

Titration of NA activity for viruses by colorimetric Assay

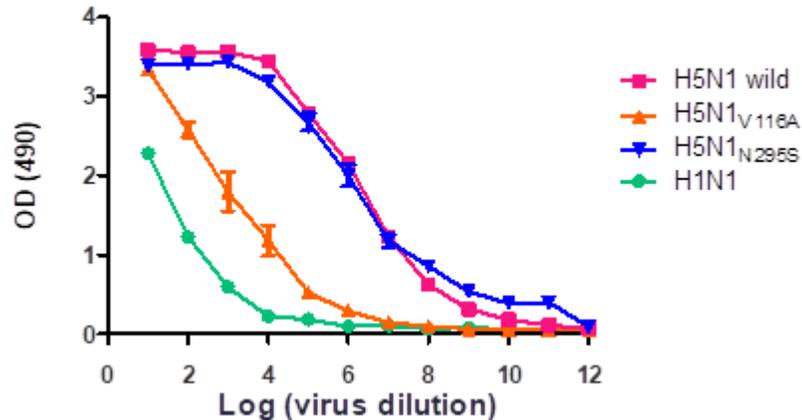


Figure S1. Titration of neuraminidase activity of H5N1_{wild}, H5N1_{V116A}, H5N1_{N295S}, and H1N1 viruses.

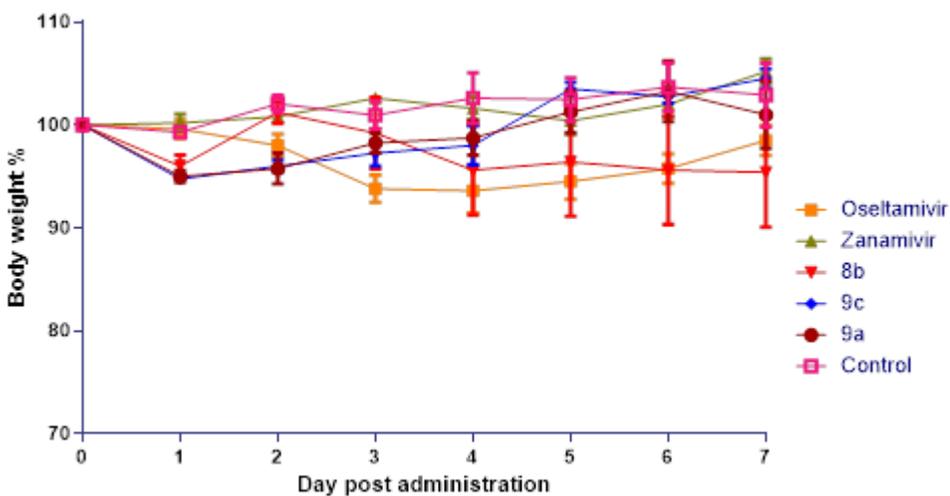


Figure S2. Safety of docked synthetic compounds (given as 3 doses), zanamivir, and oseltamivir compared with that of control (1X PBS). The safest compounds were **9c** and **9a**, which, like zanamivir, did not affect body weight. **Compound 8b**, like oseltamivir, had a slight effect on body weight.

