

## SUPPORTING INFORMATION

# Antitubercular Nucleosides that Inhibit Siderophore Biosynthesis: SAR of the Glycosyl Domain

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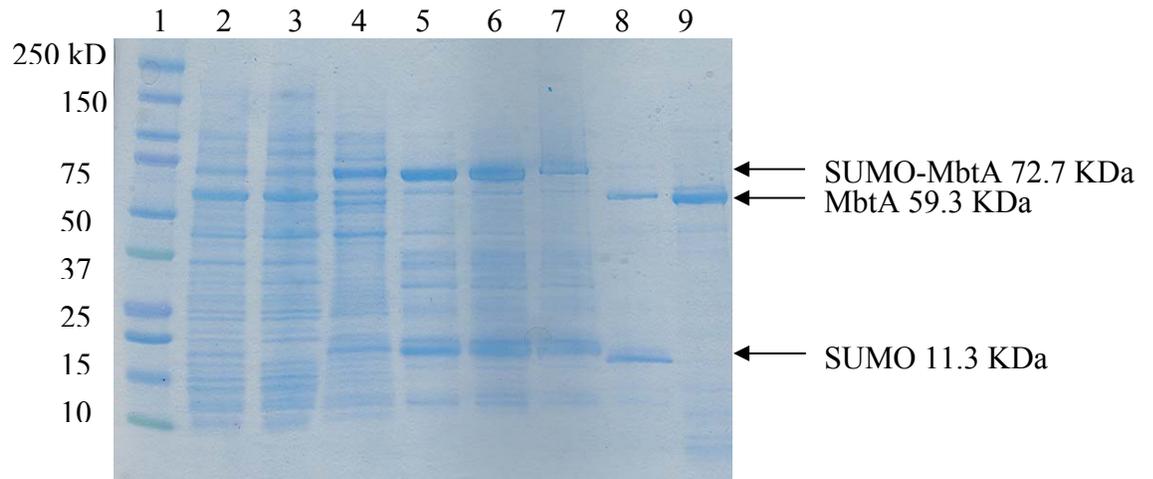


Figure S1: Purification of MbtA

1) molecular weight marker. 2) total soluble fraction. 3) Ni-NTA column flow through. 4) Ni-NTA column wash. 5) Ni-NTA column elution 6) PD-10 elution 7) PD-10 elution from fraction frozen overnight 8) SUMO protease digestion products 9) Purified MbtA

