SUPPORTING INFORMATION

A novel compound active against SARS-CoV-2 targeting Uridylate-specific endoribonuclease (NendoU/NSP15): *In silico* and *in vitro* investigations

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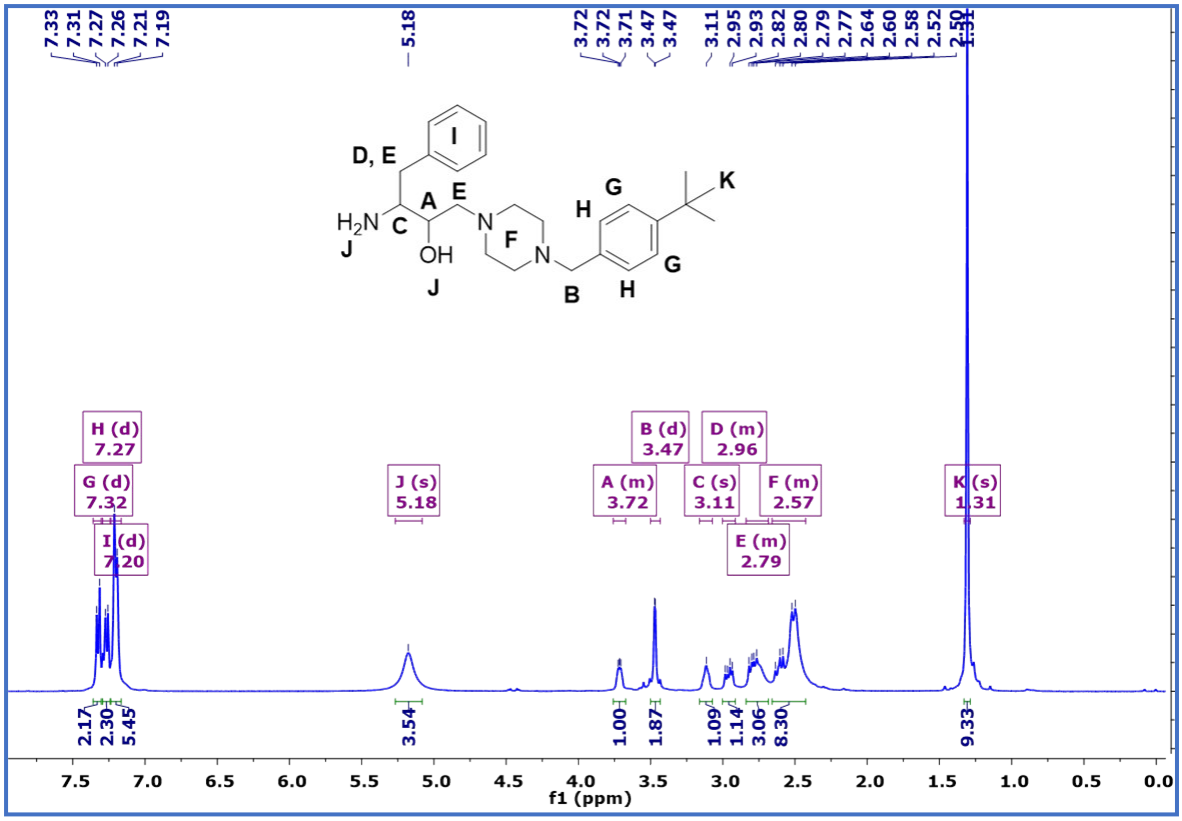

Figure S1. ^{1}H NMR spectrum of compound, **IV** in $CDCl_3$.

