

## Supplemental Material

### Figures Captions

**Figure S1.** IR spectrum complex **3**.

**Figure S2.** IR spectrum complex **4**.

**Figure S3.** IR spectrum complex **5**.

**Figure S4.** IR spectrum complex **6**.

**Figure S5.**  $^1\text{H}$  NMR spectrum in  $\text{CD}_3\text{CN}$  for complex **3**.

**Figure S6.**  $^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$  for complex **3**.

**Figure S7.**  $^1\text{H}$  NMR spectrum in  $\text{CD}_3\text{CN}$  for complex **4**.

**Figure S8.**  $^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$  for complex **4**.

**Figure S9.**  $^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$  for complex **5**.

**Figure S10.**  $^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$  for complex **6**.

**Figure S11.**  $^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$  for acetamide.

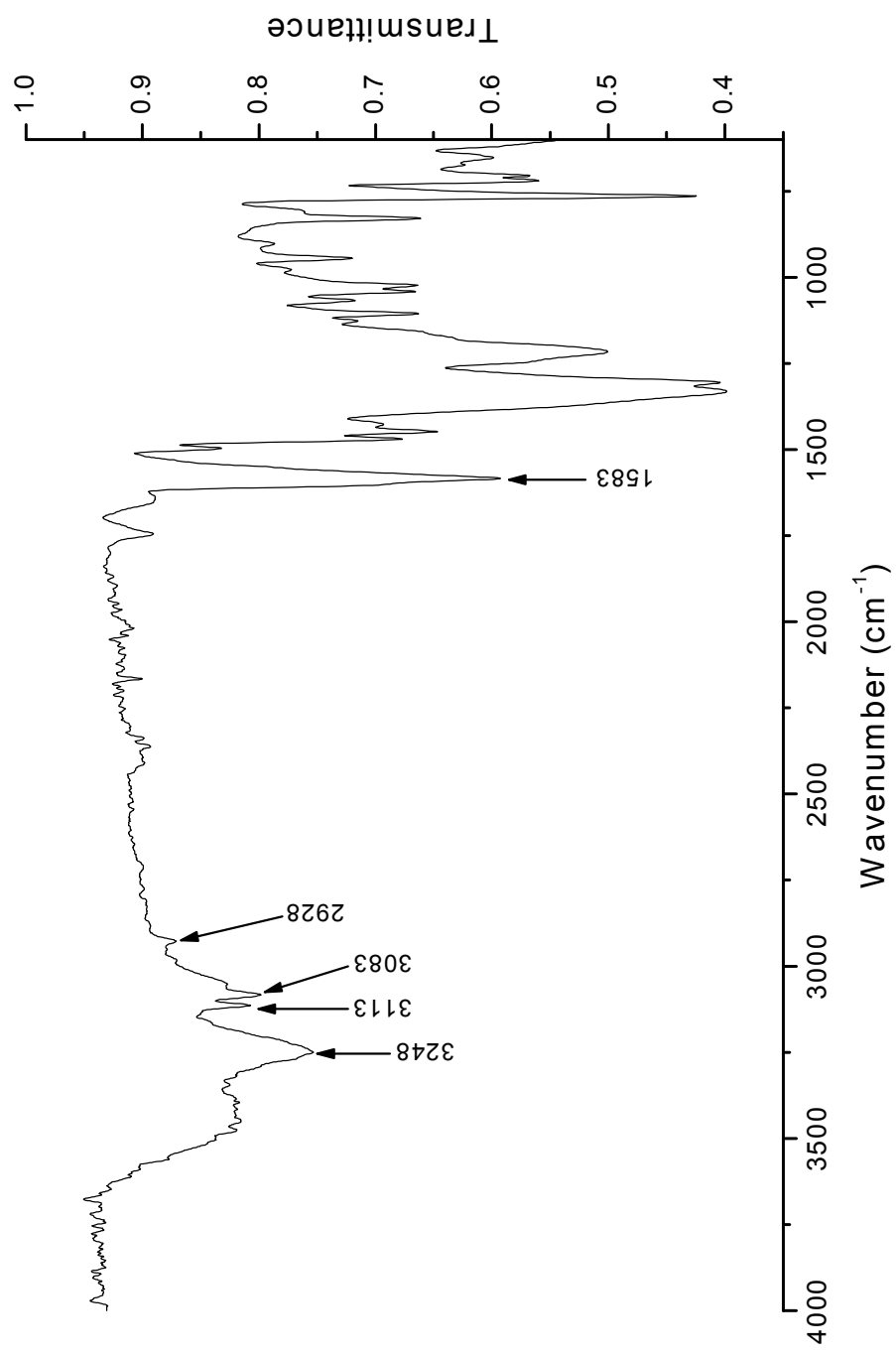


Figure S1

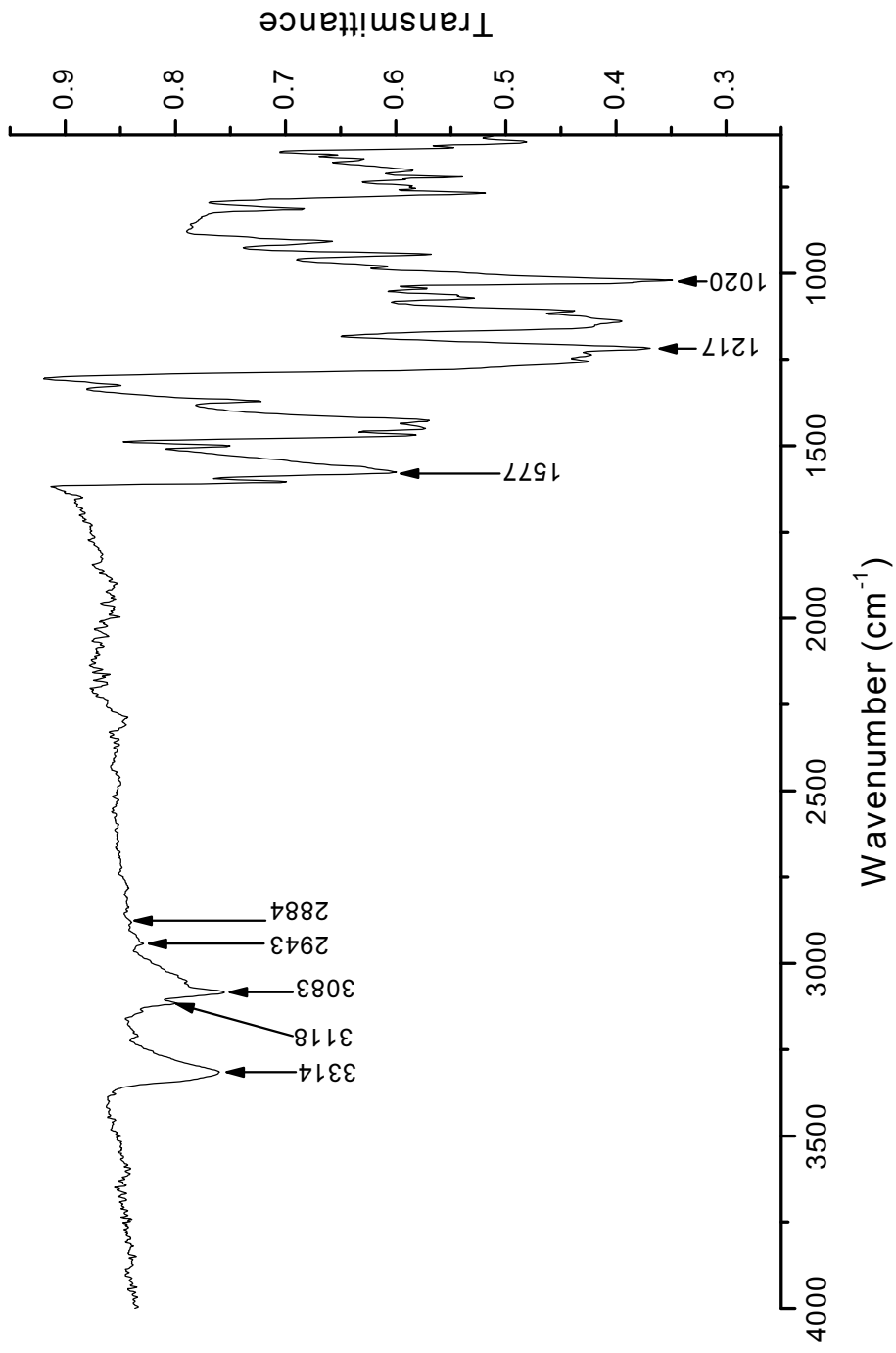


Figure S2

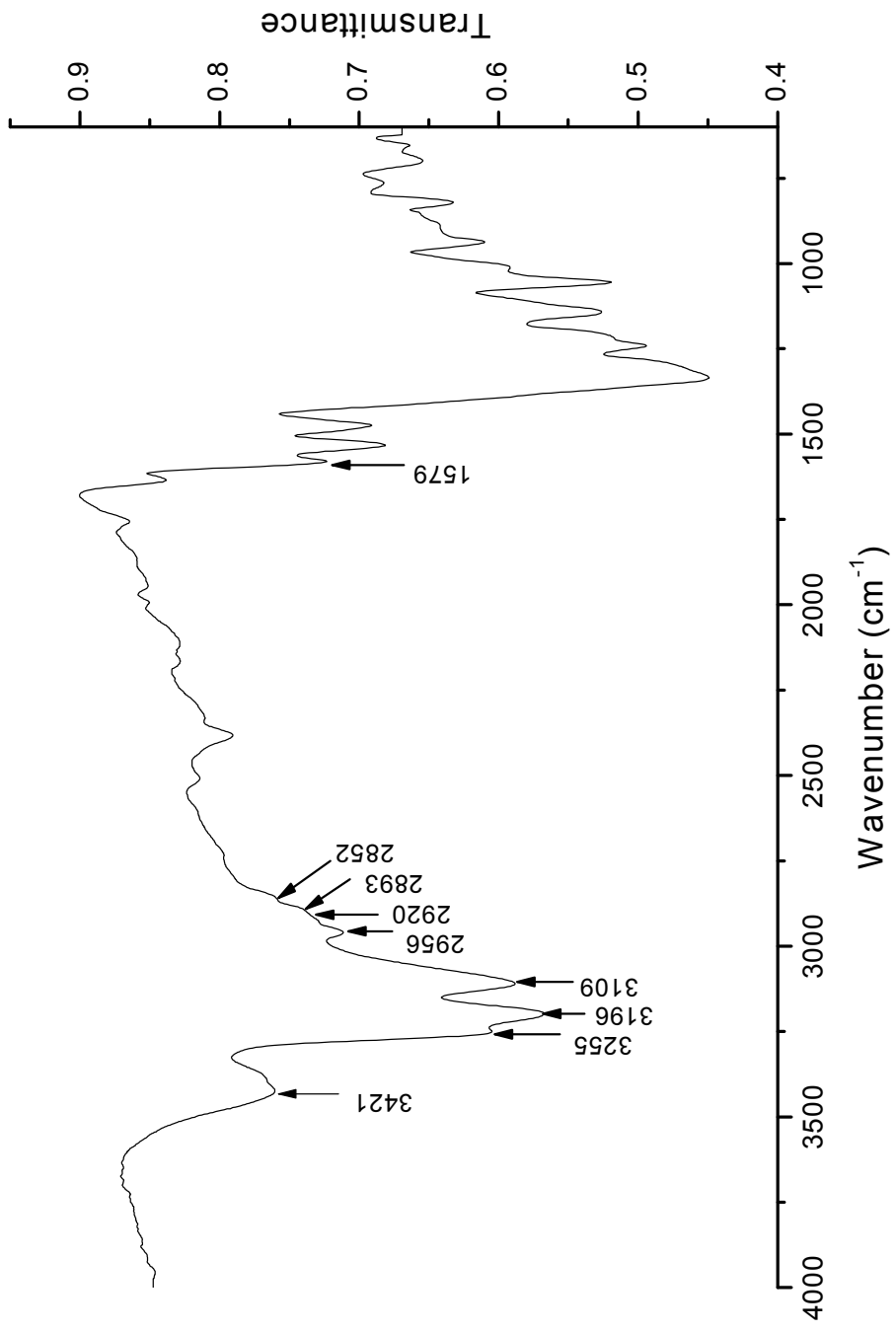


Figure S3

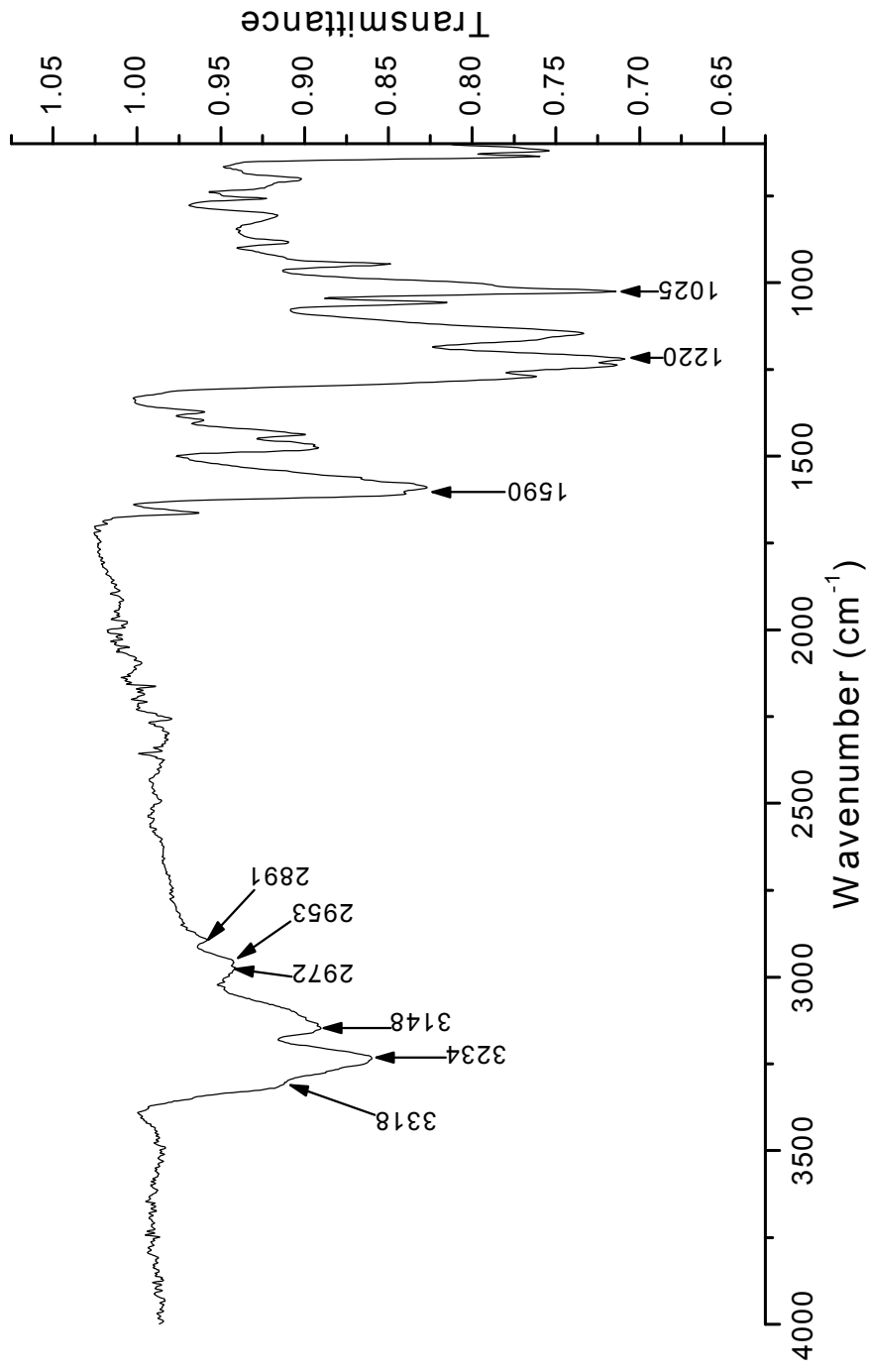


Figure S4

Pdacetamide\_crystals\_060905  
Archive directory: /export/home/vnmr1/vnmrSYS/data  
Sample directory:  
Pulse Sequence: s2pul1  
Solvent: CD3CN  
Ambient temperature  
File: Pdacetamide\_Crystals\_060905  
INVA-500 Varian500  
Relax. delay 1.000 sec  
Pulse 36.4 degrees  
Acq. time 1.000 sec  
Width 7896.0 Hz  
512 repetitions  
OBSERVED F1 F2 499.7447109 MHz  
F1 size 32768  
F2 size 32768  
Total time 24 min, 45 sec