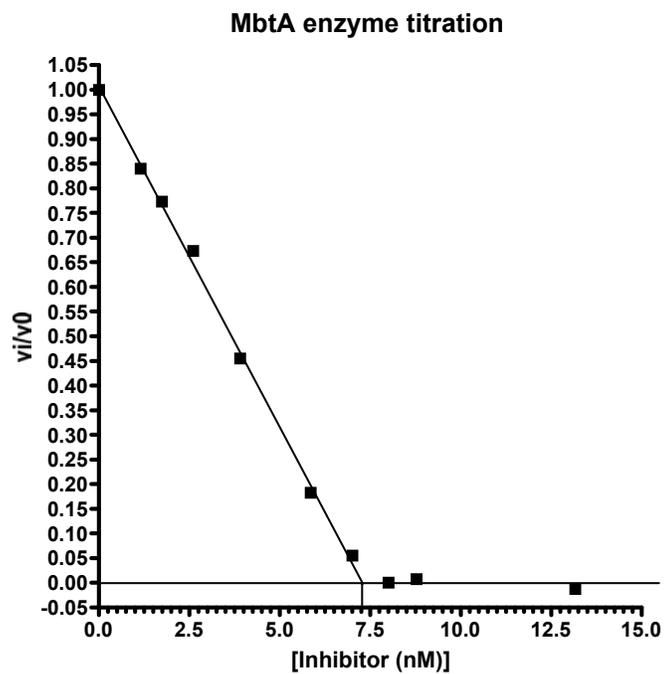


Figure S2: Titration of MbtA with analog 8

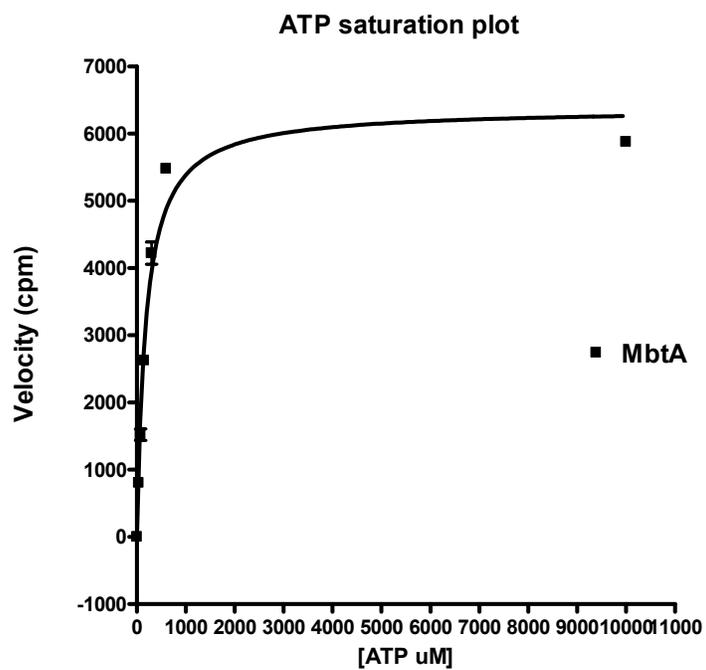


Figure S3: Saturation curve of MbtA with ATP

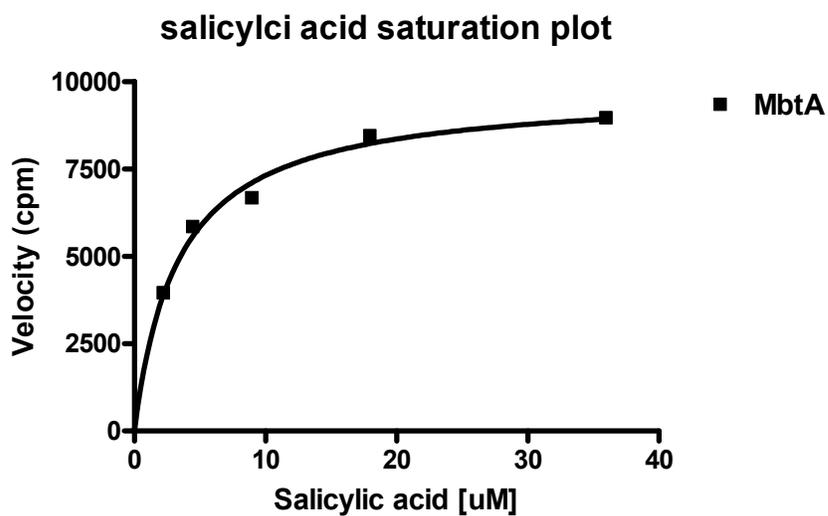


Figure S4: Saturation curve of MbtA with salicylic acid

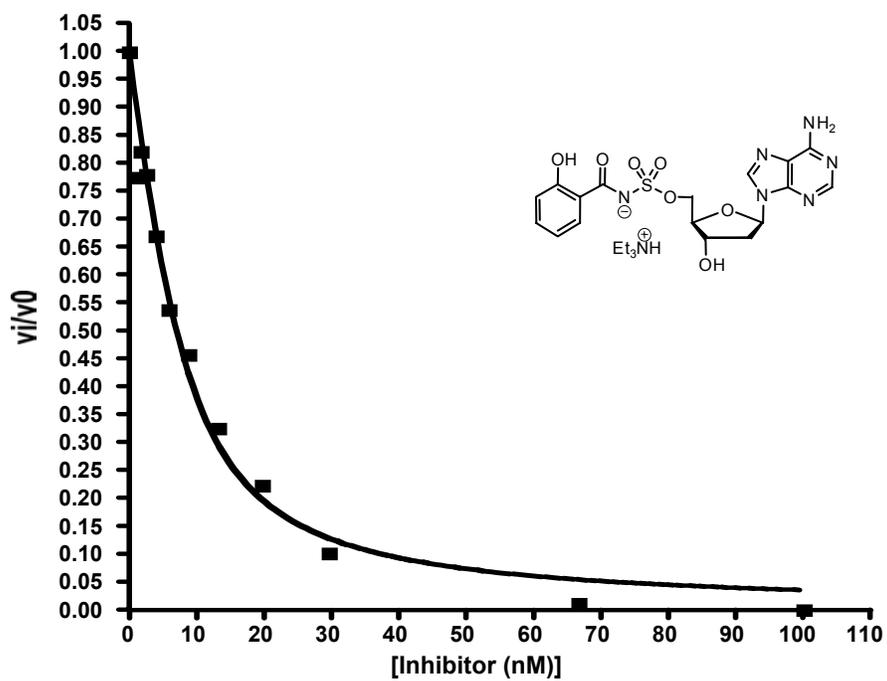


Figure S5: Dose response curve for inhibitor **9**

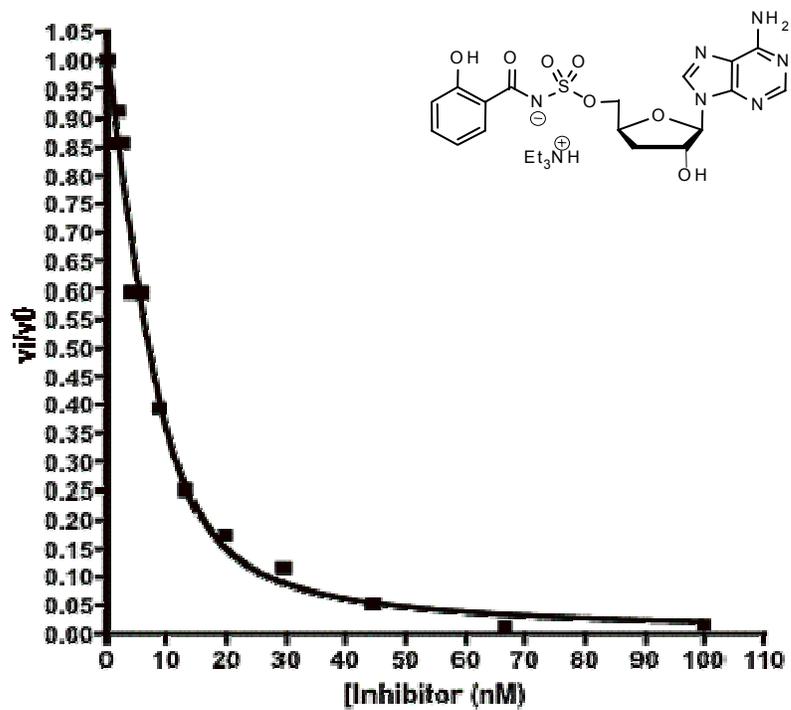


Figure S6: Dose response curve for inhibitor **10**

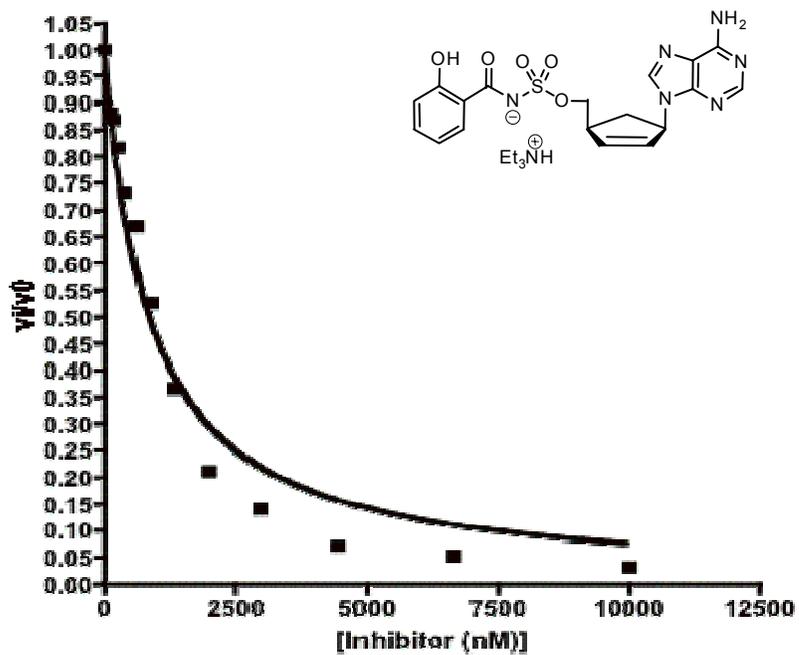


Figure S7: Dose response curve for inhibitor 11

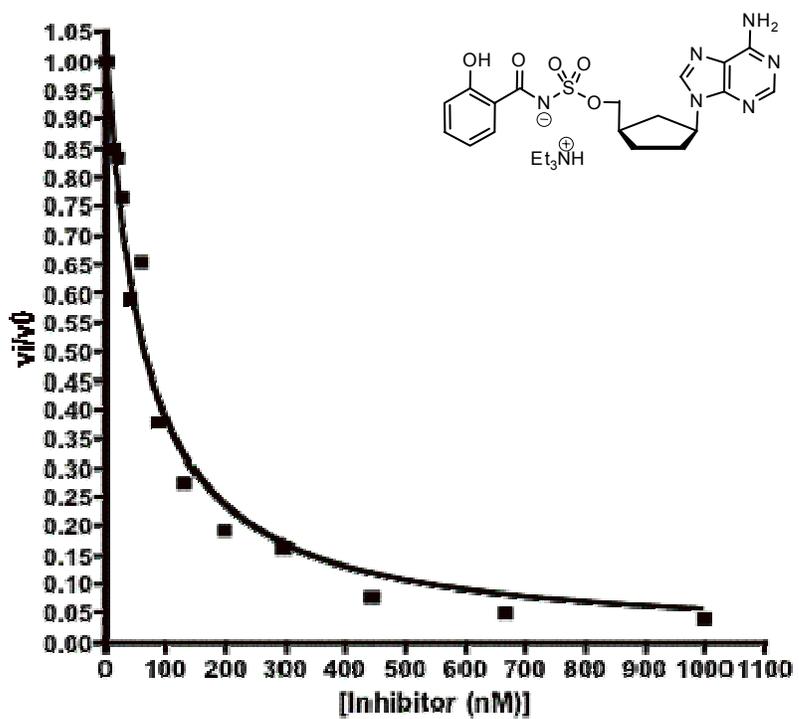