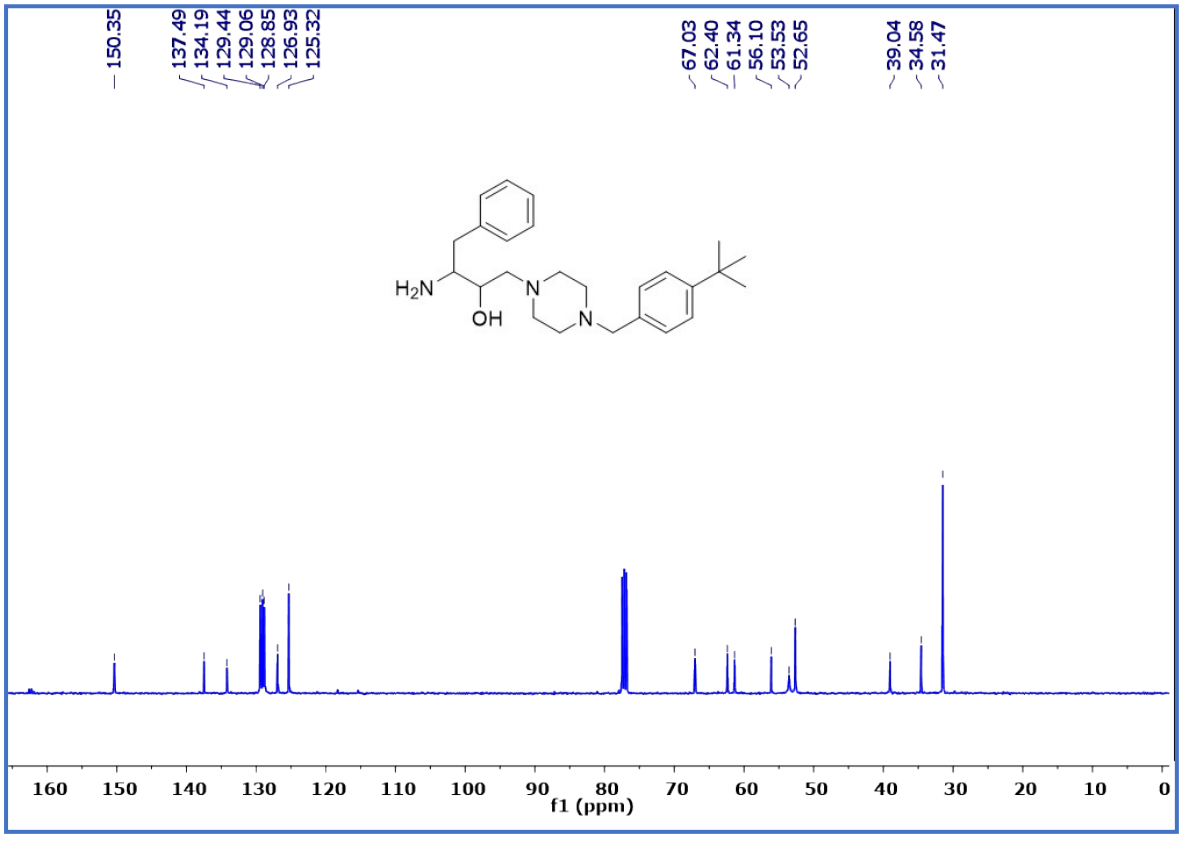

Figure S2. ^{13}C NMR spectrum of compound, **IV** in $CDCl_3$.

