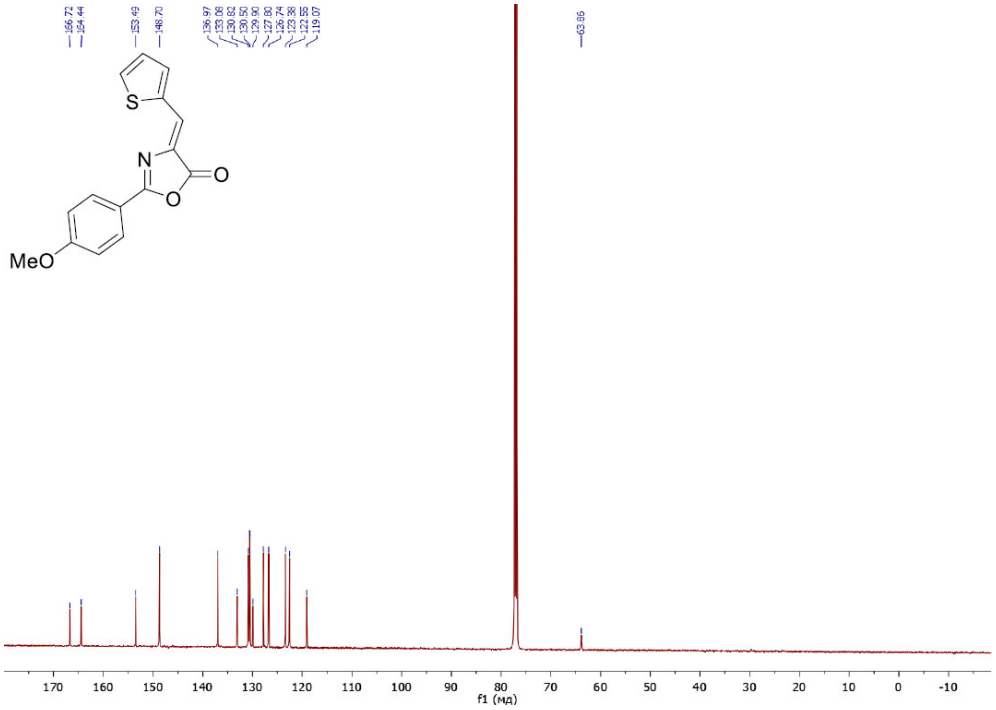

Fig. (S10). ^{13}C NMR spectrum of compound **1k** ($CDCl_3$, 126 MHz).

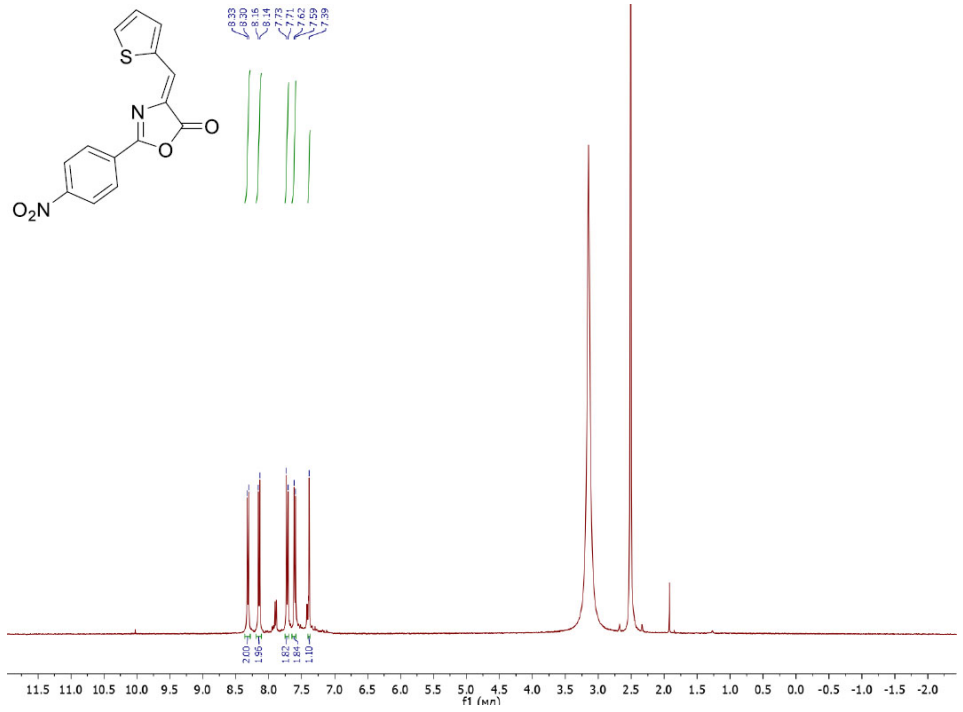

Fig. (S11). ^{1}H NMR spectrum of compound **1l** (DMSO-d_6, 400 MHz).

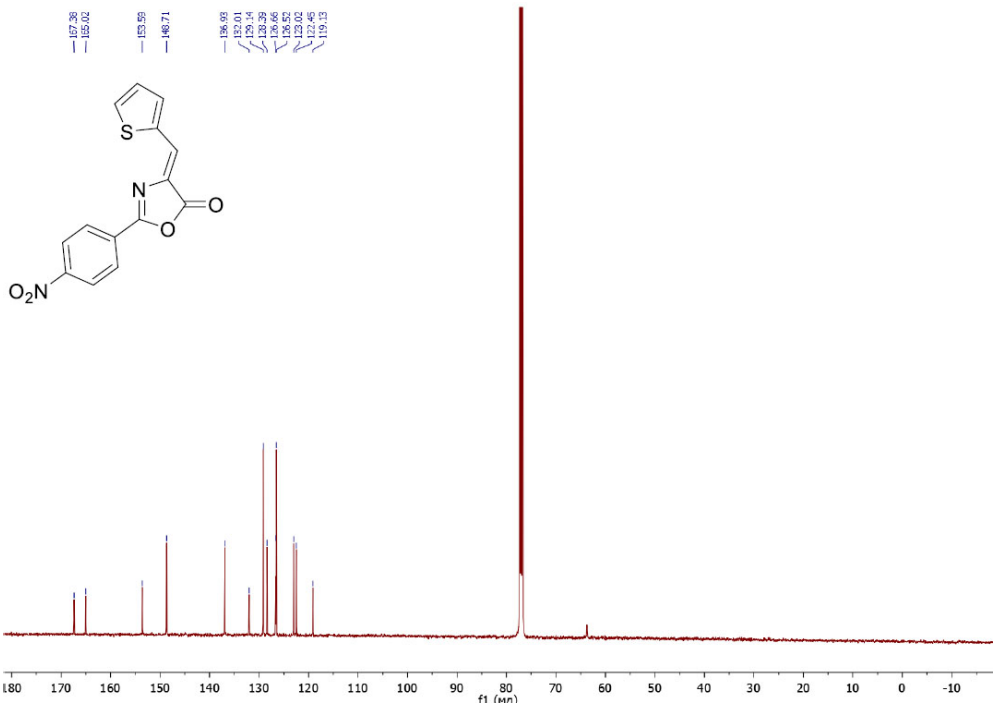

Fig. (S12). ^{13}C NMR spectrum of compound **1l** ($CDCl_3$, 126 MHz).