Figure S8: Dose response curve for inhibitor 12

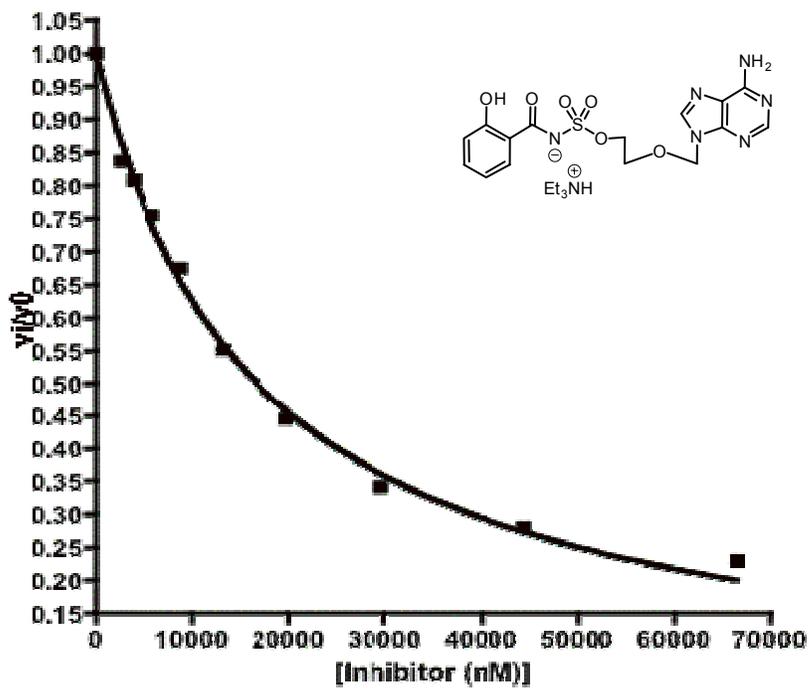


Figure S9: Dose response curve for inhibitor 12

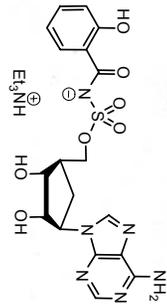
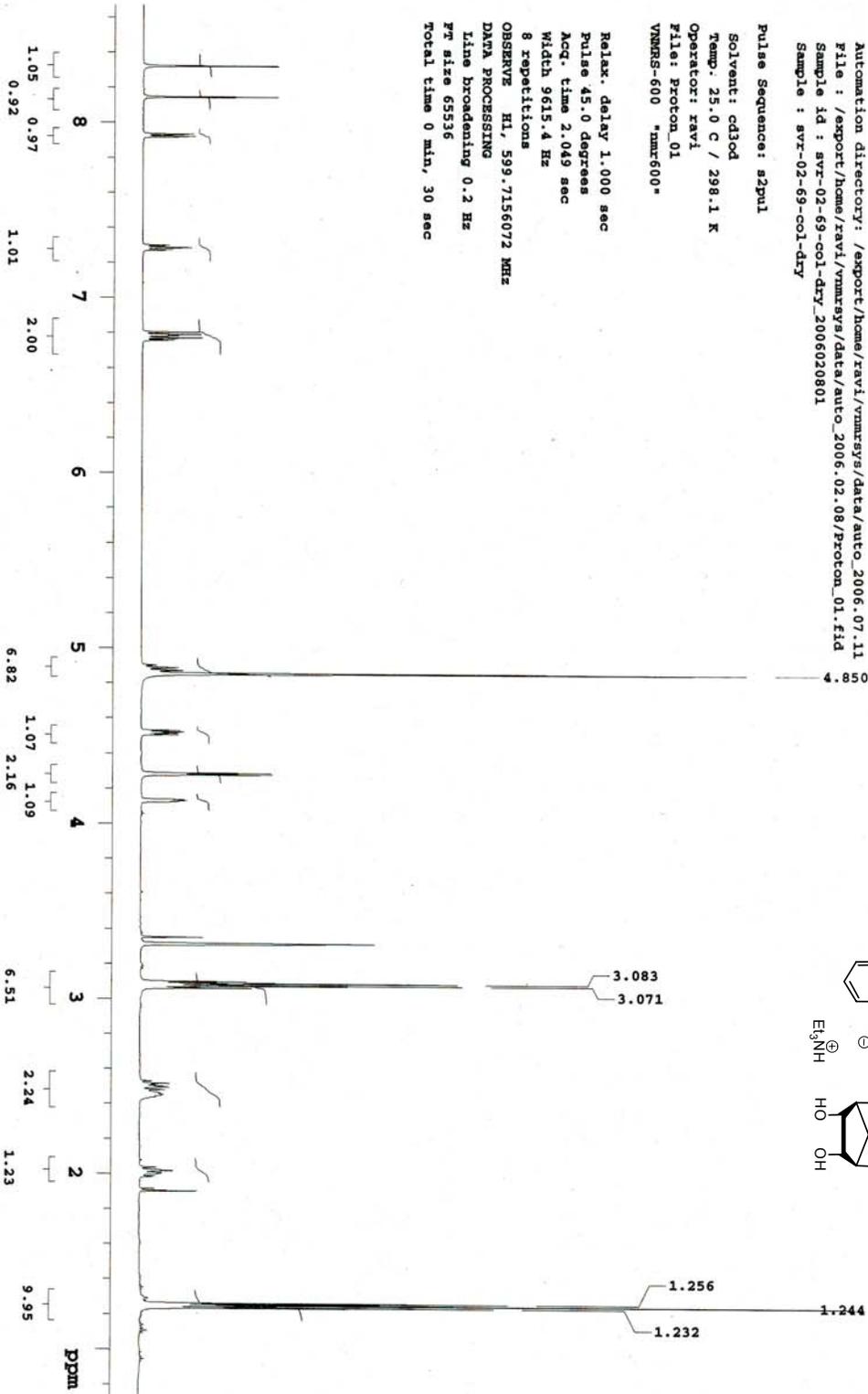
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Sample : svr-02-69-col-dry

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Operator: ravi  
File: Proton\_01  
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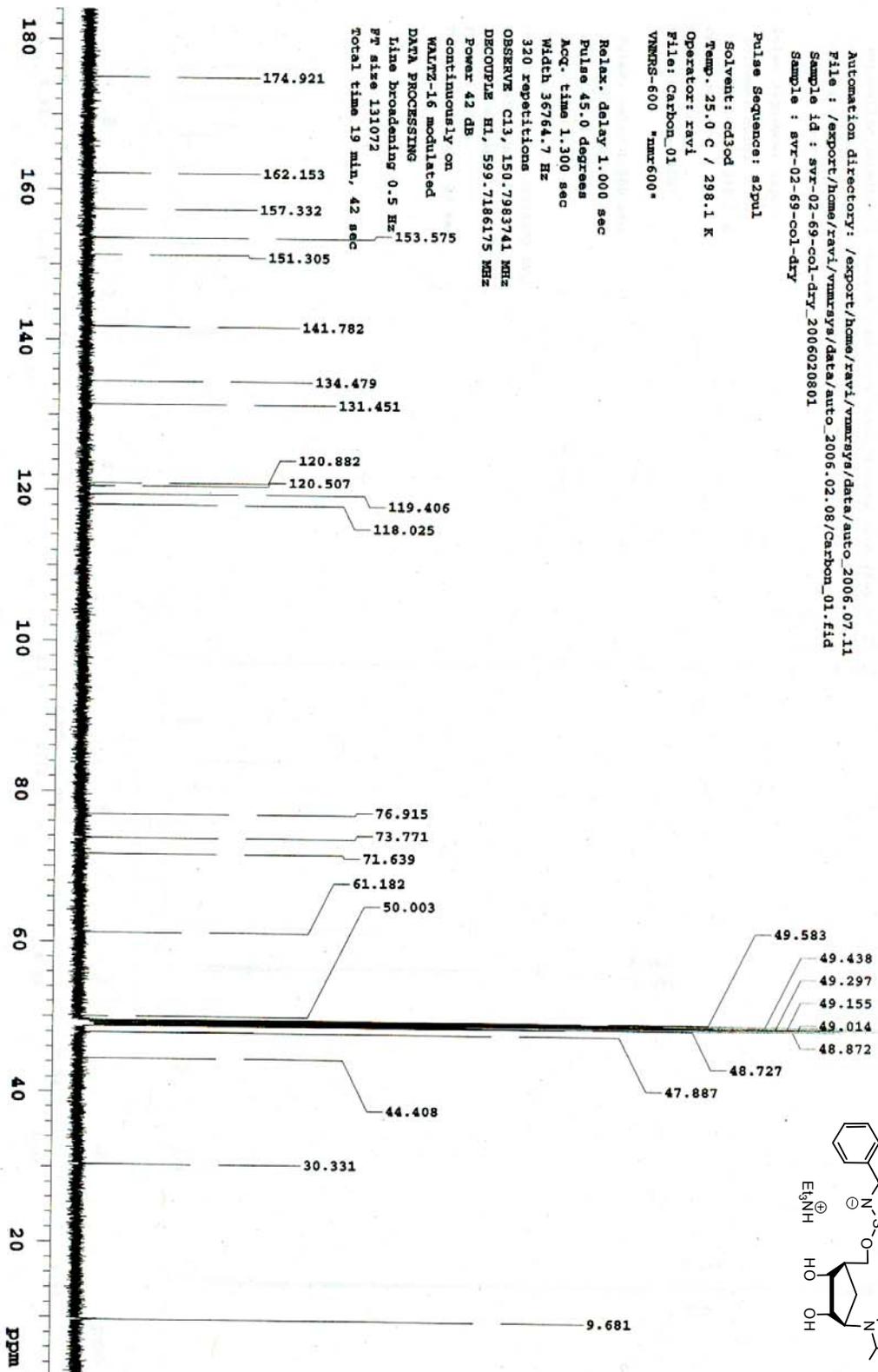
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PR size 65536  
Total time 0 min, 30 sec