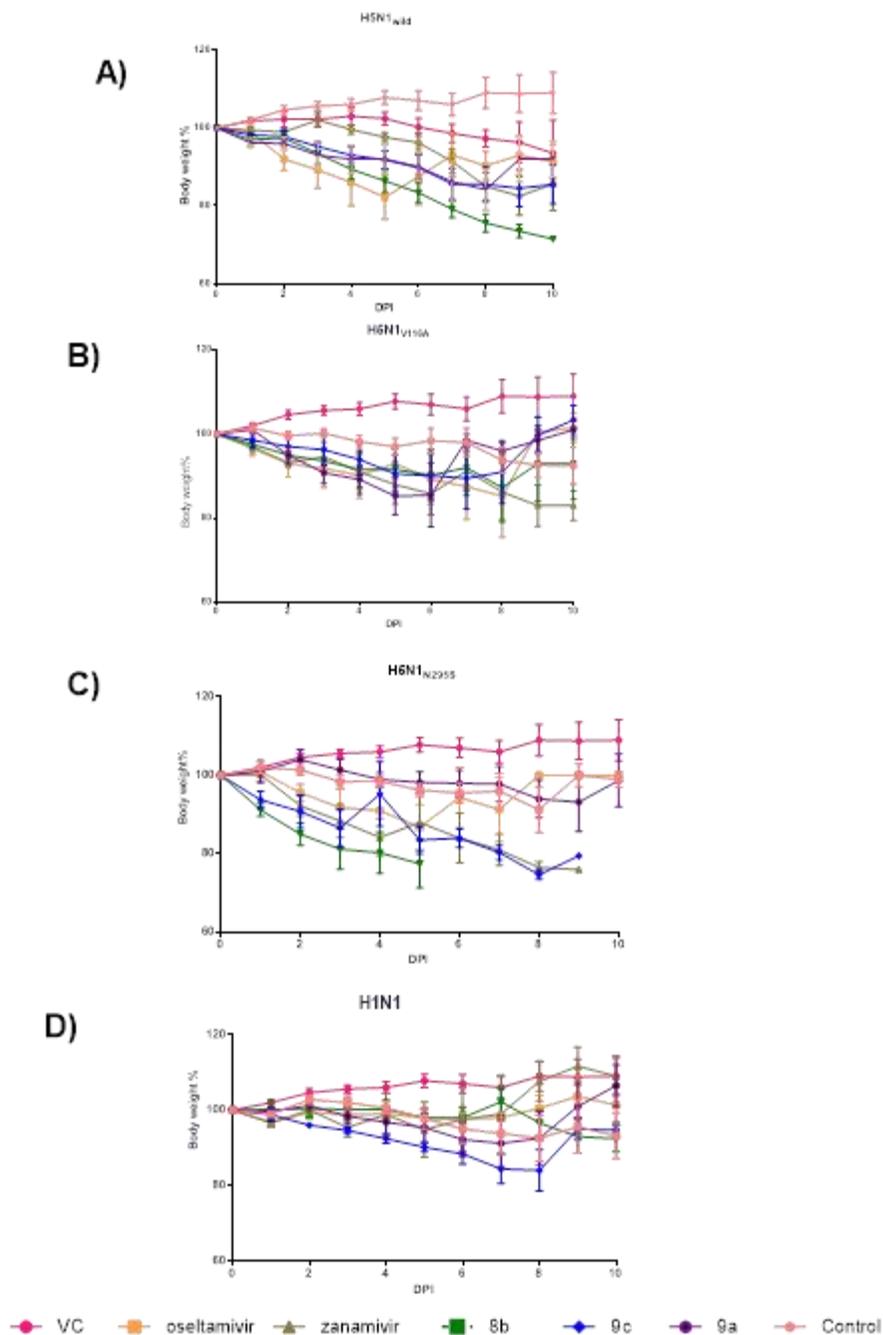
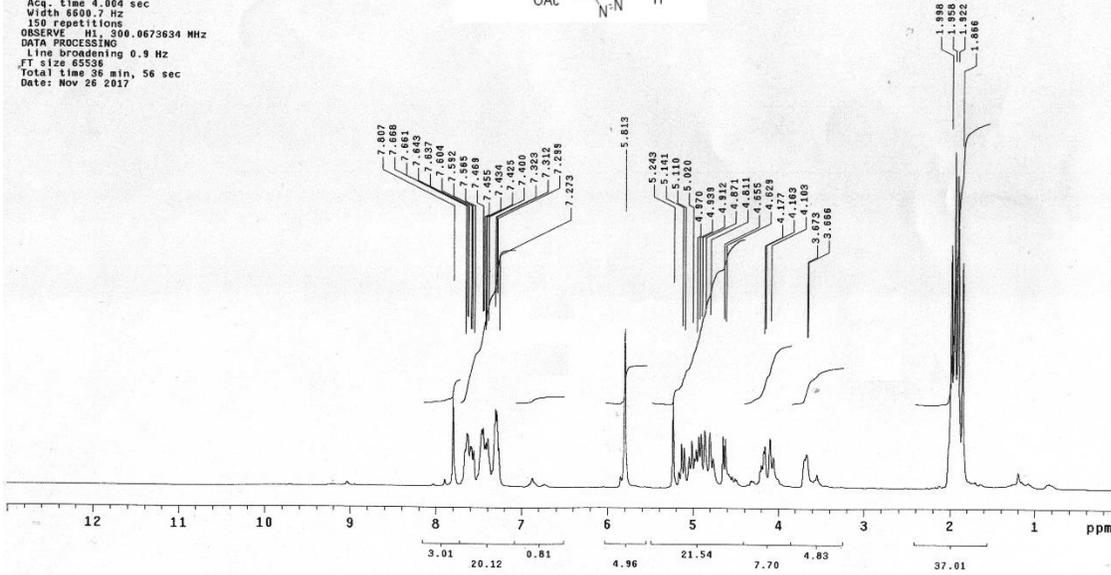
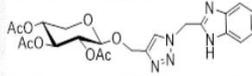