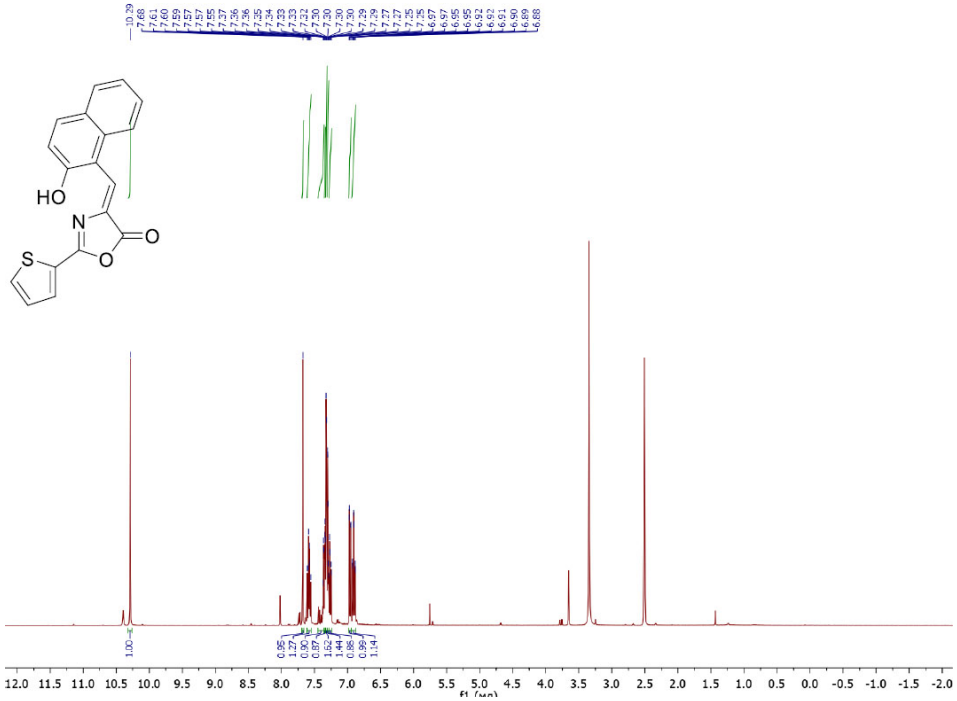

Fig. (S13). ^{1}H NMR spectrum of compound **1m** (DMSO-d_6, 400 MHz).

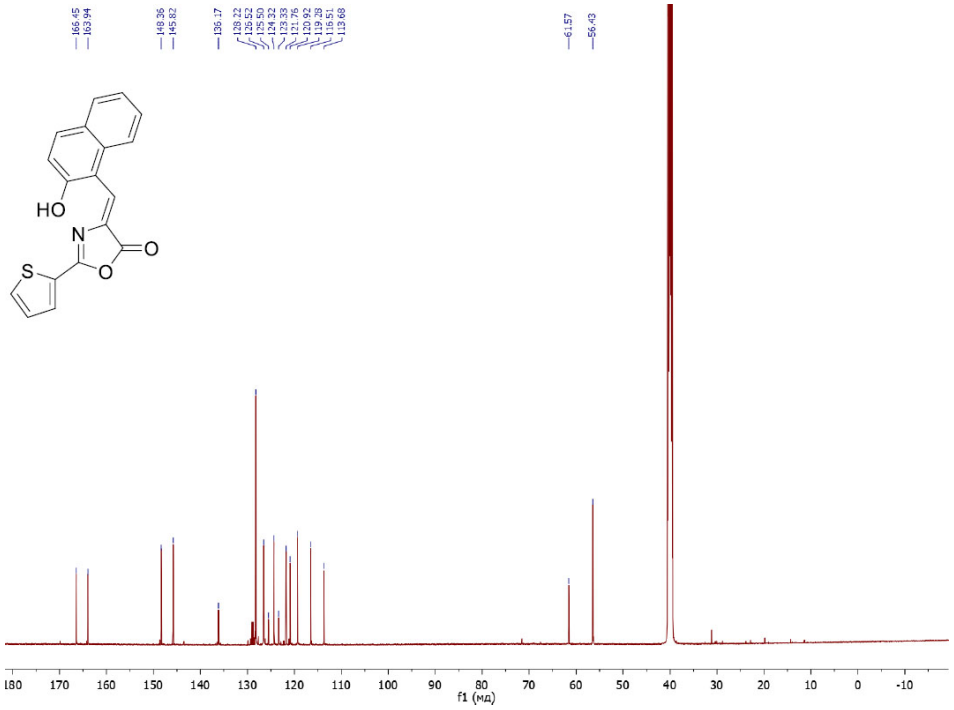

Fig. (S14). ^{13}C NMR spectrum of compound **1m** (DMSO-d_6, 126 MHz).

