

Supplementary materials for

Novel tetrahydroisoquinoline based heterocyclic compounds efficiently inhibit SARS-CoV-2 infection in vitro

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Spectra of *tert*-butyl *rel*-4-(((3*R*,4*S*)-3-(1*H*-indol-3-yl)-1-oxo-2-propyl-1,2,3,4-tetrahydroisoquinolin-4-yl)methyl)piperazine-1-carboxylate (**1**)

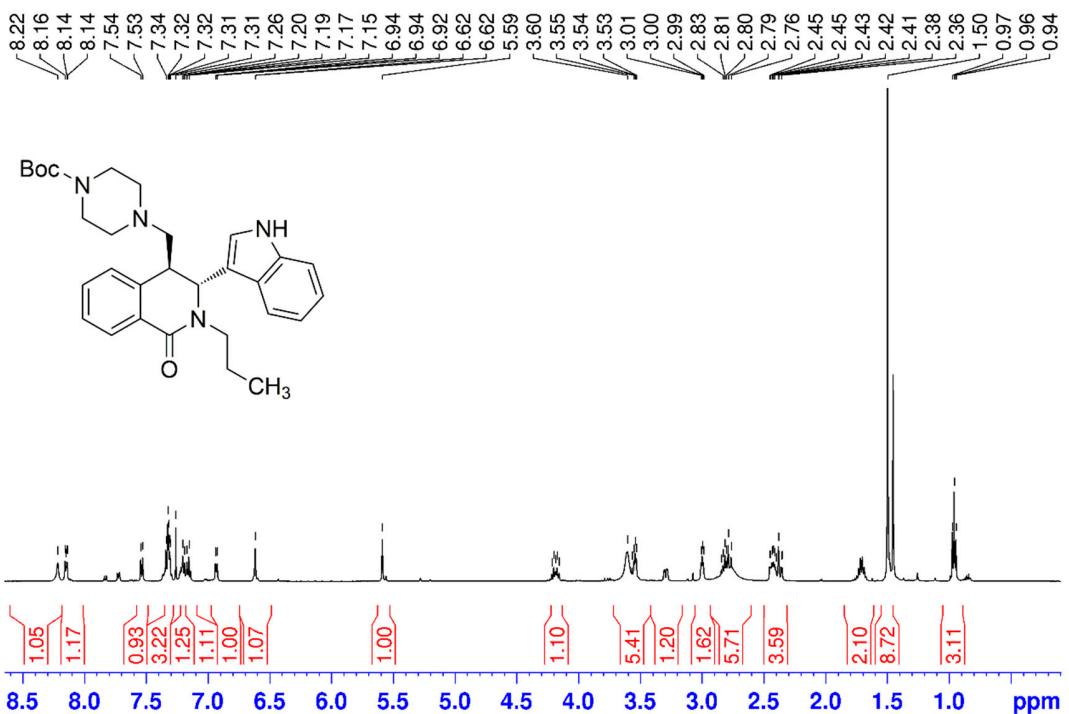


Figure S1. ^1H NMR (DMSO- d_6) of compound *trans*-**1** at 298 K.