Figure S3. Body weight loss of mice infected with different viruses that were given either synthetic compounds **8b**, **9c**, and **9a** 5 h post infection, oseltamivir or zanamivir as drug control, or no treatment (viral control [VC]). All groups were compared with an uninfected control group that was given 1X PBS instead of drugs or compounds. (A) Antiviral activity after infection with H5N1_{wild} (B) Antiviral activity after infection with H5N1_{V116A} (C) Antiviral activity after infection with H5N1_{N295S} (D) Efficacy and antiviral activity after infection with H1N1 virus.

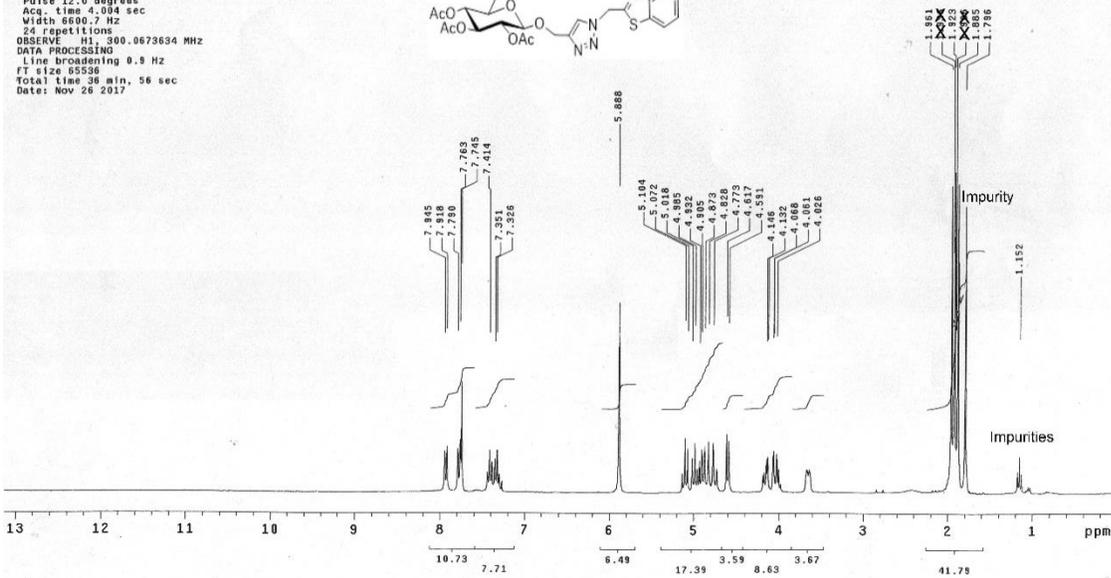
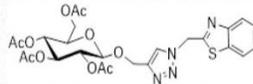
WaelAbdelHafeez-N53-CDC13-H1
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

Pulse Sequence: s2pul
 Solvent: CDC13
 Temp: 30.0 C / 303.1 K
 Mercury-300BS "NMR300"
 Relax. delay 1.000 sec
 Pulse 12.0 degrees
 Acq. time 4.004 sec
 Width 6600.7 Hz
 150 repetitions
 OBSERVE H1, 300.0673634 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65536
 Total time 36 min, 56 sec
 Date: Nov 26 2017



WaelAbdelHafeez-551-CDC13-H1
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