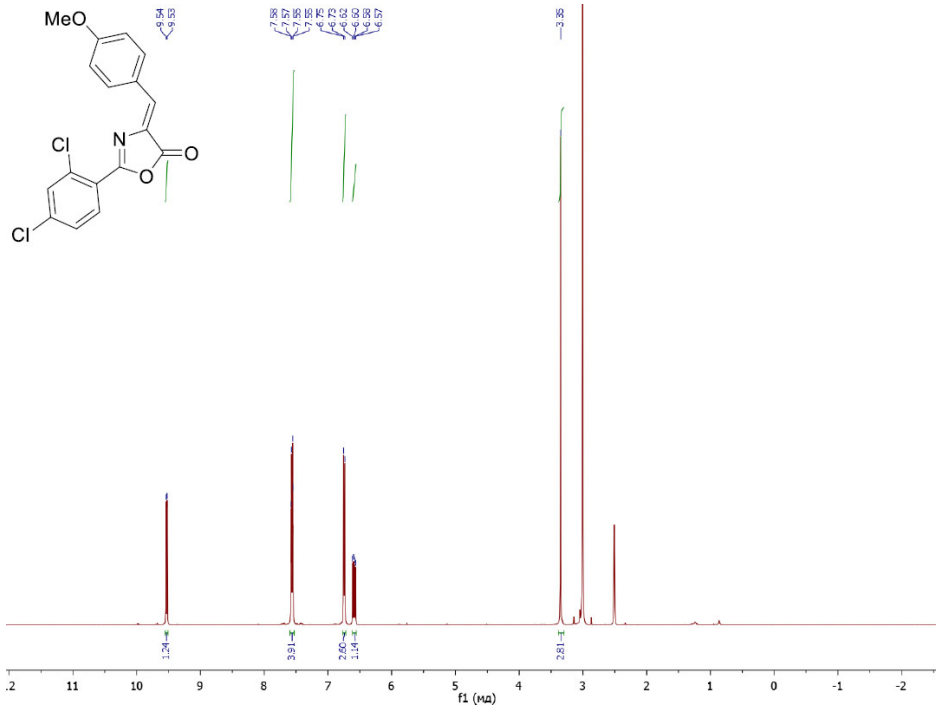

Fig. (S15). ^{1}H NMR spectrum of compound **1n** (DMSO-d_6, 500 MHz).

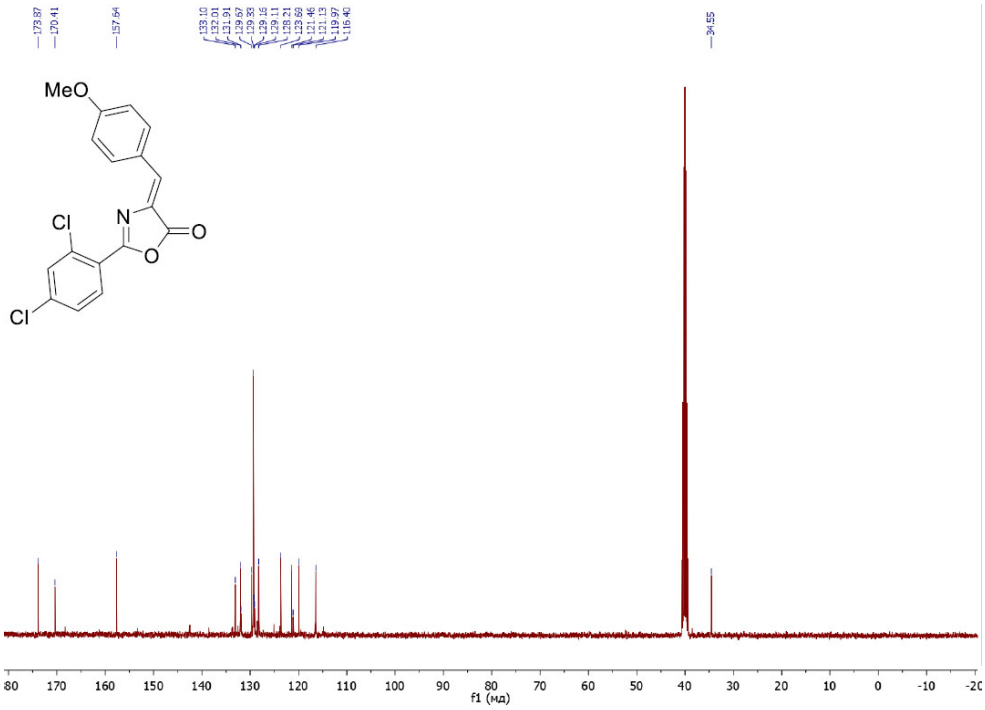

Fig. (S16). ^{13}C NMR spectrum of compound **1n** (DMSO-d_6, 101 MHz).

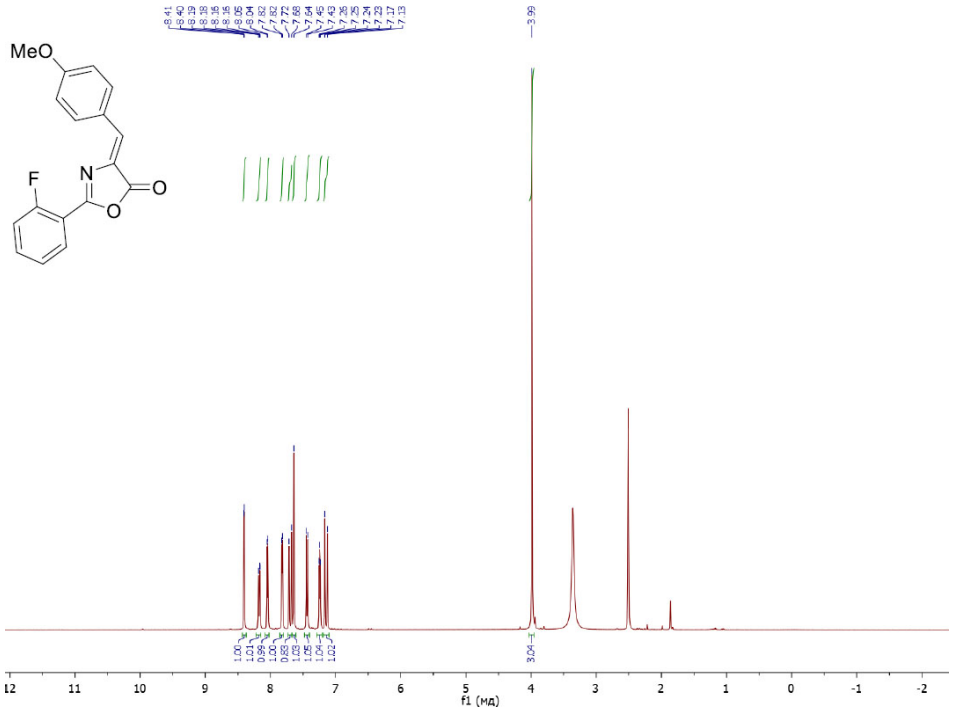

Fig. (S17). ^{1}H NMR spectrum of compound **1o** (DMSO-d_6, 400 MHz).