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Pulse Sequence: szpul  
Solvent: cd3od  
Temp: 25.0 C / 298.1 K  
Operator: ravi  
File: Carbon\_01  
VNMRS-600 \*nmr600\*

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 36764.7 Hz  
320 repetitions  
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DECUPLE H1, 599.7186175 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
PT size 131072  
Total time 19 min, 42 sec

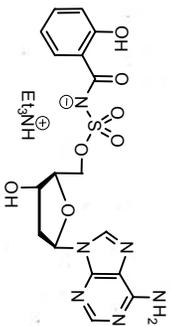
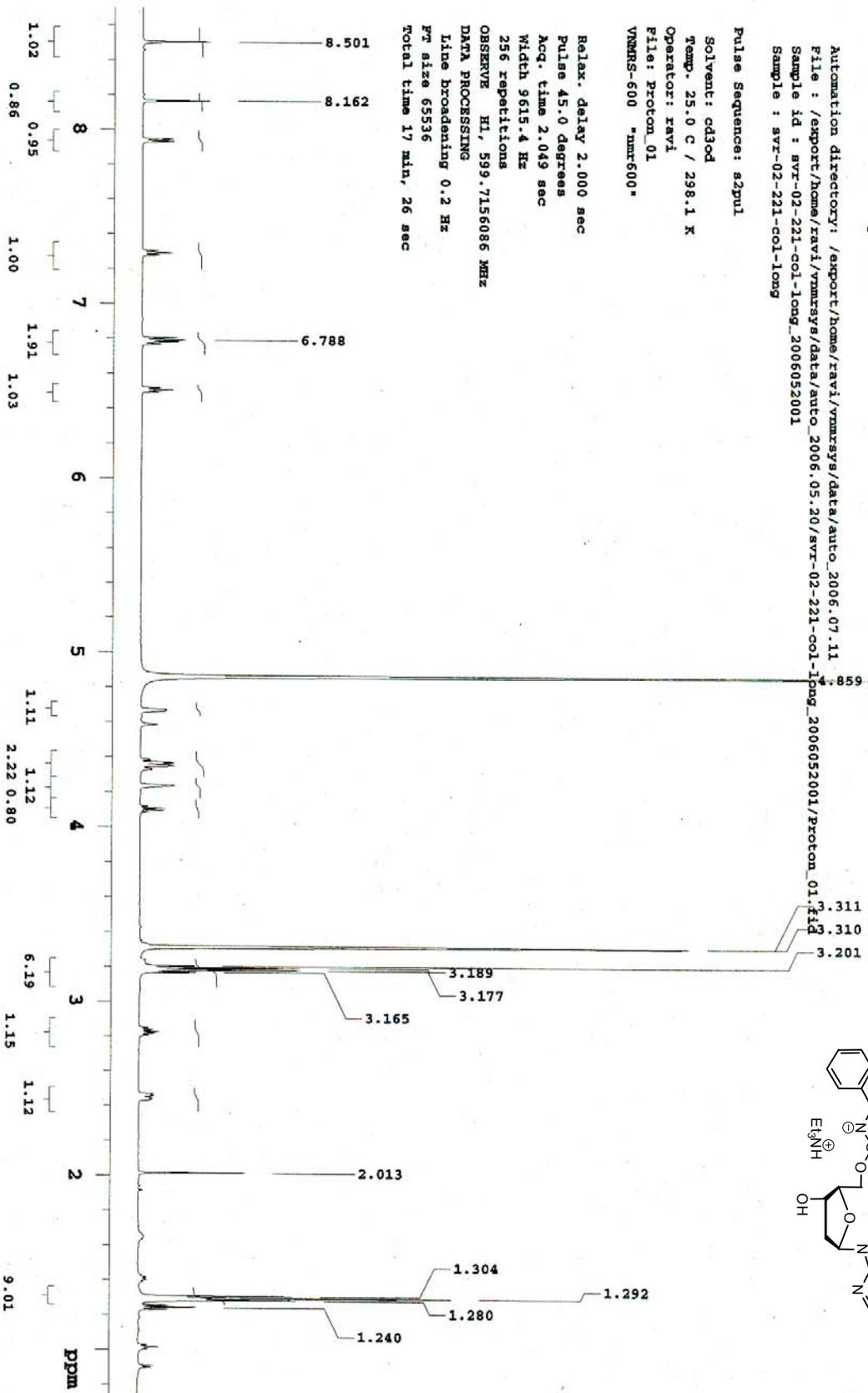


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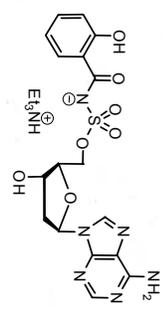
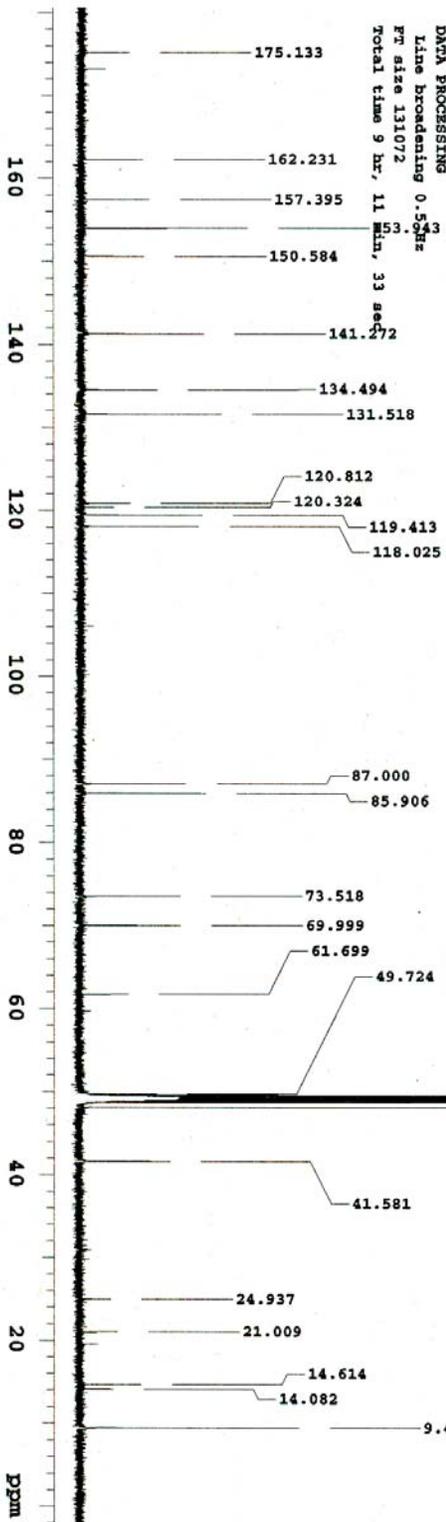
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 Sample : svr-02-221-col

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 Operator: ravi  
 File: Carbon\_01  
 VNMRS-600 \*nmr600\*

Relax. delay 2.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 36764.7 Hz  
 10000 repetitions  
 OBSERVE C13, 150.7983713 MHz  
 DECOUPLE H1, 599.7186175 MHz  
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 continuously on  
 FALTR-16 modulated  
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 FT size 131072  
 Total time 9 hr, 11 min, 33 sec