Pulse Sequence: s2pul
 Solvent: CDC13
 Temp: 30.0 C / 303.1 K
 Mercury-300BS "NMR300"
 Relax. delay 1.000 sec
 Pulse 12.0 degrees
 Acq. time 4.004 sec
 Width 6600.7 Hz
 24 repetitions
 OBSERVE H1, 300.0673634 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65536
 Total time 36 min, 56 sec
 Date: Nov 26 2017

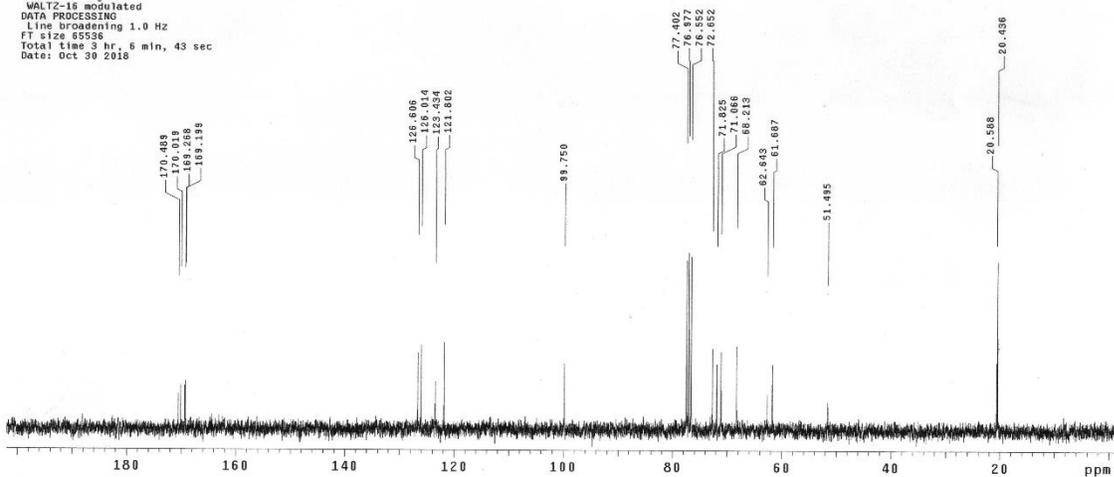
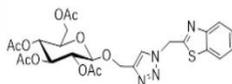


TarekSaad-SS1-CDCL3-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp: 30.0 C / 303.1 K
Mercury-300SB "NMR300"

Pulse 67.5 degrees
Acq. time 1.747 sec
Width 18761.7 Hz
328 repetitions
OBSERVE C13, 75.4520062 MHz
DECOUPLE H1, 300.0688576 MHz
Power 10 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 3 hr, 6 min, 43 sec
Date: Oct 30 2018

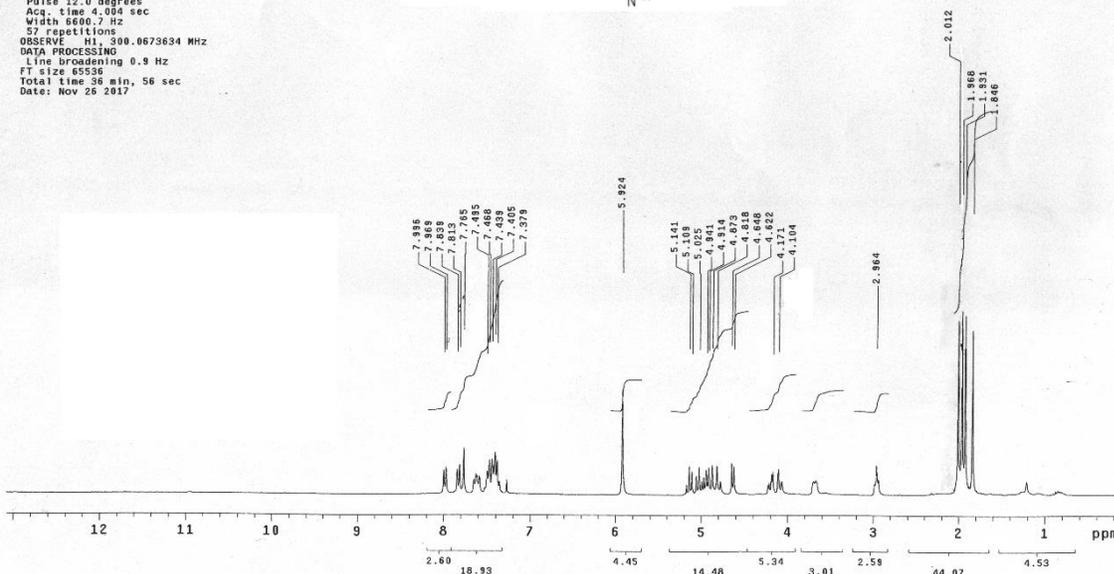
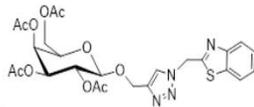