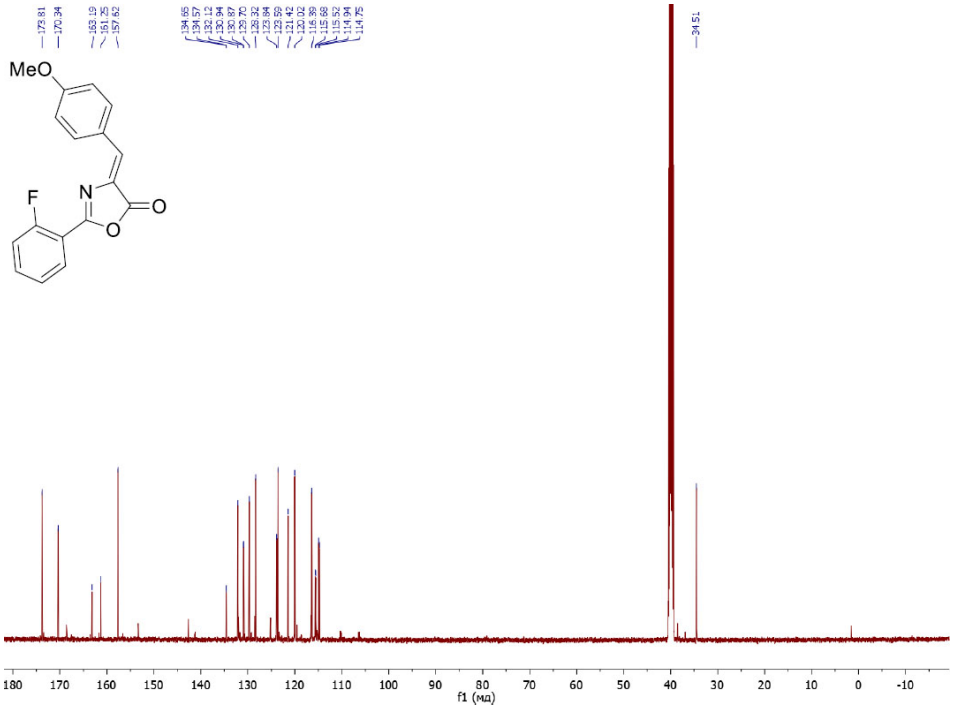

Fig. (S18). ^{13}C NMR spectrum of compound **1o** (DMSO-d_6, 126 MHz).

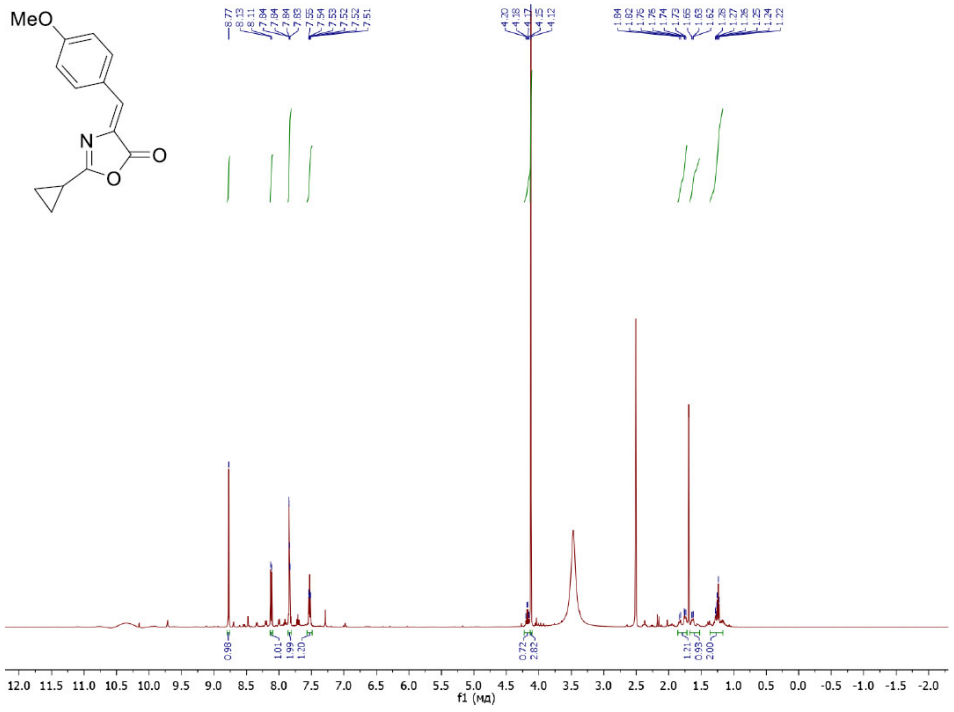

Fig. (S19). ^{1}H NMR spectrum of compound **1p** (DMSO-d_6, 500 MHz).

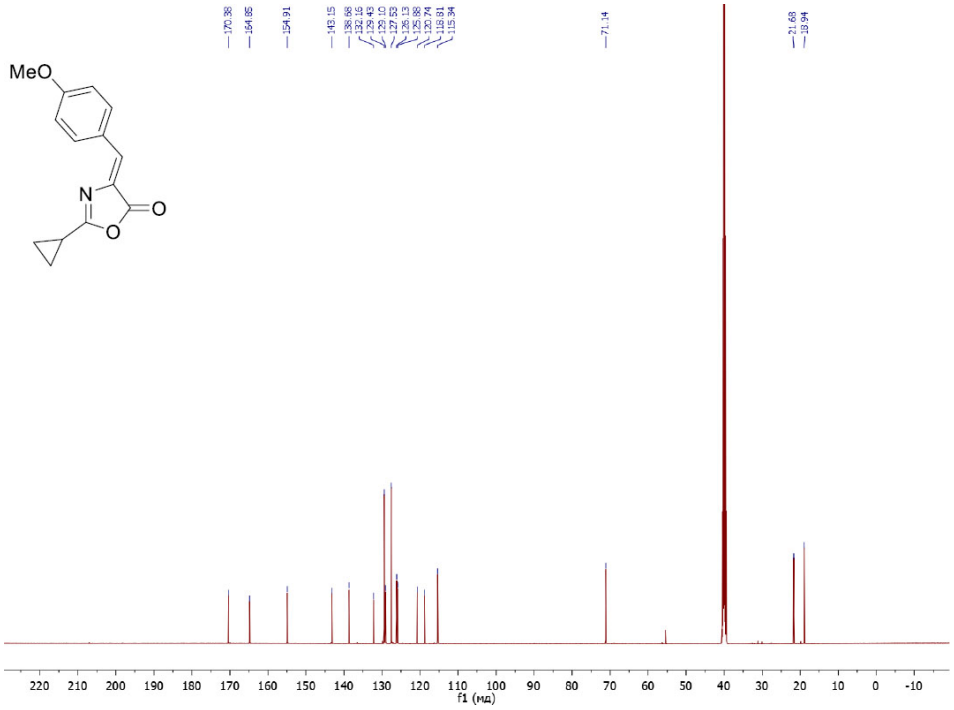

Fig. (S20). ^{13}C NMR spectrum of compound **1p** (DMSO-d_6, 126 MHz).