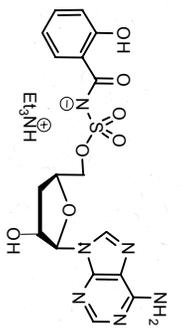
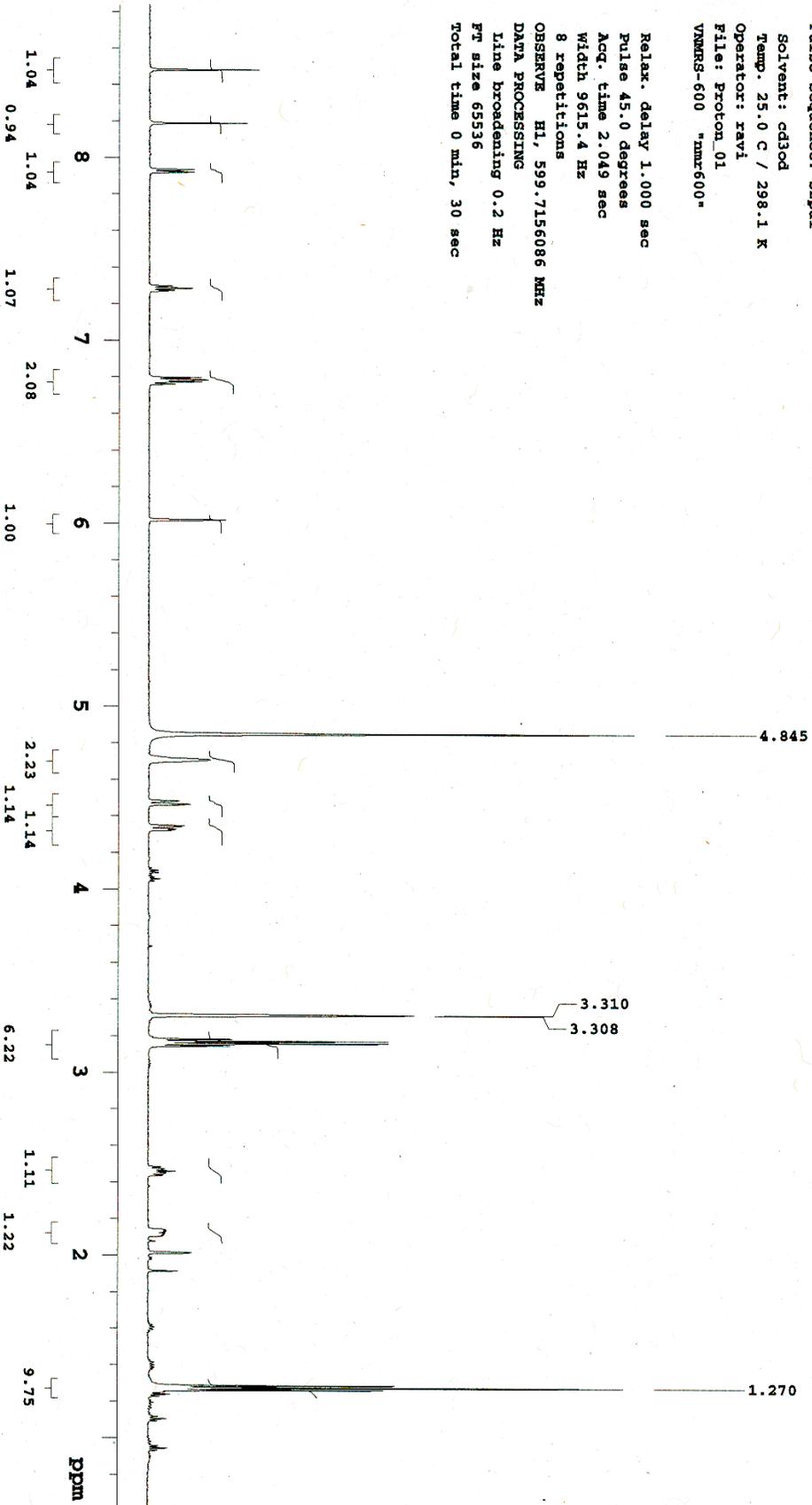
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Sample : svr-02-129-col

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Operator: ravi  
File: Proton\_01  
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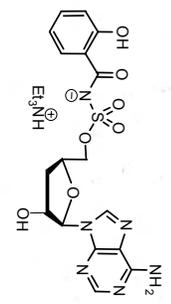
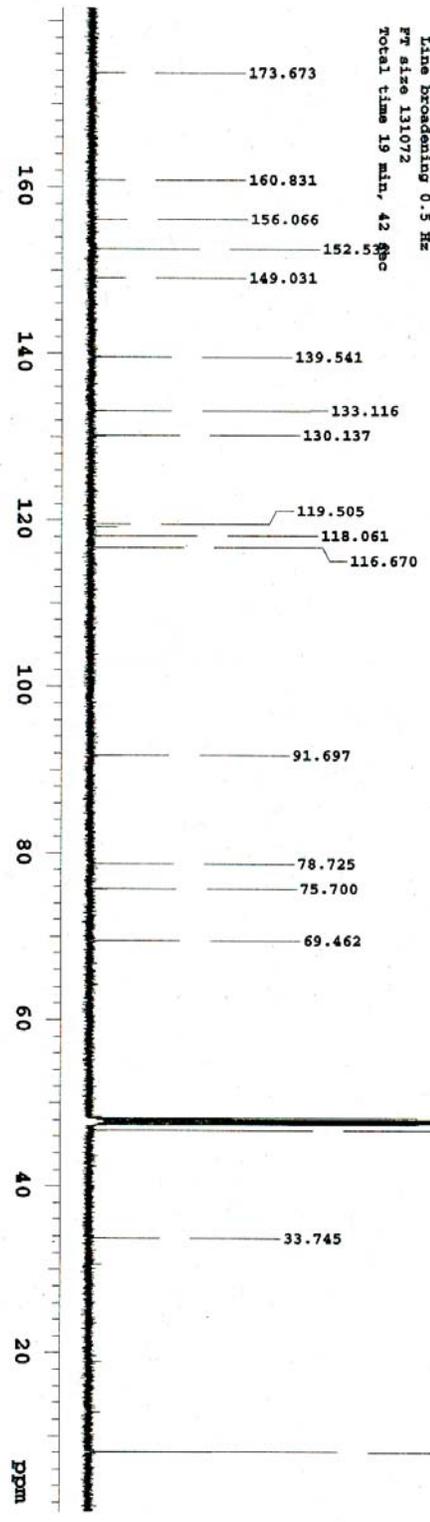
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DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 0 min, 30 sec



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 Sample : svr-02-129-co1

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 Temp. 25.0 C / 298.1 K  
 Operator: ravi  
 File: Carbon\_01  
 VNMRS-600 \*nmr600\*

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 36764.7 Hz  
 368 repetitions  
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 DECOUPLE H1, 599.7185175 MHz  
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 continuously on  
 WALTZ-16 modulated  
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 FT size 131072  
 Total time 19 min, 42 sec