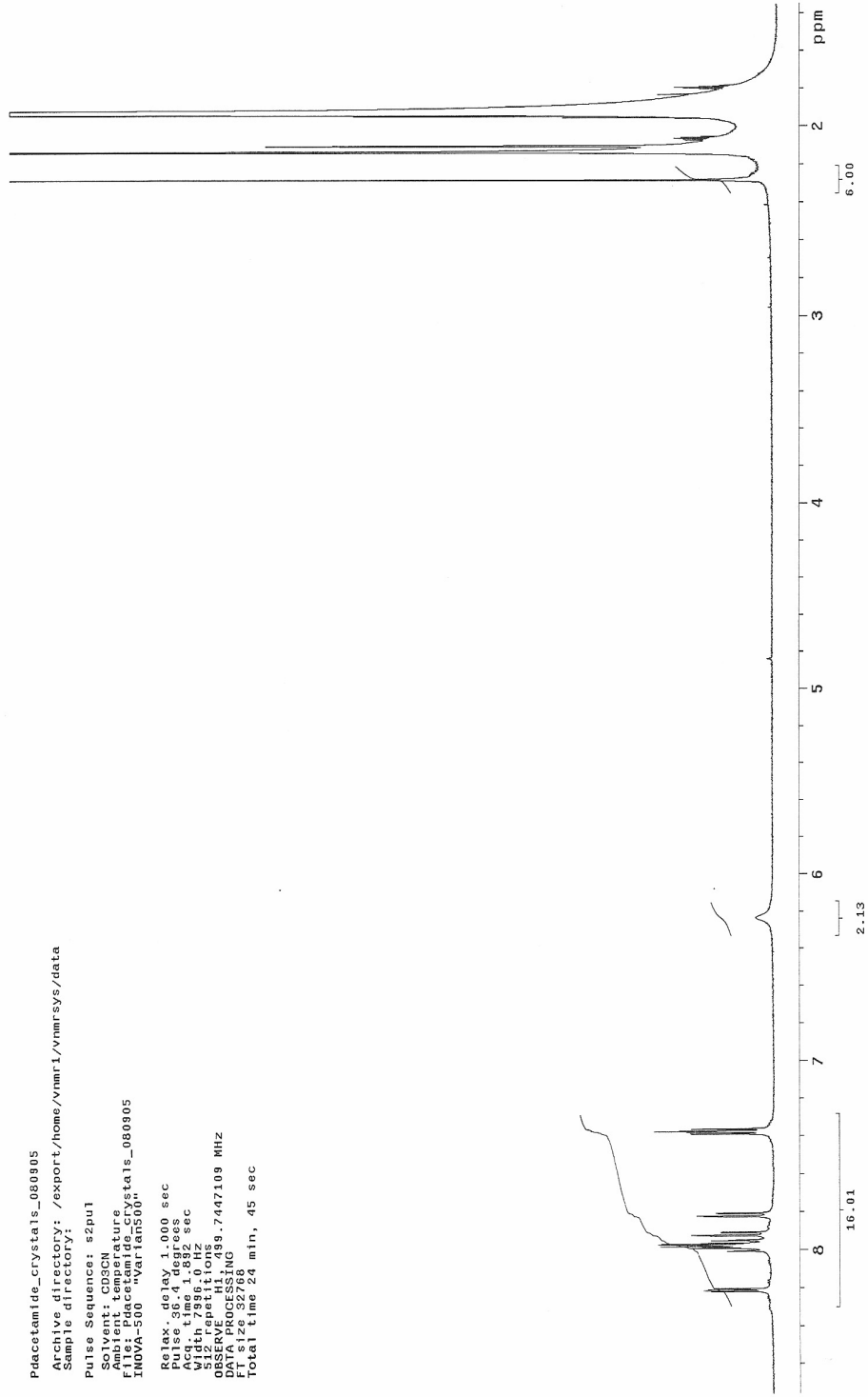


Figure S5

Pdbpy\_acetamide\_N03\_D20\_112106  
Pulse Sequence: presat  
Solvent: d2o  
Temp: 25.0 C / 298.1 K  
PROBHD: 5mm QNP1H  
PULPROG: zgpg30  
INSTR: spect  
Relax. delay: 2.000 sec  
Pulse: 45.0 degrees  
PC: 100.00000000  
Width: 999.0 Hz  
256 Repetitions  
085KRVOCES51MG .6859297 MHz  
FT size: 65536  
Total time: 25 min, 30 sec

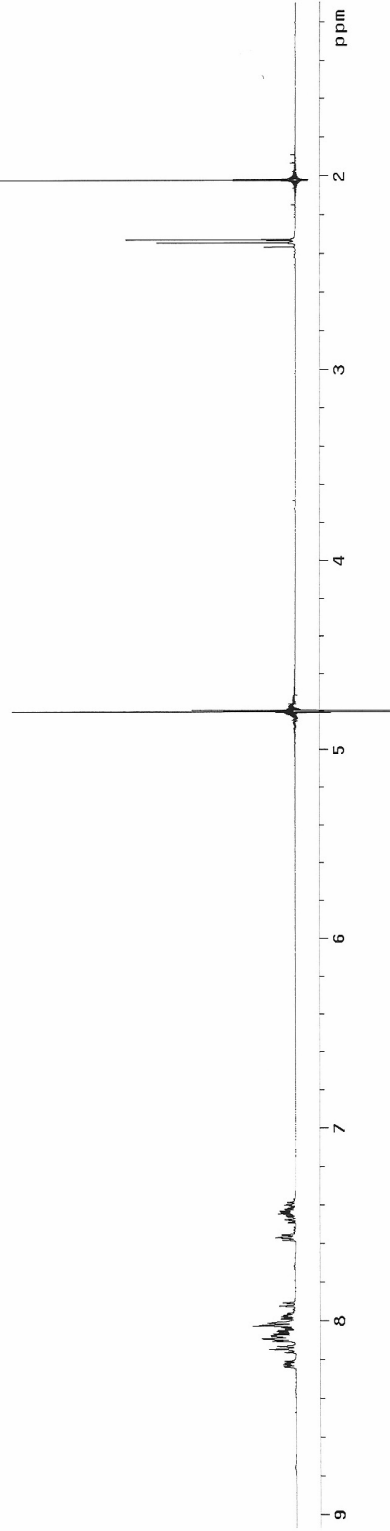


Figure S6

PdbpyOTF\_acetamide\_CD3CN\_012807  
Archive directory: /export/home/vnmr1/vnmrSYS/data  
Sample directory:  
File: PROTON  
Pulse Sequence: s2pul  
Solvent: CD3CN  
Ambient temperature:  
INOVA-500 "Inova500"  
Relax. delay 1.000 sec  
Pulse 38.4 degrees  
Acq. time 1.892 sec  
v1  
v2  
512 Repetitions  
OBSERVE\_H1, 499.6873786 MHZ  
DATA PROCESSING  
Total time 24 min, 45 sec