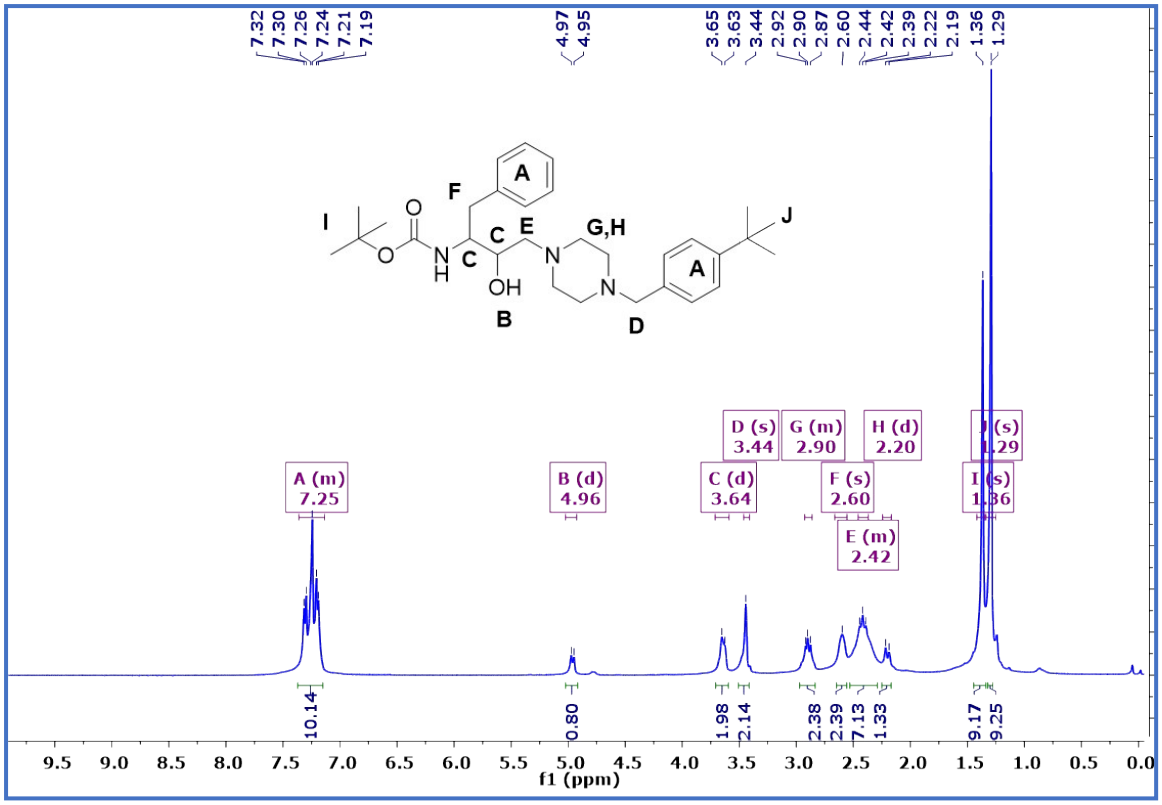

Figure S3. ^{1}H NMR spectrum of compound, **III** in $CDCl_3$.