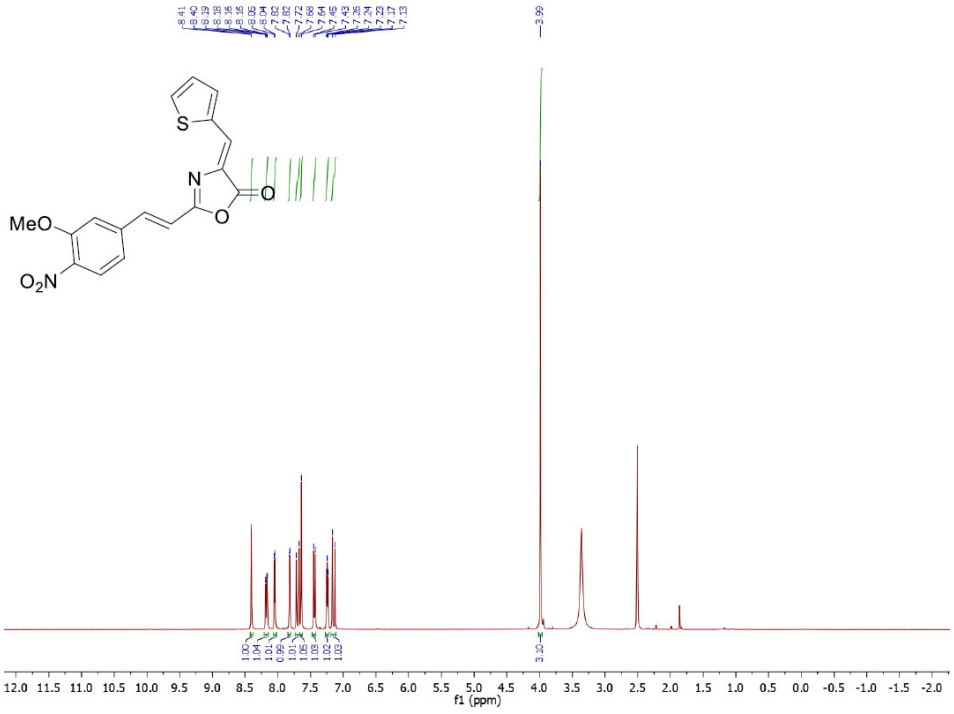

Fig. (S21). ^{1}H NMR spectrum of compound **1q** (DMSO-d_6, 400 MHz).

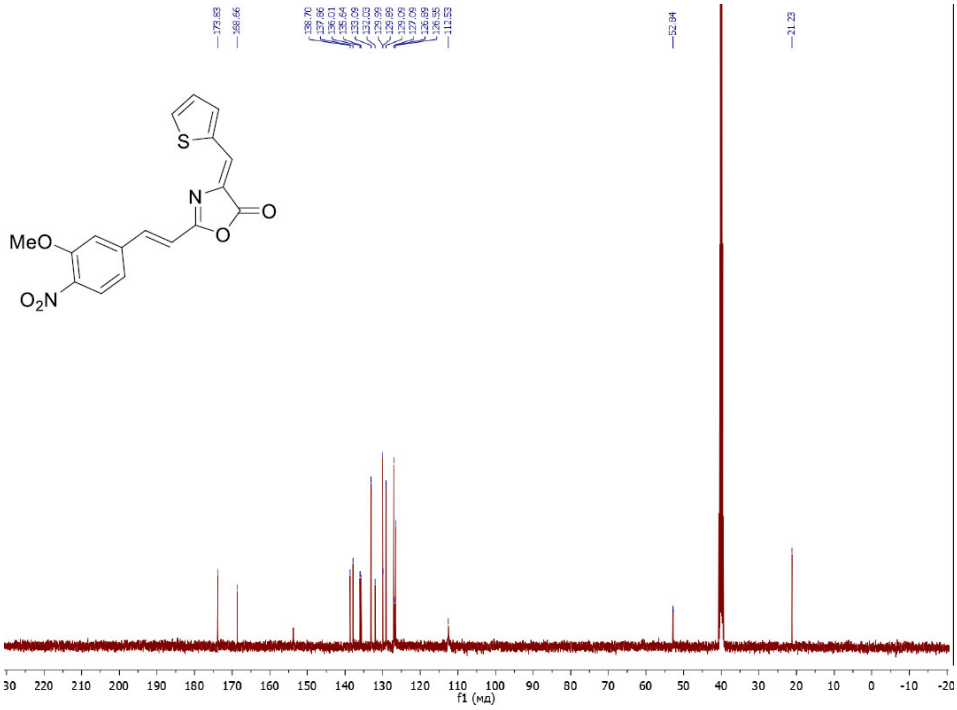

Fig. (S22). ^{13}C NMR spectrum of compound **1q** (DMSO-d_6, 101 MHz).