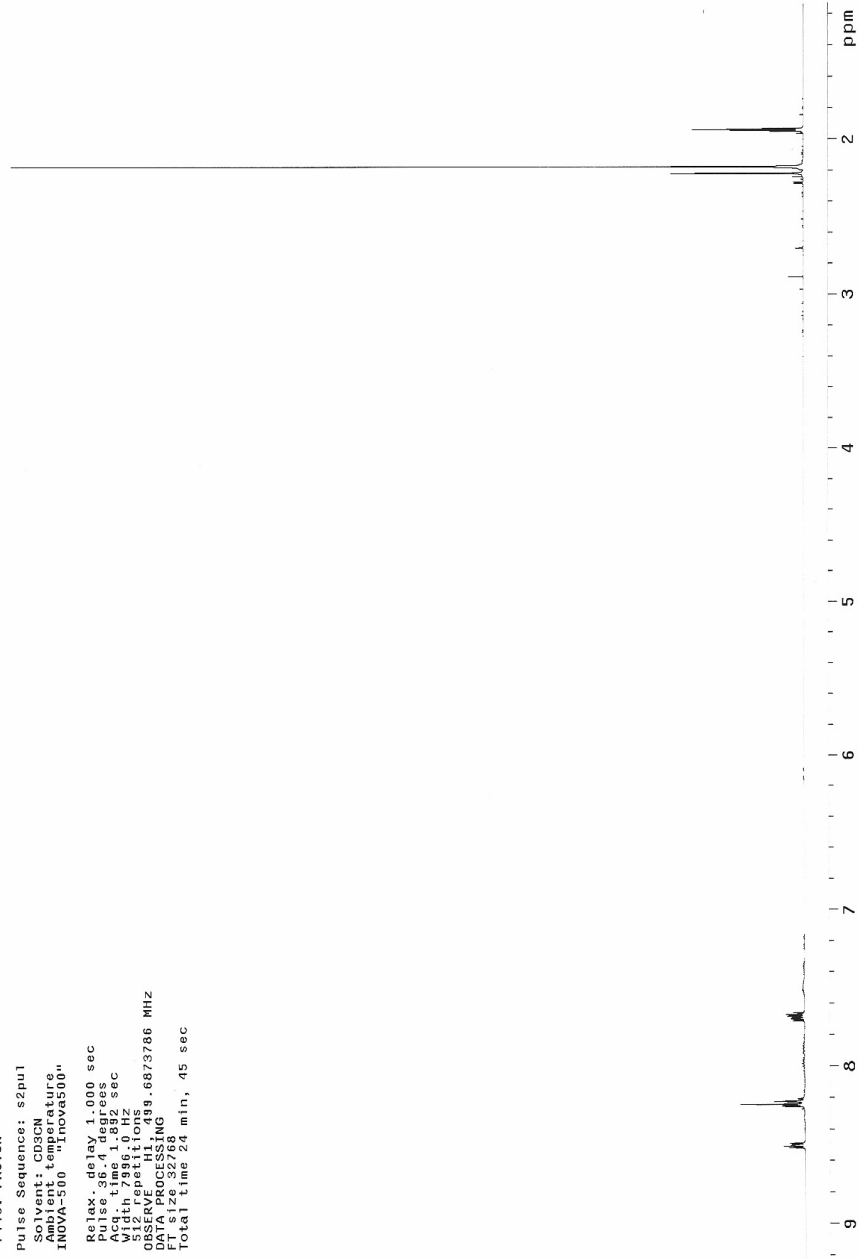


Figure S7



Pdbpy0Tf\_acetamide\_D2O\_101106  
Pulse Sequence: presat  
Solvent: d2o  
Temp: 625.0 C / 298.1 K  
F1: Pdbpy0Tf\_acetamide\_D2O\_101106  
INOVA-500 1HNOVS500"  
Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Width 12.000 sec  
Width 995.0 Hz  
128 repetitions  
ASCP: PROCESSING  
FT size 65536  
Total time 12 min, 51 sec