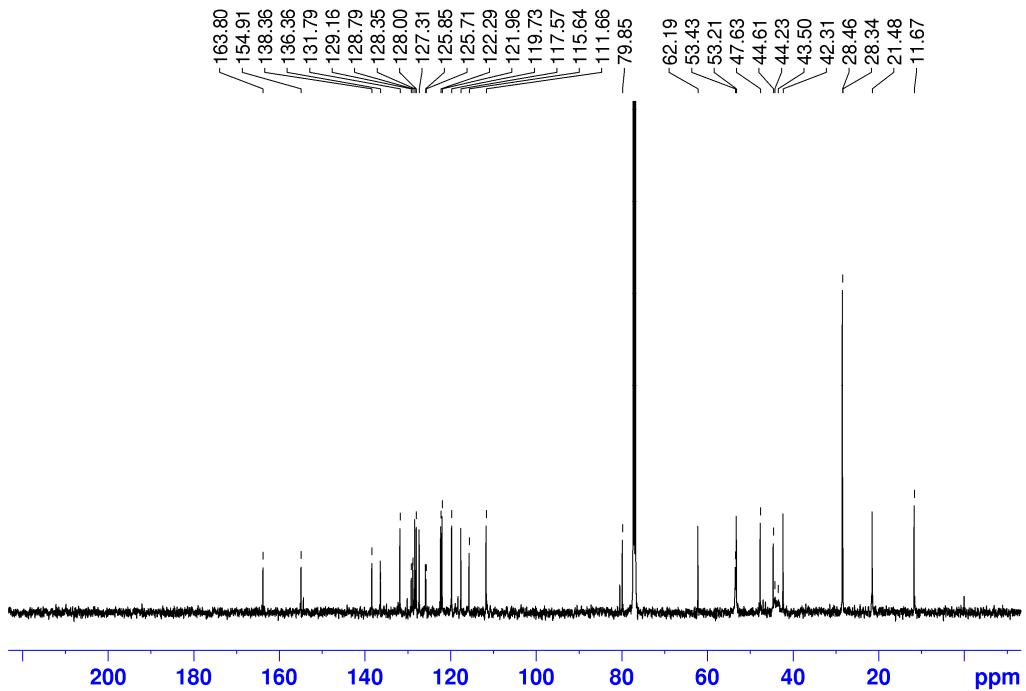
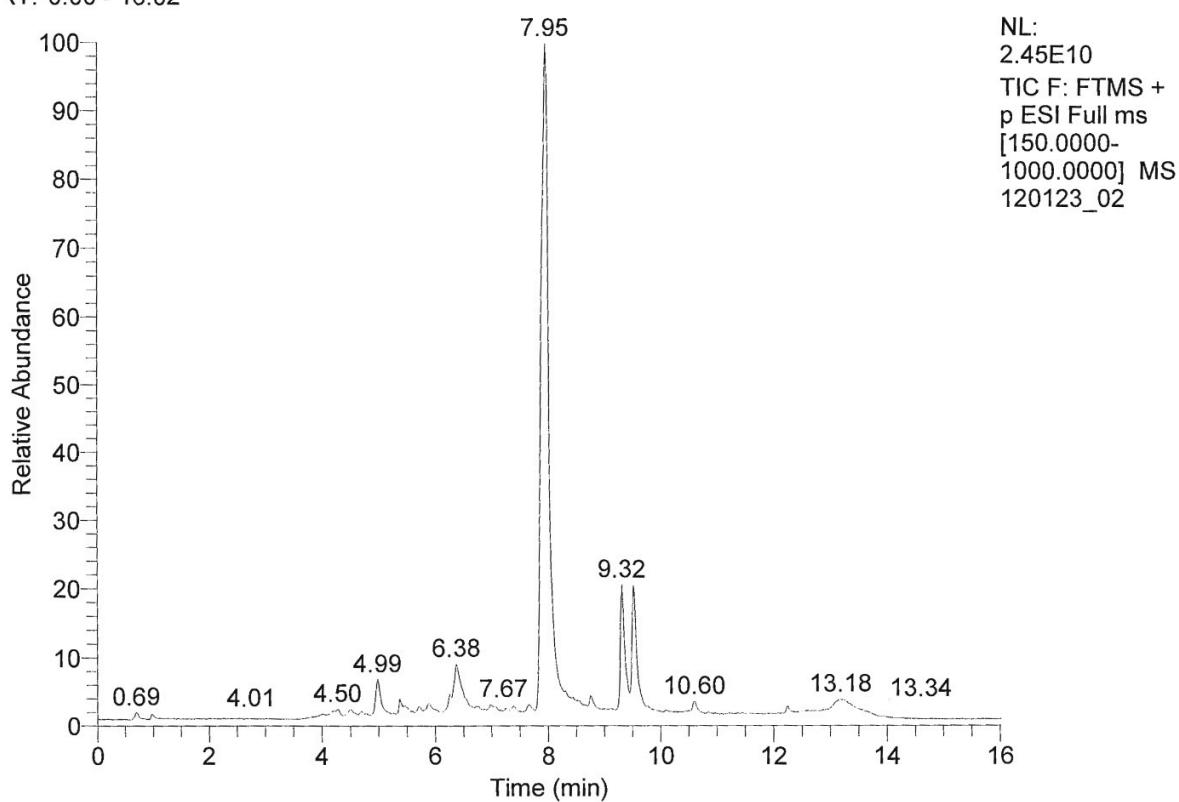


Figure S2. ^{13}C NMR (DMSO- d_6) of compound *trans*-**1** at 298 K.