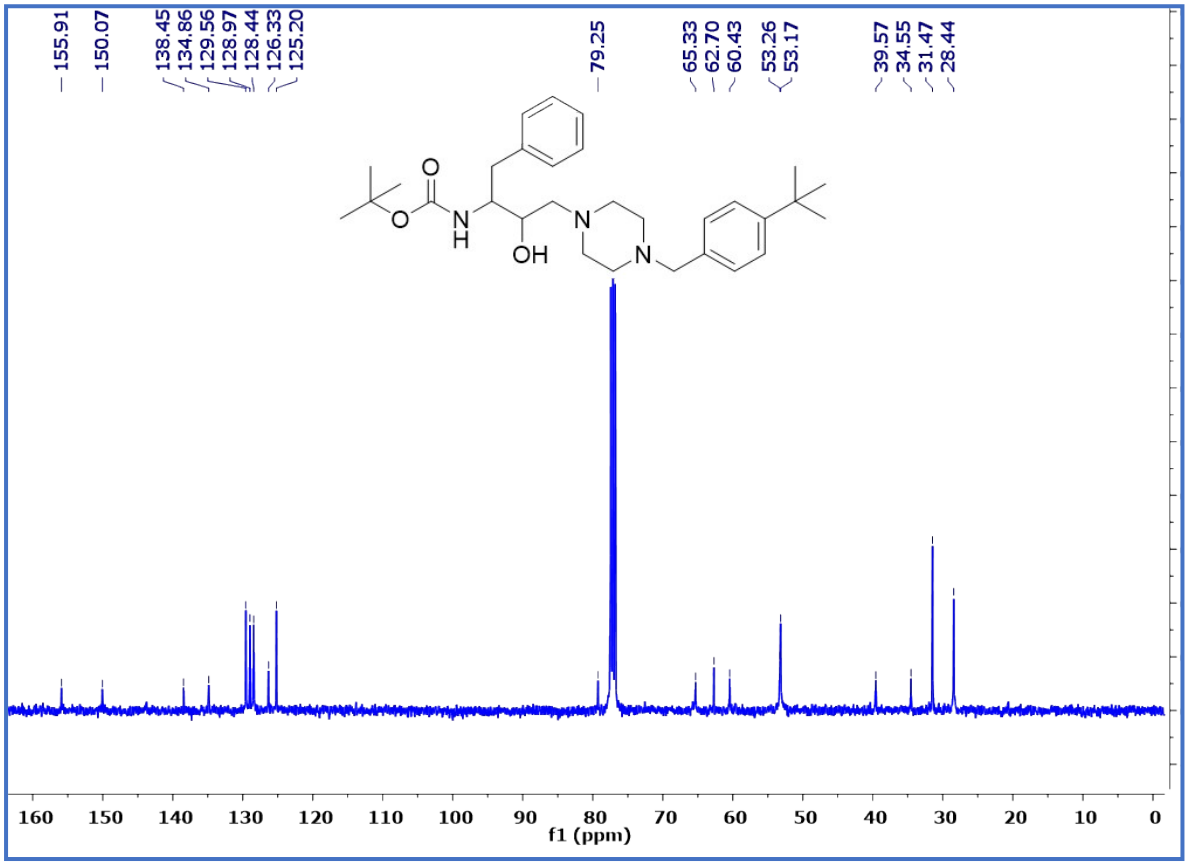

Figure S4. ^{13}C NMR spectrum of compound, **III** in $CDCl_3$.