WaelAbdelHafeez-552-CDCl3-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Temp: 30.0 C / 303.1 K
Mercury-300SB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
57 repetitions
OBSERVE H1, 300.0673634 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 36 min, 56 sec
Date: Nov 26 2017

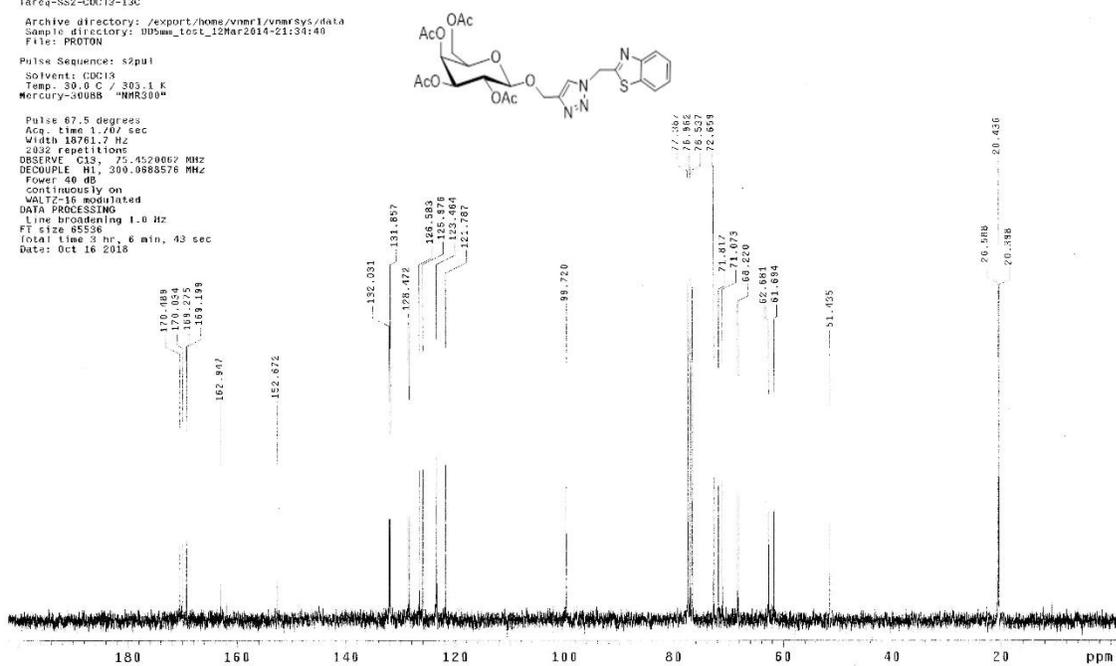


Tarea-S2-CDC13-130

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDC13
Temp: 30.0 C / 303.1 K
Mercury-300RB "NMR300"

Pulse 67.5 degrees
Acq. time 1.407 sec
Width 18761.7 Hz
3322 repetitions
OBSERVE C13, 75.4520667 MHz
DECOUPLE H1, 300.0688576 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85536
Total time 3 hr, 6 min, 43 sec
Date: Oct 16 2018