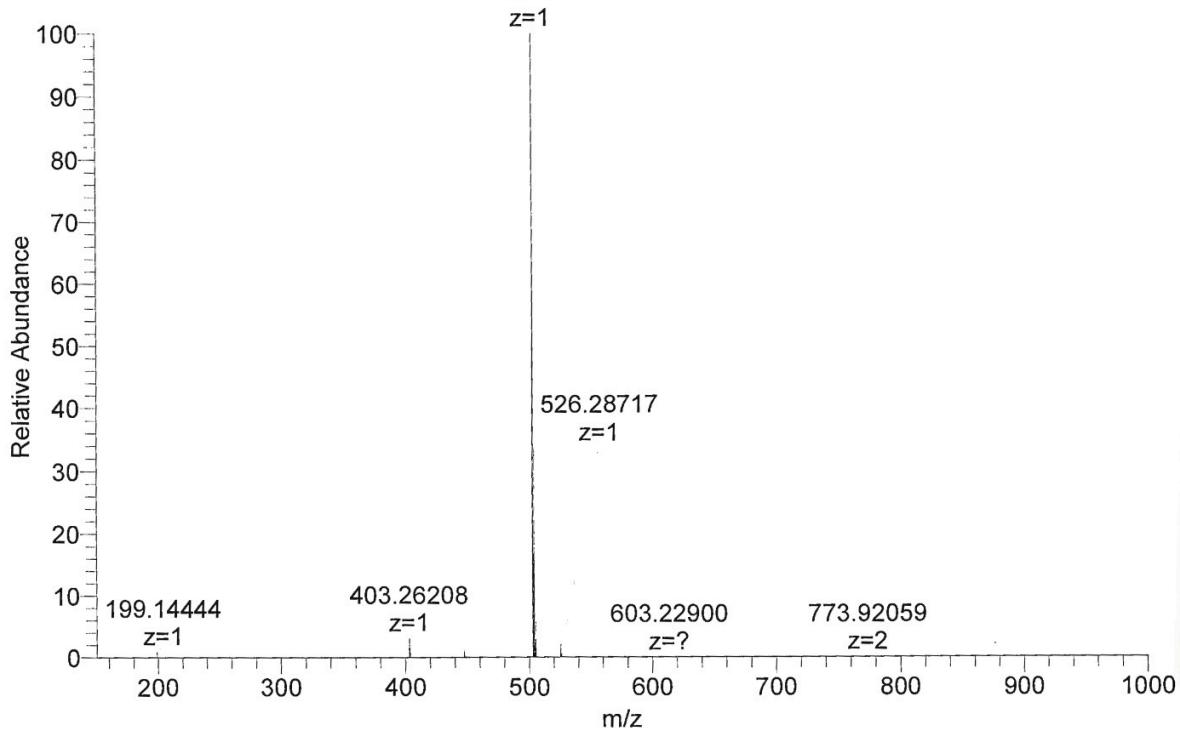
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120123_02 #593 RT: 7.93 AV: 1 NL: 1.28E10

T: FTMS + p ESI Full ms [150.0000-1000.0000]

503.30753

Figure S3. HRMS spectrum of compound *trans*-1.

Spectra of *rel*-(3*R*,4*S*)-3-(1*H*-indol-3-yl)-4-(piperazin-1-ylmethyl)-2-propyl-3,4-dihydroisoquinolin-1(2*H*)-one (**2**)