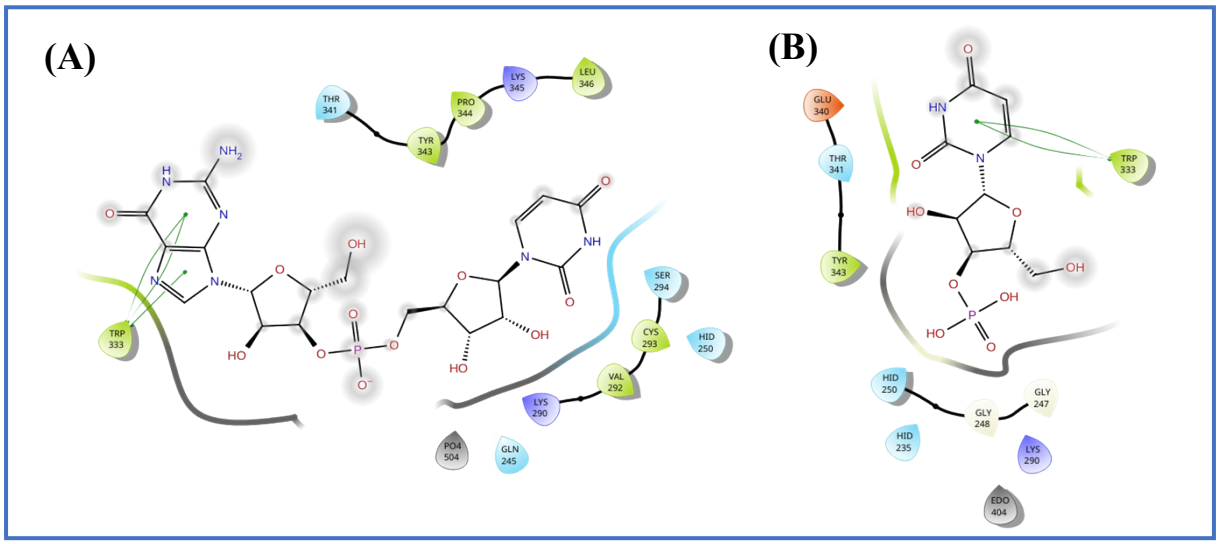

Figure S5. Schematic representation of 2D interaction maps of: A) nucleotide (active site bound substrate); and **B**) 3'-uridinemonophosphate (3'-UMP; Active site bound product) against NendoU enzyme of SARS-CoV-2.