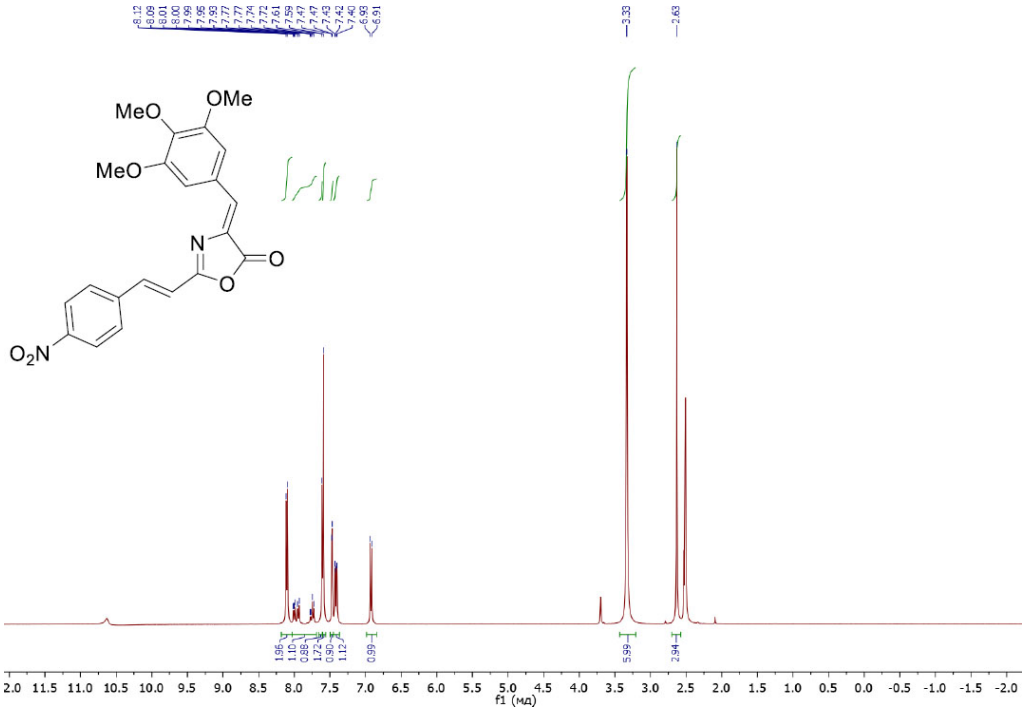

Fig. (S23). ^{1}H NMR spectrum of compound **1r** (DMSO-d_6, 400 MHz).

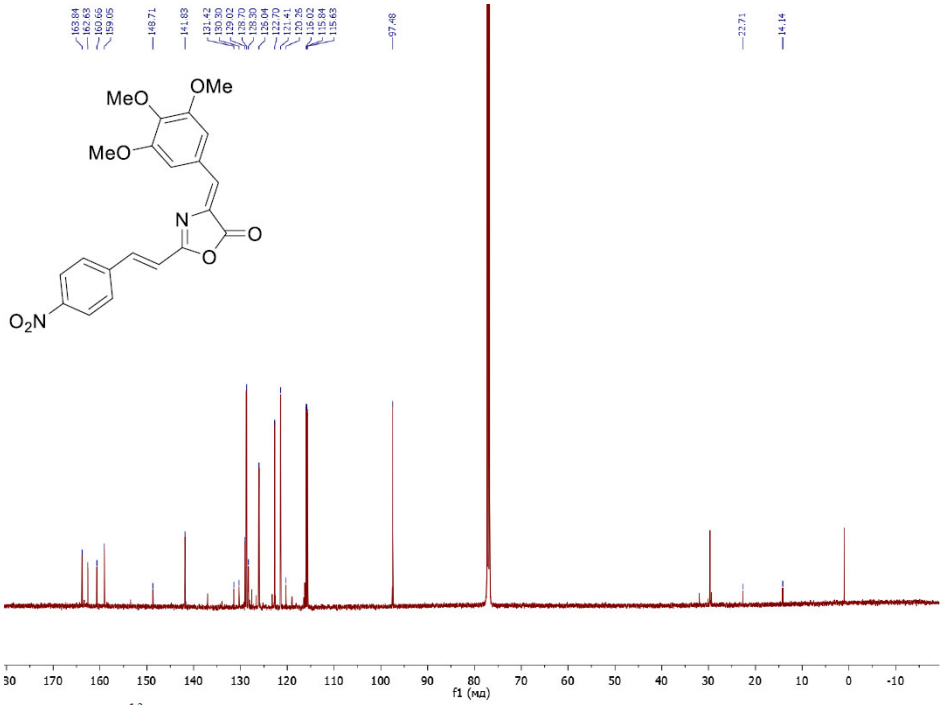

Fig. (S24). ^{13}C NMR spectrum of compound **1r** ($CDCl_3$, 126 MHz).

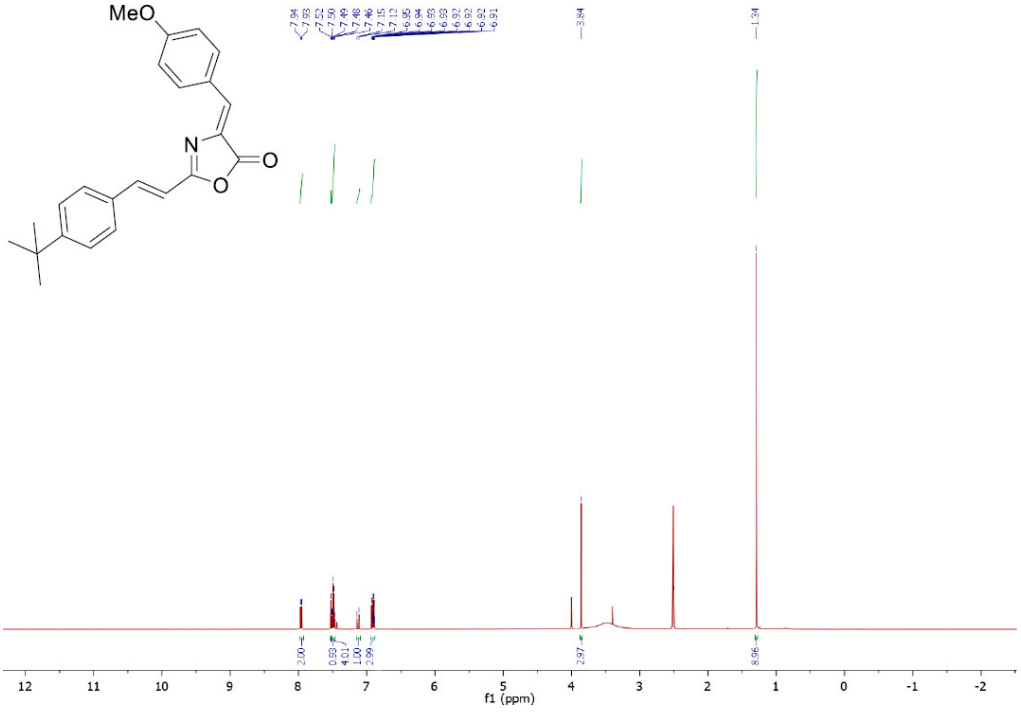

Fig. (S25). ^{1}H NMR spectrum of compound **1s** (DMSO-d_6, 500 MHz).