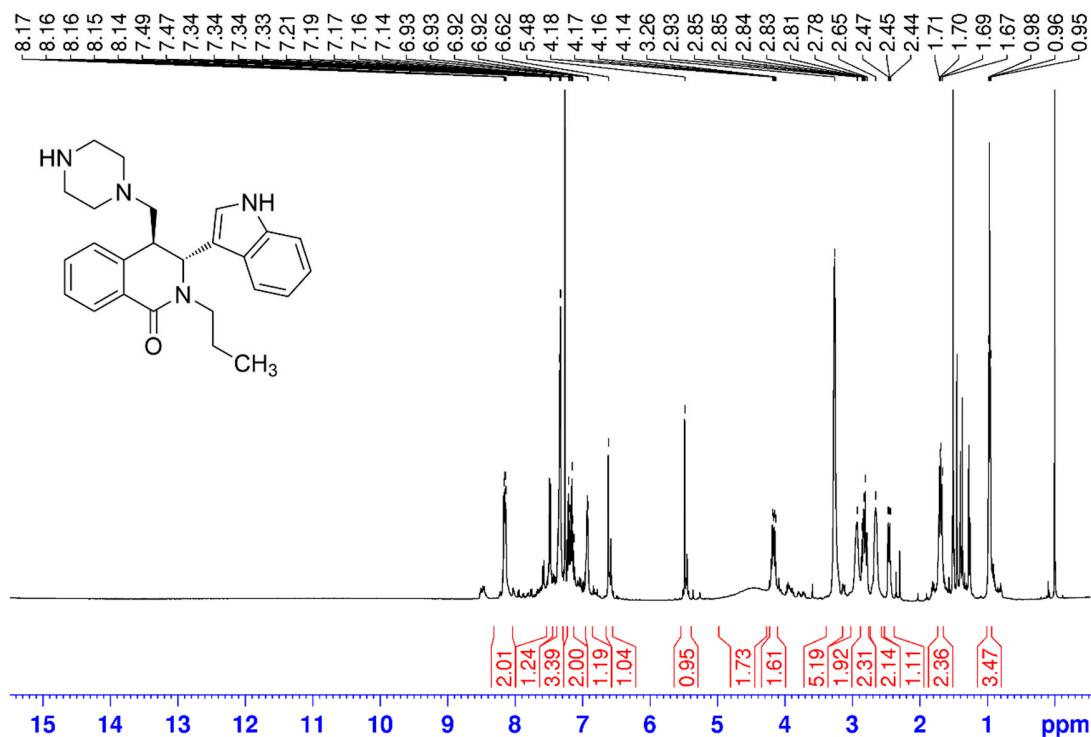


Figure S4. ¹H NMR (CDCl₃) of compound *trans*-**2** at 298 K.