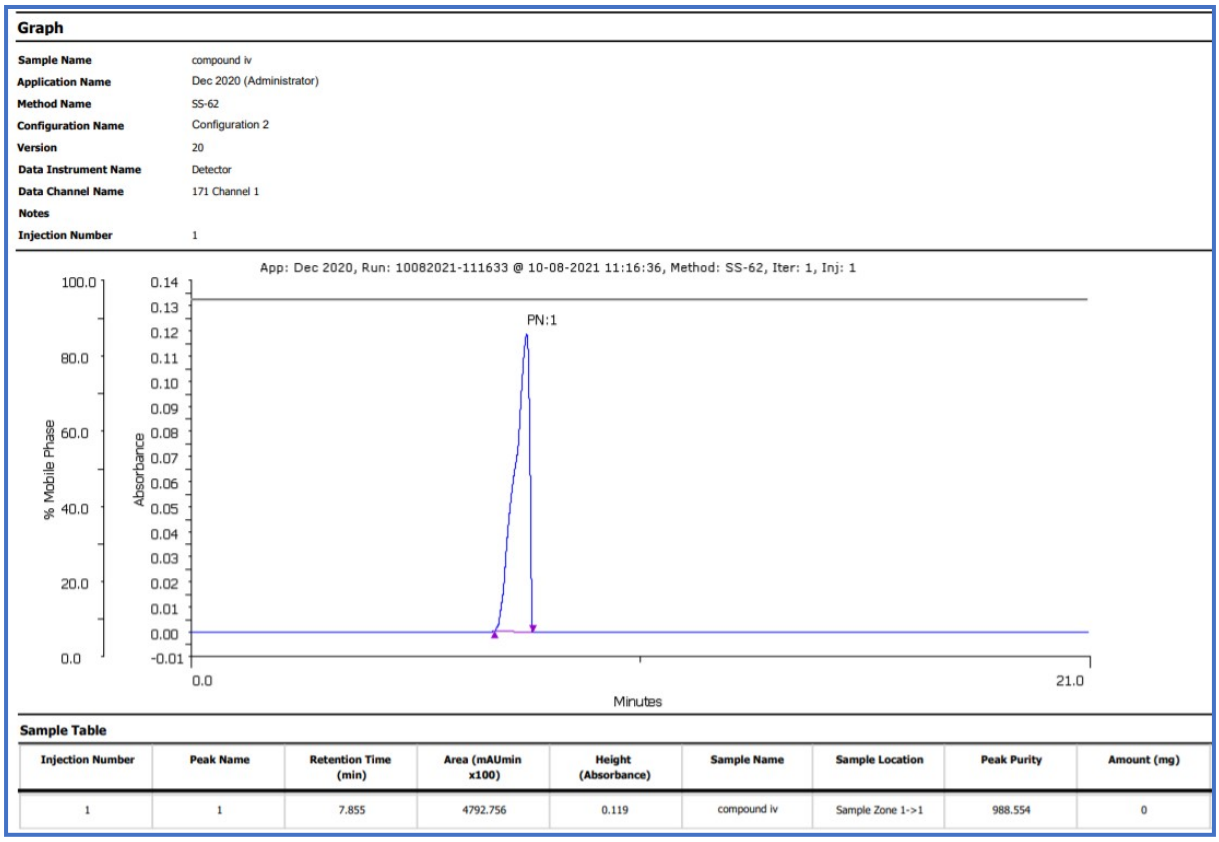

Figure S6. HPLC purity analysis for compound **IV.**

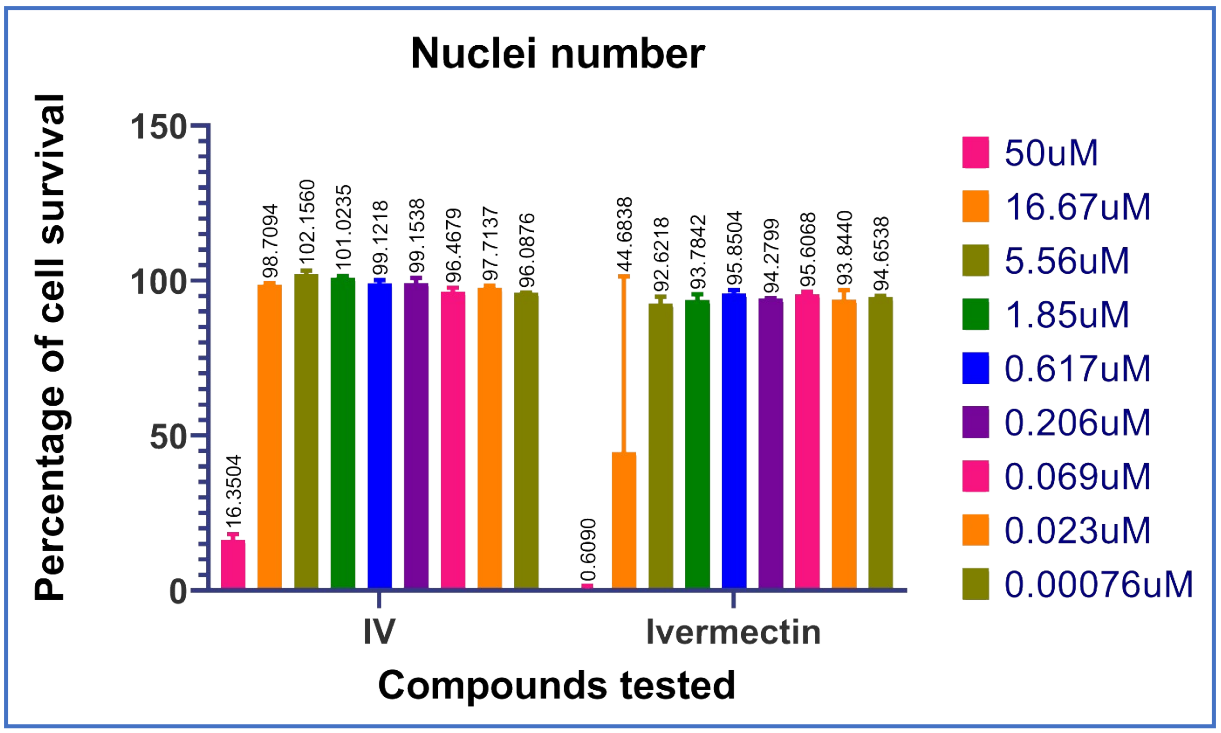

Figure S7. Cytotoxicity of Compounds tested. Effect of compounds tested on viability of Vero cell lines. Cells were seeded at 37 °C for 24 h prior to treatment with compounds. Cells were either treated with compounds (9 dilutions) for 48 h or treated with DMSO only as control. Cell viability was measured by total nuclei counting. Ivermectin showed toxicity at 16.67 µM diluted concentration while at 50 µM it completely wiped down the Vero cell population. Compound **IV** showed some toxicity at 50 µM concentration which is nearly three times its IC50 value. Compound **IV** was far less cytotoxic to Vero cell line compared to FDA approved drug ivermectin.