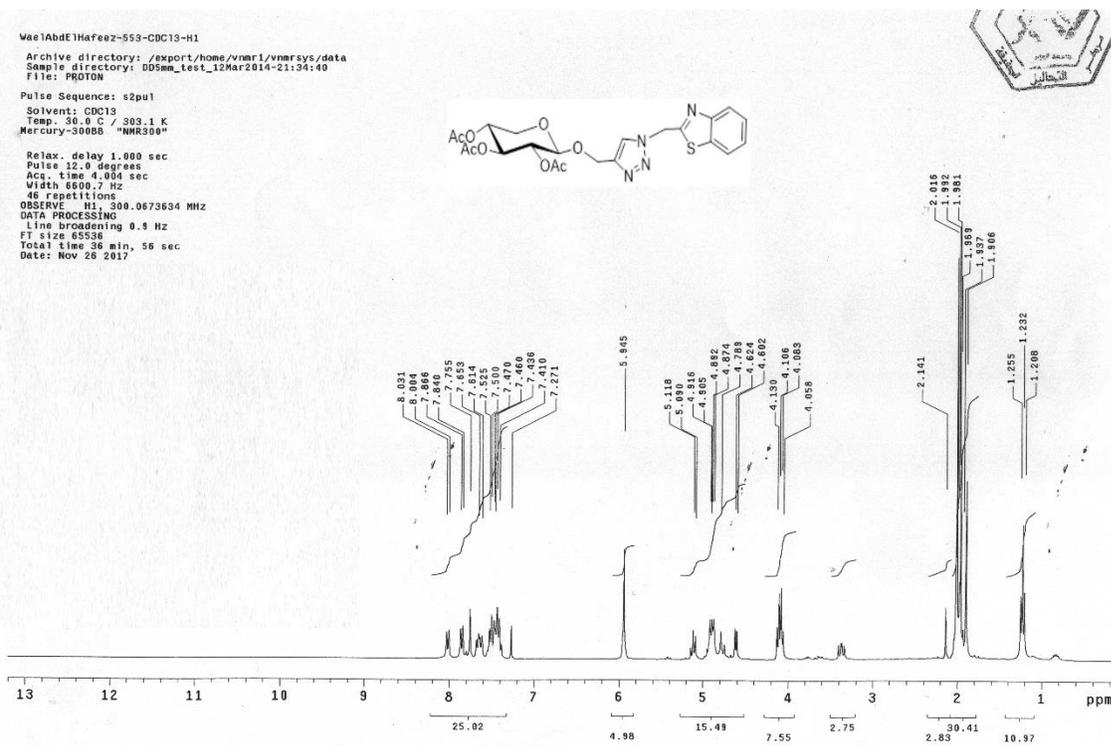


WaelAbdElHafeez-553-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDC13
Temp: 30.0 C / 303.1 K
Mercury-300RB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.904 sec
Width 6600.7 Hz
46 repetitions
OBSERVE H1, 300.0673634 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 85536
Total time 36 min, 56 sec
Date: Nov 26 2017

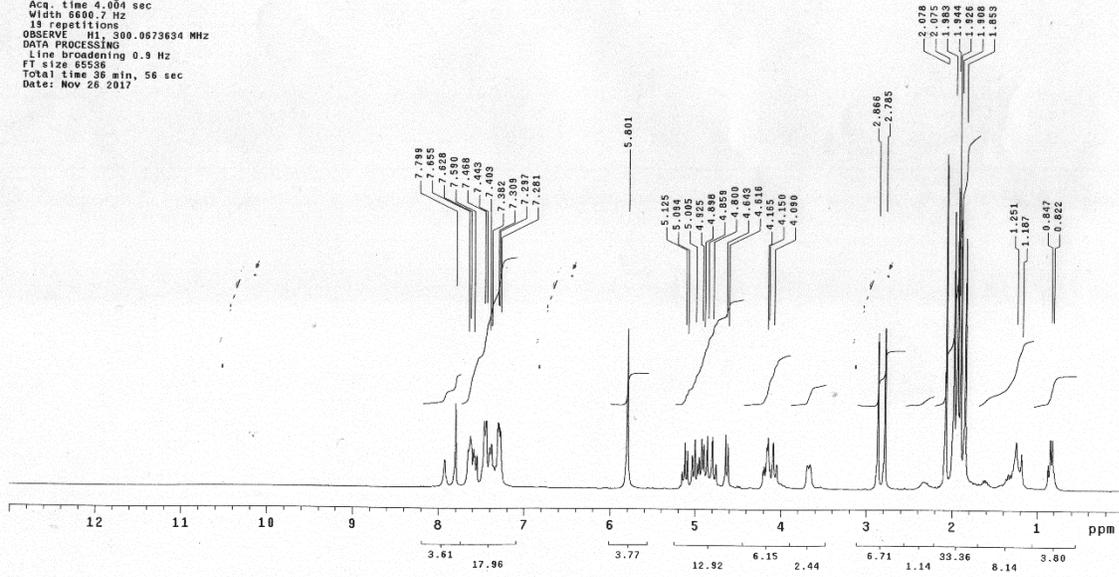


Wae1AbdE1HaFeez-051-CDCl3-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
18 repetitions
OBSERVE H1, 300.0673634 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 36 min, 56 sec
Date: Nov 26 2017