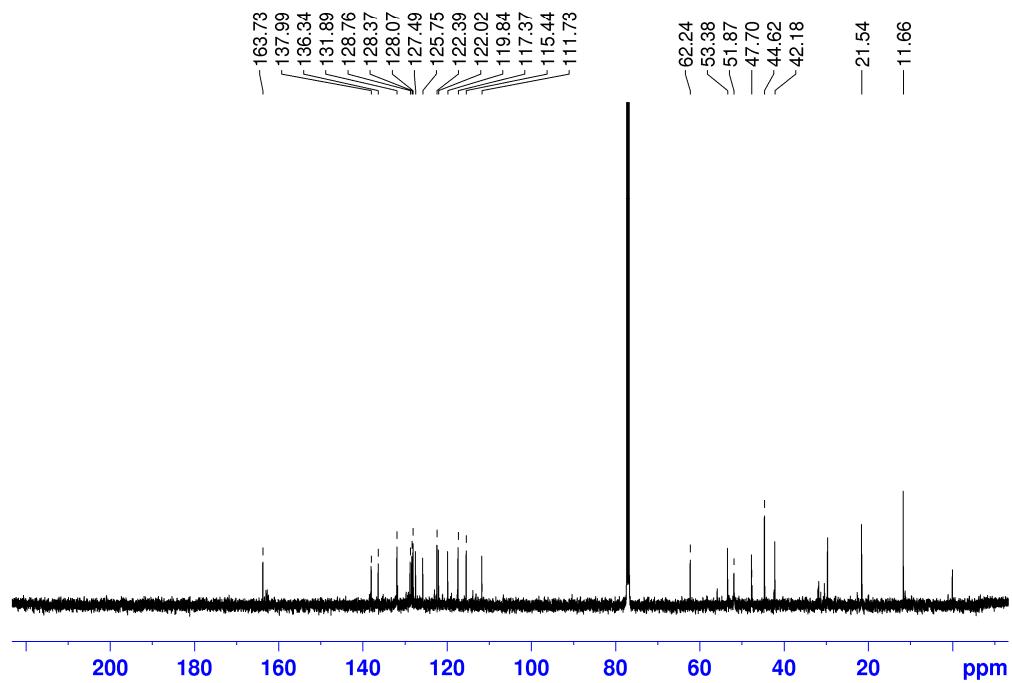
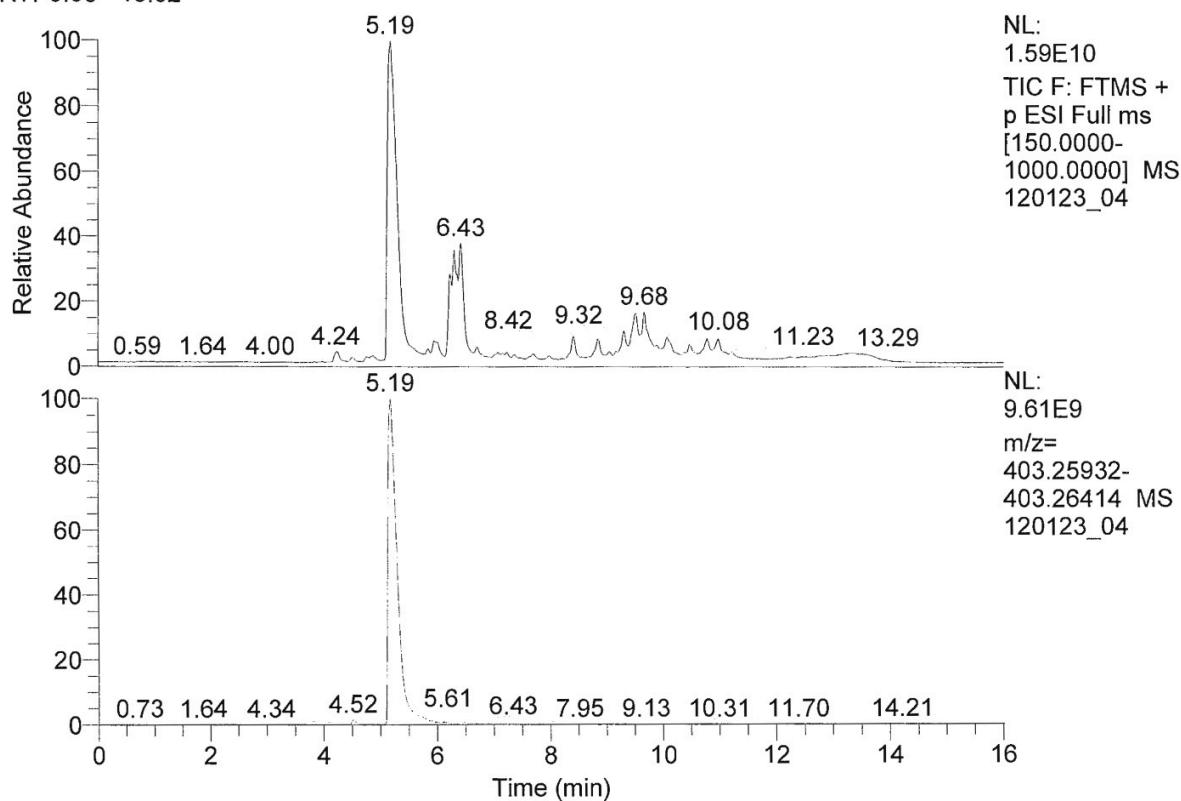


Figure S5. ¹³C NMR (CDCl₃) of compound *trans*-**2** at 298 K.