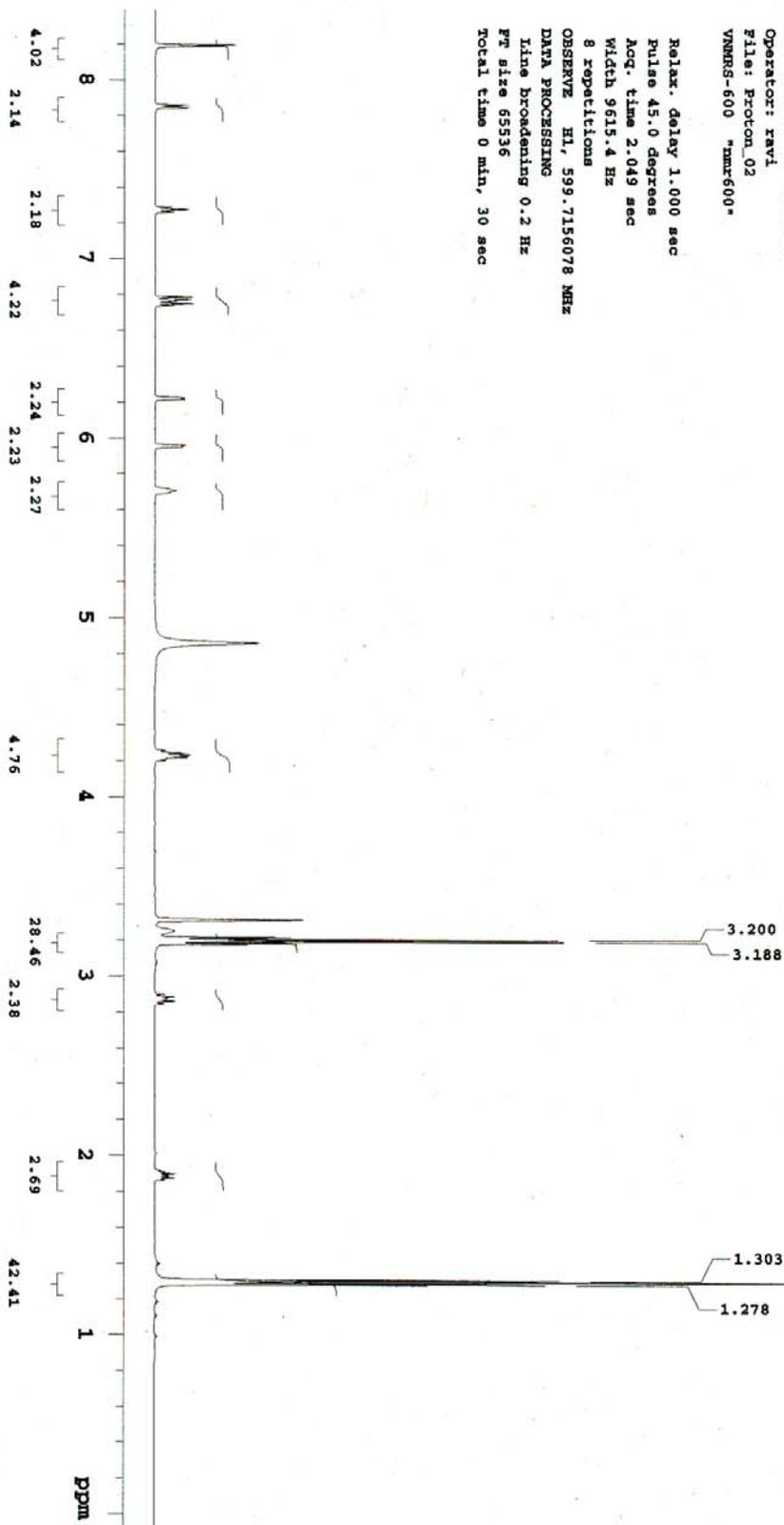


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Sample : svr-02-135-col

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Operator: ravi  
File: Proton\_02  
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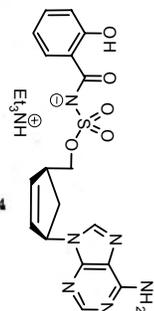
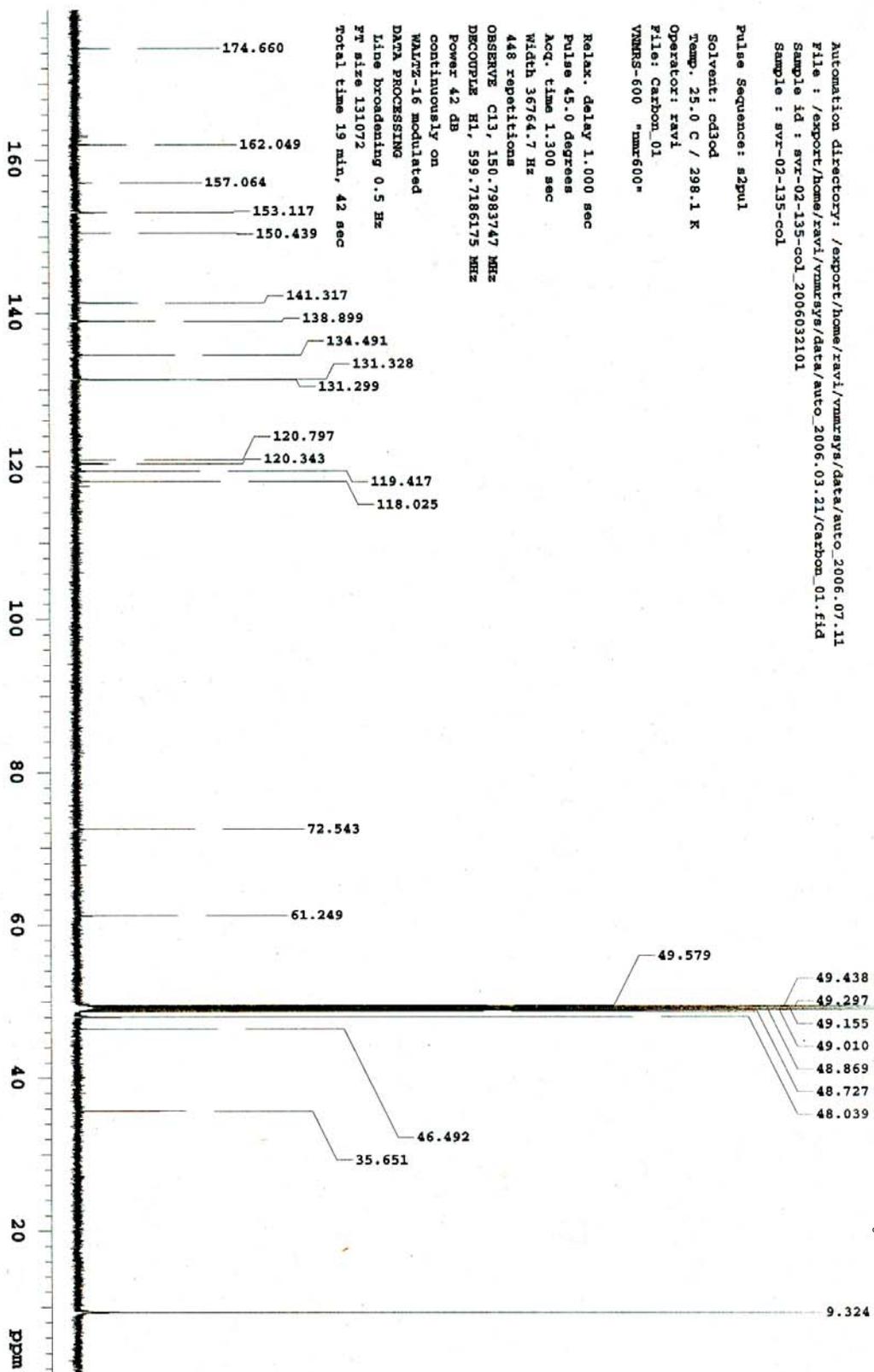
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line broadening 0.2 Hz  
PR size 65536  
Total time 0 min, 30 sec



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Sample : svr-02-135-col

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Temp. 25.0 C / 298.1 K  
Operator: ravi  
File: Carbon\_01  
VNMRS-600 "nmr600"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 36764.7 Hz  
448 repetitions  
OBSERVE C13, 150.7983747 MHz  
DECUPLE H1, 599.7185175 MHz  
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continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
SF size 131072  
Total time 19 min, 42 sec