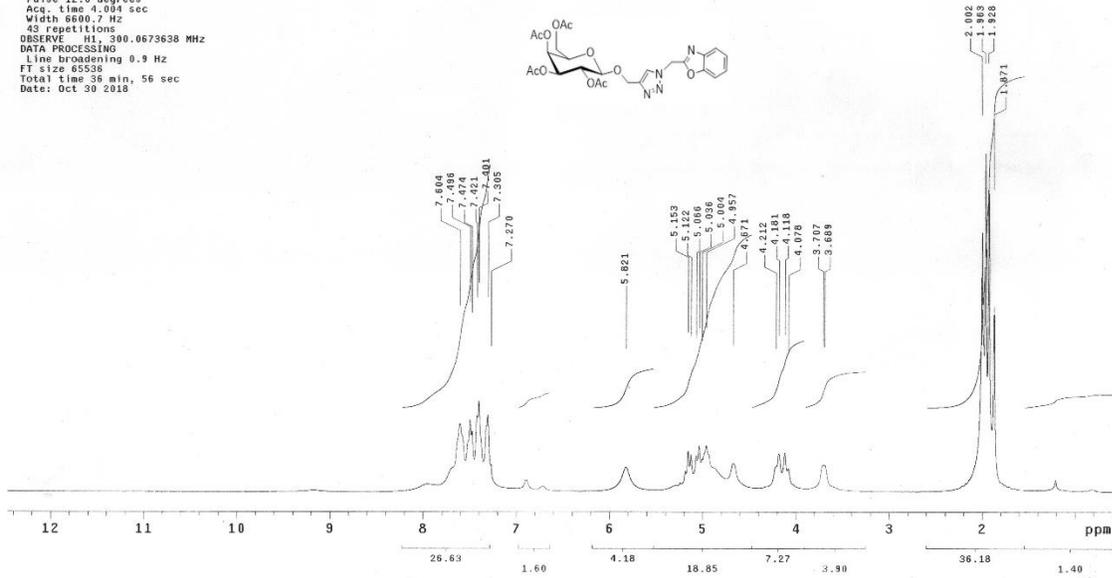
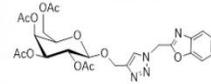


TareqSaad-052-CDCl3-1H

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Temp: 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
43 repetitions
OBSERVE H1, 300.0673638 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 36 min, 56 sec
Date: Oct 30 2018



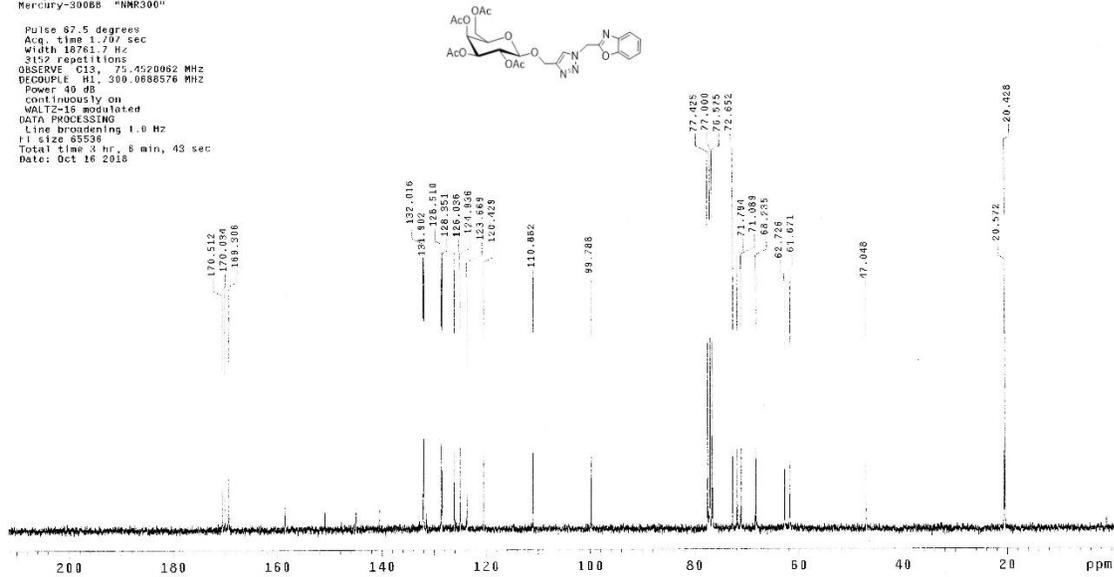
Tarek-052-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul