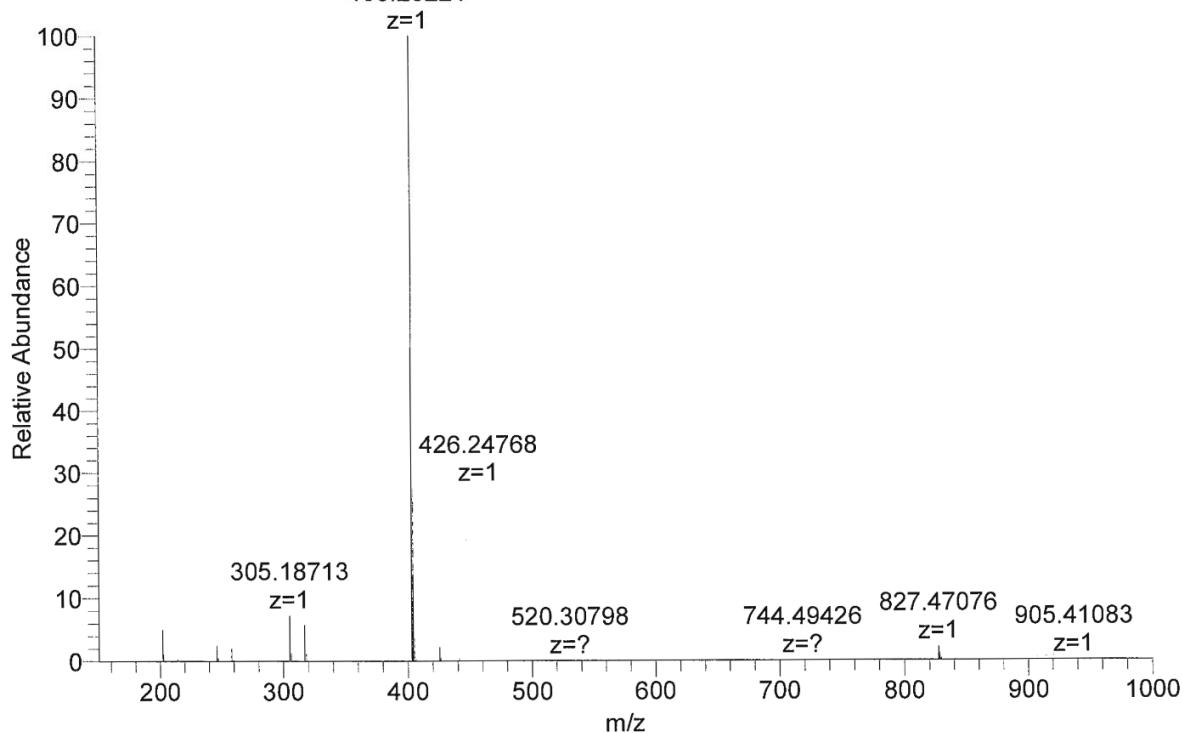
RT: 0.00 - 16.02



120123_04 #392 RT: 5.24 AV: 1 NL: 7.32E9

T: FTMS + p ESI Full ms [150.0000-1000.0000]

403.26221

Figure S6. HRMS spectrum of compound *trans*-2.

General structure of compounds *trans*-3 - *trans*-9

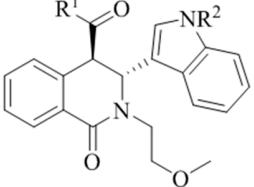
	$R^1 =$	$R^2 =$	
	$-\text{N}(\text{CH}_2\text{CH}_2\text{OCH}_3)\text{NH}-$	H	<i>trans</i> -3
	$-\text{N}(\text{CH}_2\text{CH}_2\text{OCH}_3)\text{NHC}(=\text{O})\text{OC}(\text{CH}_3)_3-$	H	<i>trans</i> -4
	$-\text{N}(\text{CH}_2\text{CH}_2\text{O})\text{NH}-$	H	<i>trans</i> -5
	$-\text{N}(\text{CH}_2\text{CH}_2\text{NH}_3^+)^+$	H	<i>trans</i> -6
	$-\text{N}(\text{CH}_2=\text{N})\text{NH}-$	H	<i>trans</i> -7
	$\text{H}_3\text{N}^+\text{C}(\text{CH}_3)_2\text{C}(=\text{O})\text{NHCH}_3-$	H	<i>trans</i> -8
	$\text{H}_3\text{N}^+\text{C}(\text{CH}_3)_2\text{C}(=\text{O})\text{NHCH}_3-$	$\text{CH}_2\text{N}(\text{CH}_3)_2\text{CH}_2-$	<i>trans</i> -9

Figure S7. General structure of compounds *trans*-3 - *trans*-9