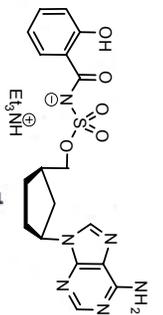
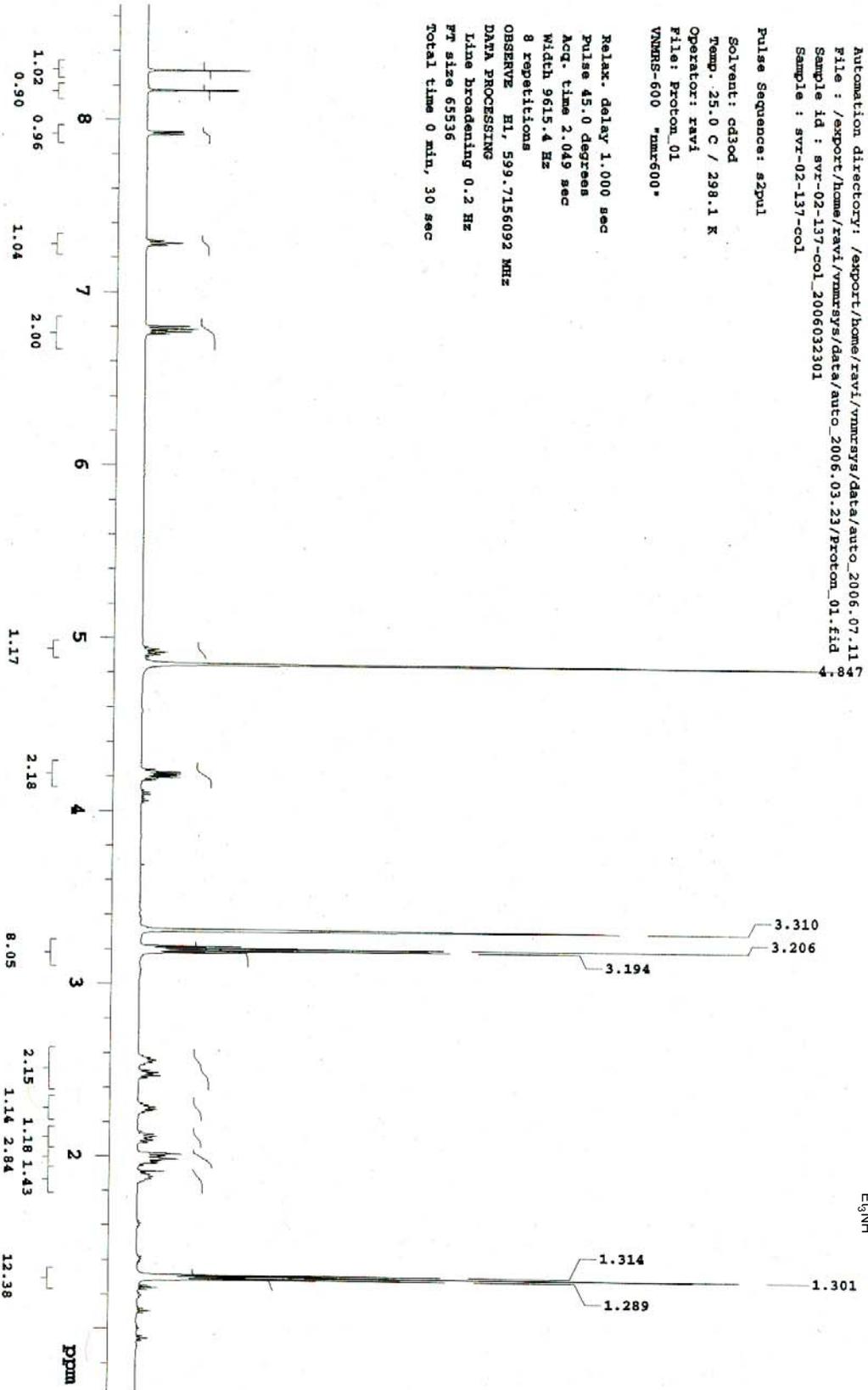


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Sample : svr-02-137-col

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File: Proton\_01  
VNMRS-600 \*nmr600\*

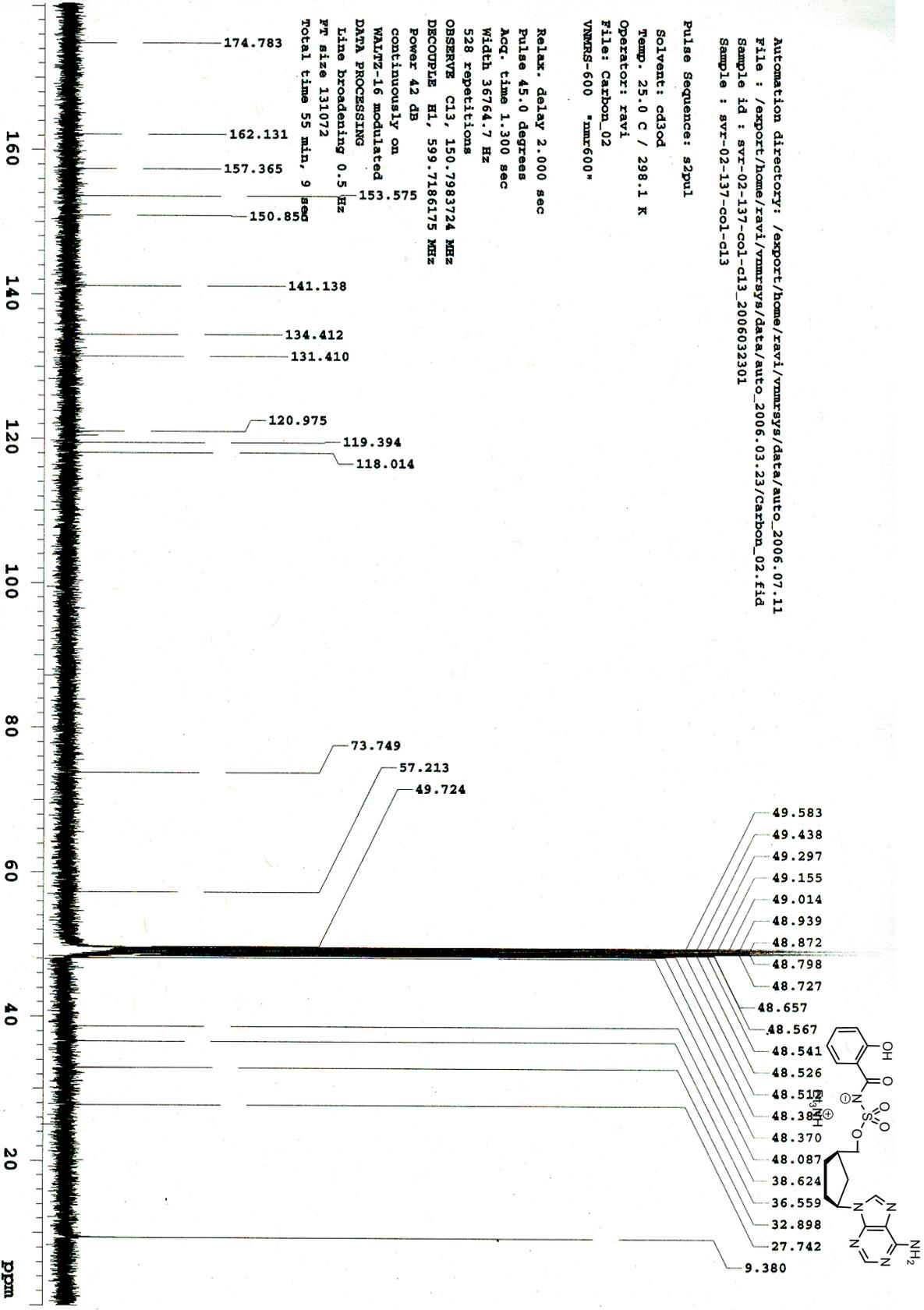
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DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 0 min, 30 sec



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 Sample : svr-02-137-col-cl3

Pulse Sequence: s2pul  
 Solvent: cd3od  
 Temp. 25.0 C / 298.1 K  
 Operator: ravi  
 File: Carbon\_02  
 VNMRS-600 "nmr600"

Relax. delay 2.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.300 sec  
 Width 36764.7 Hz  
 528 repetitions  
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 DECOUPLE H1, 599.7186175 MHz  
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 continuously on  
 VALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 131072  
 Total time 55 min, 9 sec