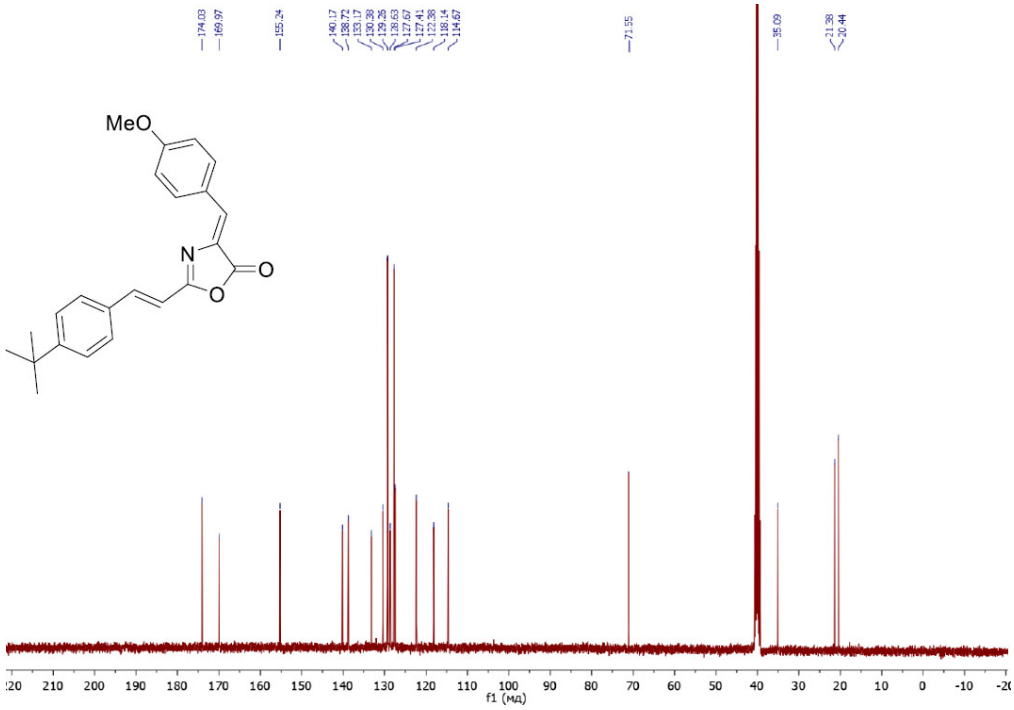

Fig. (S26). ^{13}C NMR spectrum of compound **1s** (DMSO-d_6, 126 MHz).

Fig. (S27). Molecular weight marker for HELA cell line.

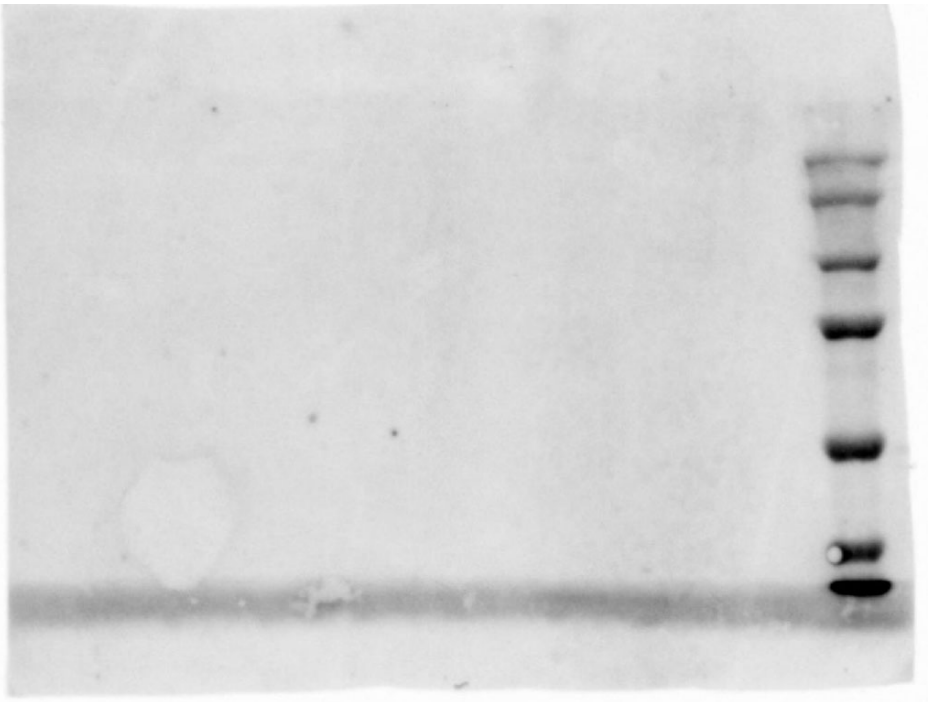

Fig. (S28). Molecular weight marker for SH-SY5Y cell line.

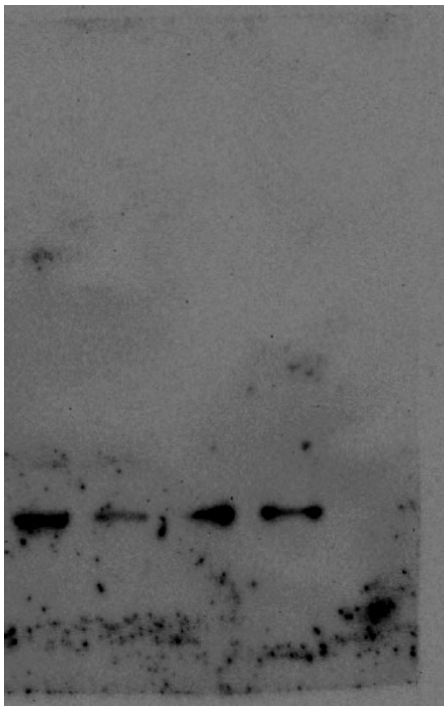

Fig. (S29). Beta actin in blotting for SH-SY5Y cell line.

Fig. (S30). Beta actin in blotting for HELA cell line.

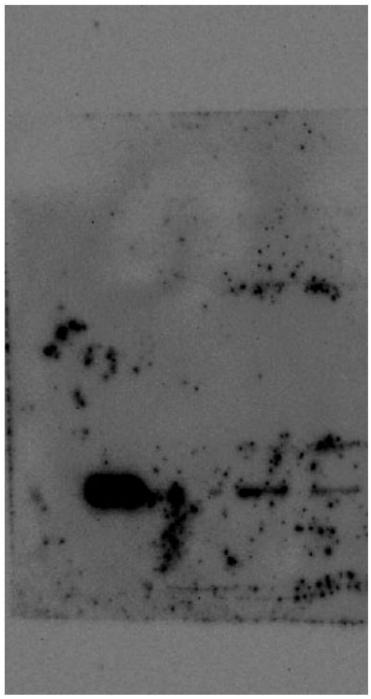

Fig. (S31). Beta actin in blotting for U251 cell line.