Solvent: CDC13
Temp: 30.0 C / 303.1 K
Mercury-30006 "NMR300"

Pulse 67.5 degrees
Acq. time 1.797 sec
Width 10761.7 Hz
3152 repetitions
OBSERVE C13, 75.4520962 MHz
DECOUPLE H1, 300.0688576 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
F1 size 65536
Total time 4 hr, 6 min, 43 sec
Date: Oct 16 2018



Vae1AbdE1Hafeez-053-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul

Solvent: CDC13
Temp: 30.0 C / 303.1 K
Mercury-30006 "NMR300"

Relax. delay 1.000 sec
Pulse 12.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
35 repetitions
OBSERVE H1, 300.0673634 MHz
DATA PROCESSING
Line broadening 0.9 Hz
F1 size 65536
Total time 38 min, 56 sec
Date: Nov 25 2017

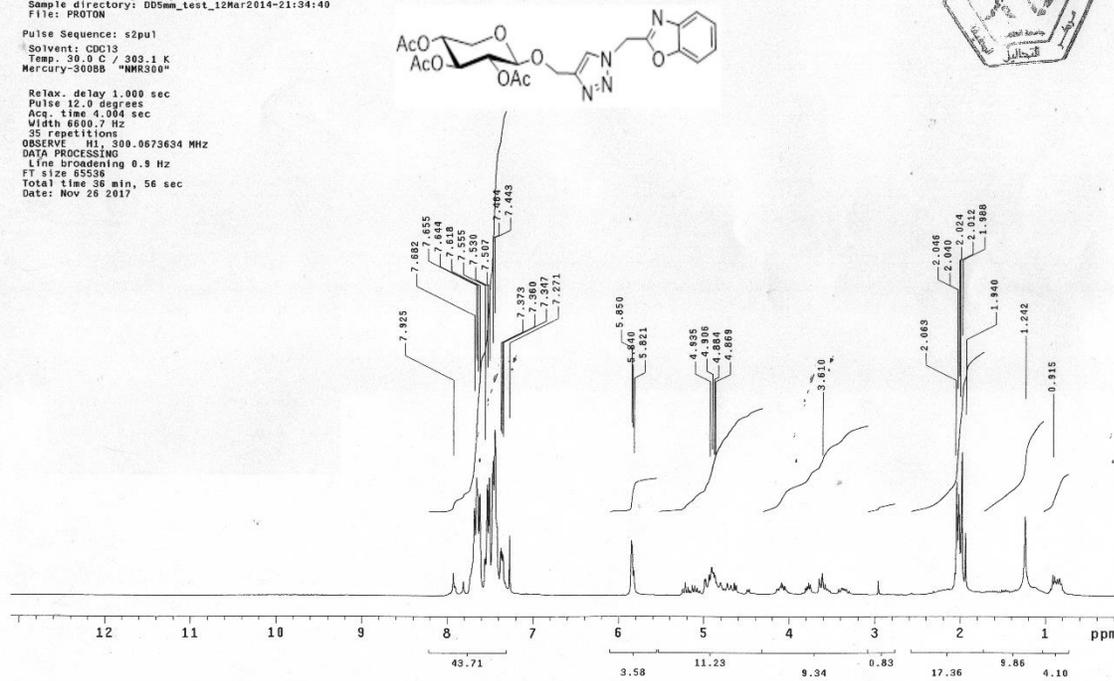


Figure S4 : NMR spectra obtained by using a JEOL EX-500 spectrometer and (CDC13) with TMS as internal standard