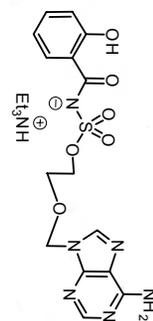
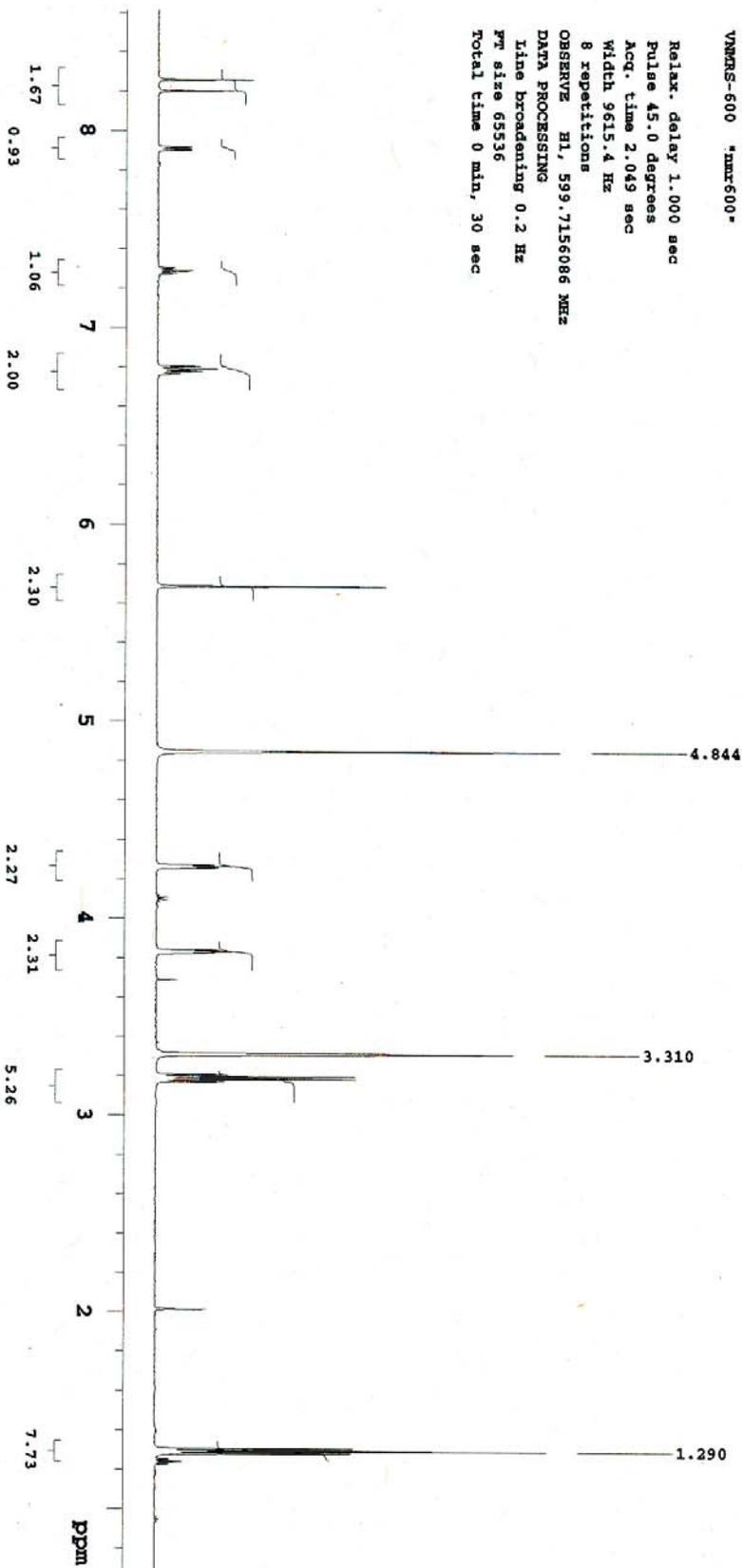


STANDARD 1H OBSERVE - profile

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Sample: svr-02-103-col

Pulse Sequence: s2pnl  
Solvent: cd3od  
Temp: 25.0 C / 298.1 K  
Operator: ravi  
File: Proton\_01  
VNMRS-600 \*nmr600\*

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
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8 repetitions  
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DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 0 min, 30 sec

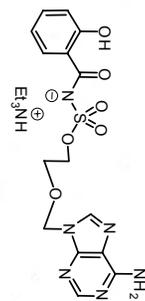
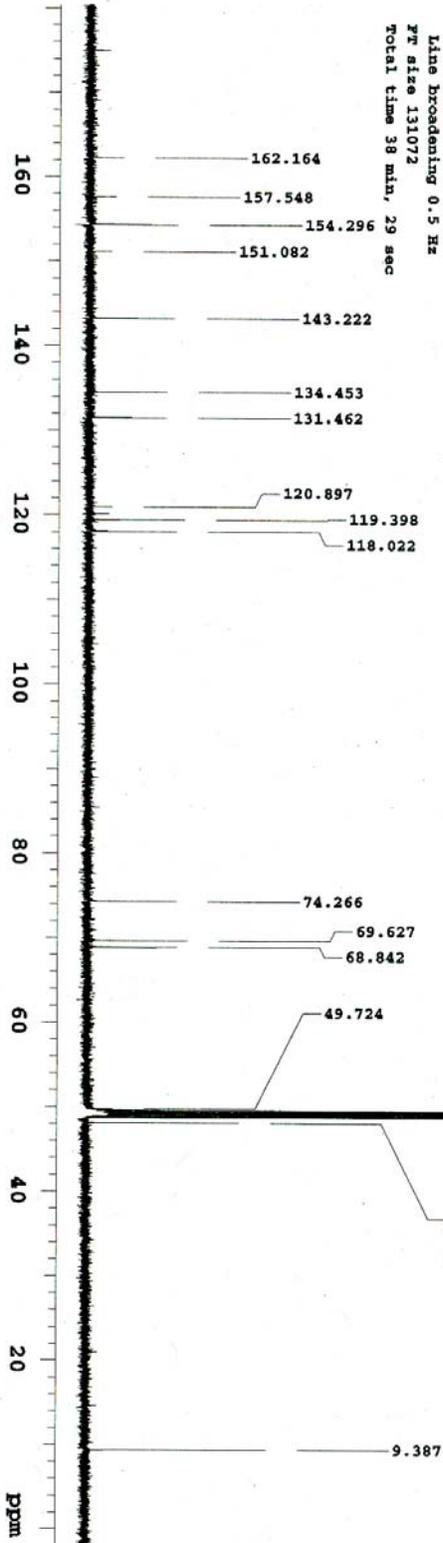


STANDARD 1H OBSERVE - profile  
STANDARD 1H OBSERVE - profile

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Sample : svr-02-103-col-cl3

Pulse Sequence: szpul  
Solvent: cd3od  
Temp. 25.0 C / 298.1 K  
Operator: ravi  
File: Carbon\_01  
VNMRS-600 \*nmr600\*

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 36764.7 Hz  
768 repetitions  
OBSERVE C13, 150.7983713 MHz  
DECOUPLE H1, 599.7186175 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
line broadening 0.5 Hz  
ZF size 131072  
Total time 38 min, 29 sec



**HPLC Purity of Inhibitors.** HPLC purity was determined for all final target inhibitors **8–13**. For all inhibitors two separate reverse-phase HPLC conditions were performed. An Agilent Eclipse XDB-C18 column (4.6 × 150 mm, 5 μm particle size) (Col 1) or Varian Microsorb MV 100-5 C18 column (4.6 X 250 mm, 5 μm particle size) (Col 2) with detection at 254 nm and the indicated HPLC conditions (Methods A–L) as described below was employed to determine the purity of inhibitors.

*Method A:* 0–20 min: gradient 10%–100% B; isocratic 20–25 min: 100% B; gradient 25–27 min: 100%–10%B; A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method B:* 0–14 min: isocratic 30% B; gradient 14–15 min: 30–100% B; isocratic 15–22 min: 100% B; A: 0.05 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method C:* 0–20 min: gradient 0%–90% B; isocratic 20–27 min: 90% B. A: 0.01 M ammonium formate; B: 90% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.8 ml/min, Col 1.

*Method D:* 0–18 min: isocratic 25% B; gradient 18–20 min: 25–100% B; isocratic 20–23 min: 100% B, A: 0.01 M ammonium formate; B: 90% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.8 ml/min, Col 1.

*Method E:* 0–20 min: gradient 10%–100% B; isocratic 20–25 min: 100% B; gradient 25–27 min: 100%–10%B; A: 0.05 M ammonium formate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method F:* 0–30 min: gradient 10%–100% B; isocratic 30–35 min: 100% B; gradient 35–37 min: 100%–10%B; A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method G:* 0–30 min: gradient 10%–100% B; isocratic 30–35 min: 100% B; gradient 35–37 min: 100%–10%B; A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method H:* 0–20 min: gradient 10%–100% B; isocratic 20–25 min: 100% B; gradient 25–27 min: 100%–10%B; A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method I:* 0–20 min: gradient 10-100% B; isocratic 20-22 min: 100% B; gradient 22–24 min: 100–10% B; isocratic 24–30 min: 100% B, A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

*Method J:* 0-30 min: isocratic 55% B; 30–35 min: gradient 55-100% B; 30–40 min: gradient 100–55% B. A: 0.04 M triethylammonium bicarbonate; B: 70% CH<sub>3</sub>CN-H<sub>2</sub>O, flow rate 0.5 ml/min, Col 2.

**Table S1.** HPLC Purity of Inhibitors

Inhibitor	Method	Retention time	Purity
8	A	11.7	99%
	B	11.2	97%
9	C	9.3	96%
	D	3.5	96%
10	E	17.3	96%
	F	20.1	94%
11	G	21.3	80%
12	H	18.5	82%
13	I	17.5	98%
	J	20.1	97%