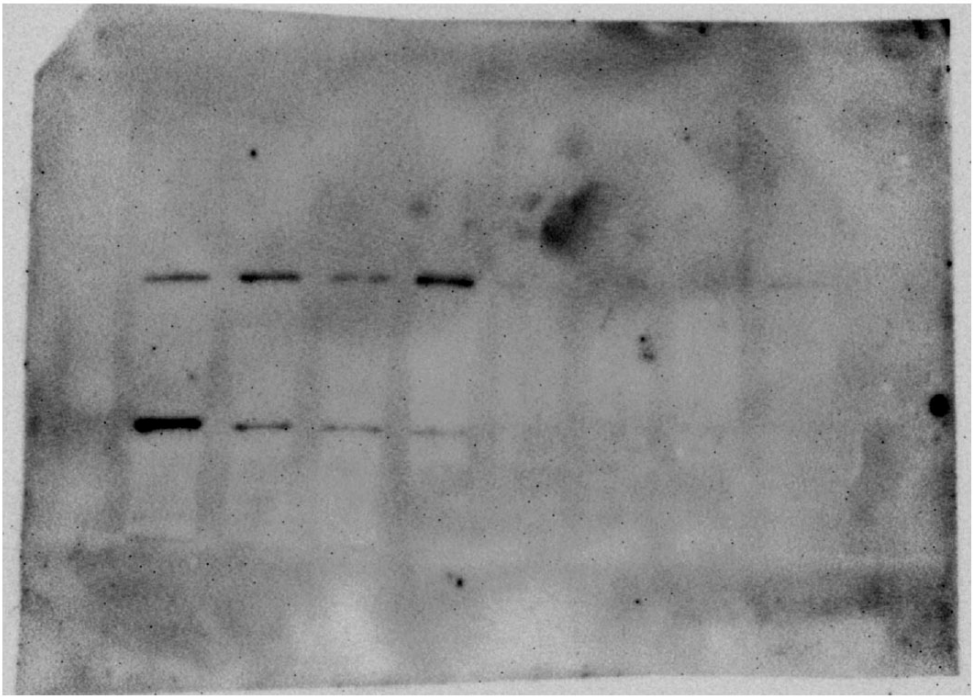

Fig. (S32). Blotting Image for TrxR1 in HELA cell line.

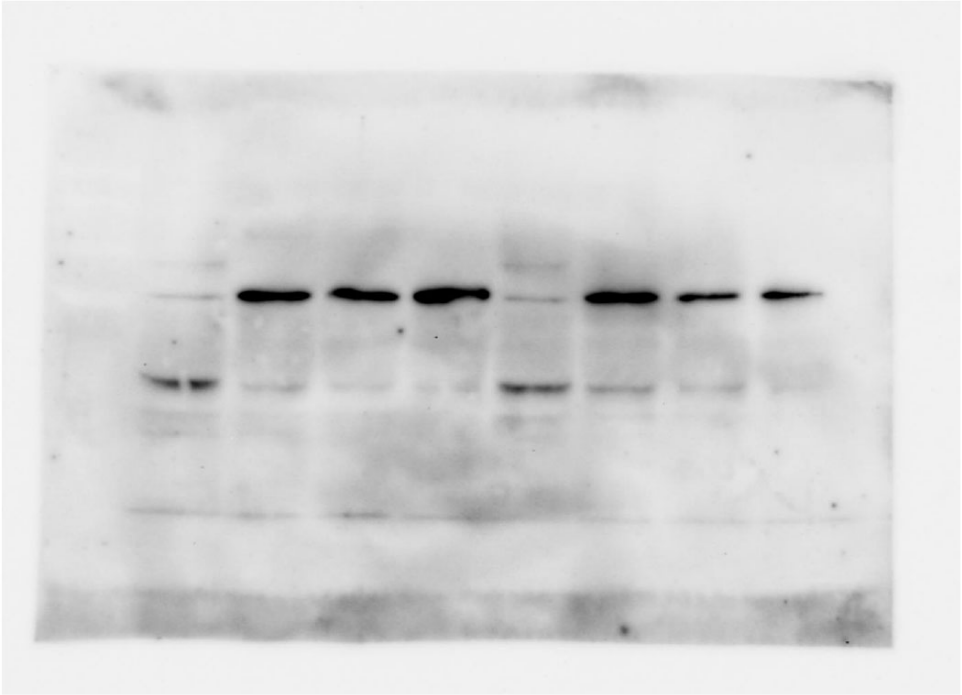

Fig. (S33). Blotting Image for TrxR1 in SH-SY5Y cell line.

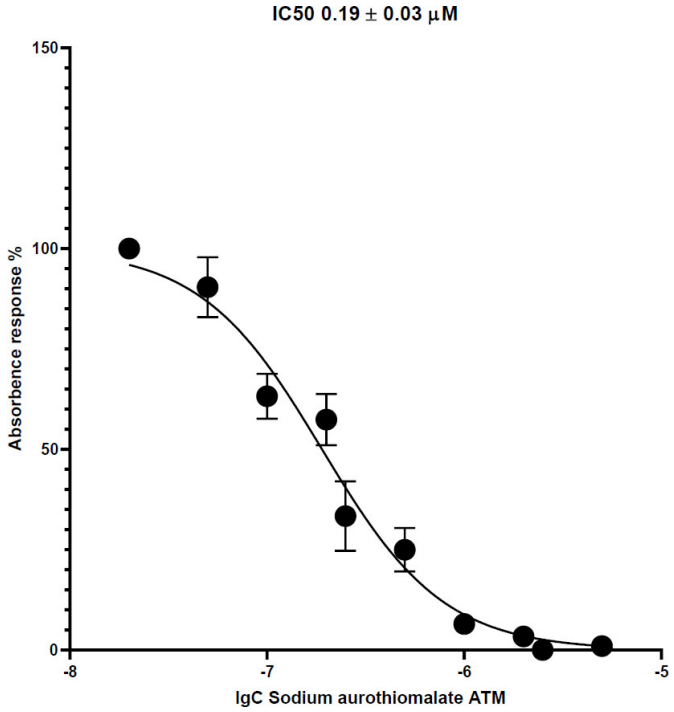

Fig. (S34). TrxR inhibition by for Sodium aurothiomalate ATM (dose response curve).