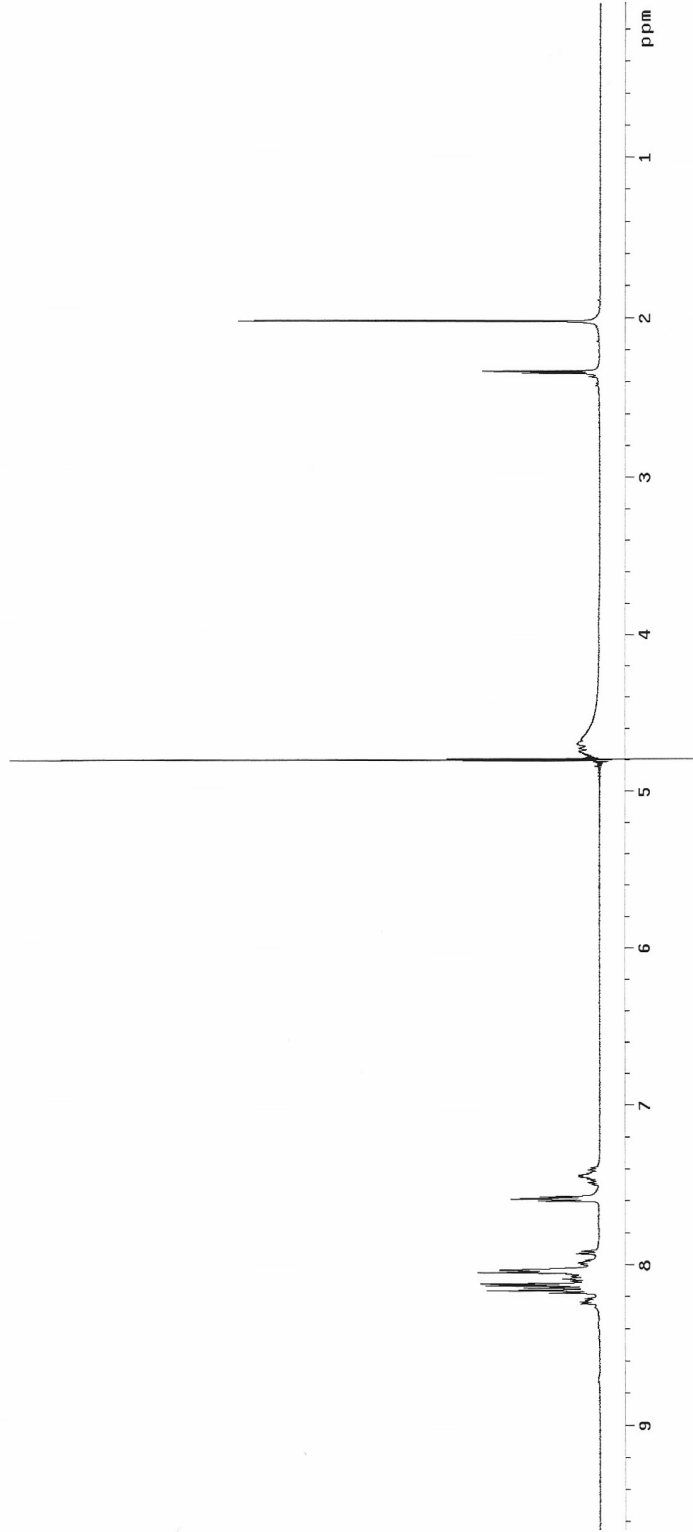


Figure S8



Pden\_acetamide\_0Tf\_D20\_110106  
Pulse Sequence: presat  
Solvent: d2o  
Temp: 25.0 C / 298.1 K  
File: Pden\_acetamide\_0Tf\_D20\_110106  
INOVA-500 "Inova500"  
Relax\_delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.922 sec  
V68h 39810Hz  
V68p 39810Hz  
OBSERVE H1, 499.6859303 MHZ  
DATA PROCESSING  
Total time 12 min, 51 sec

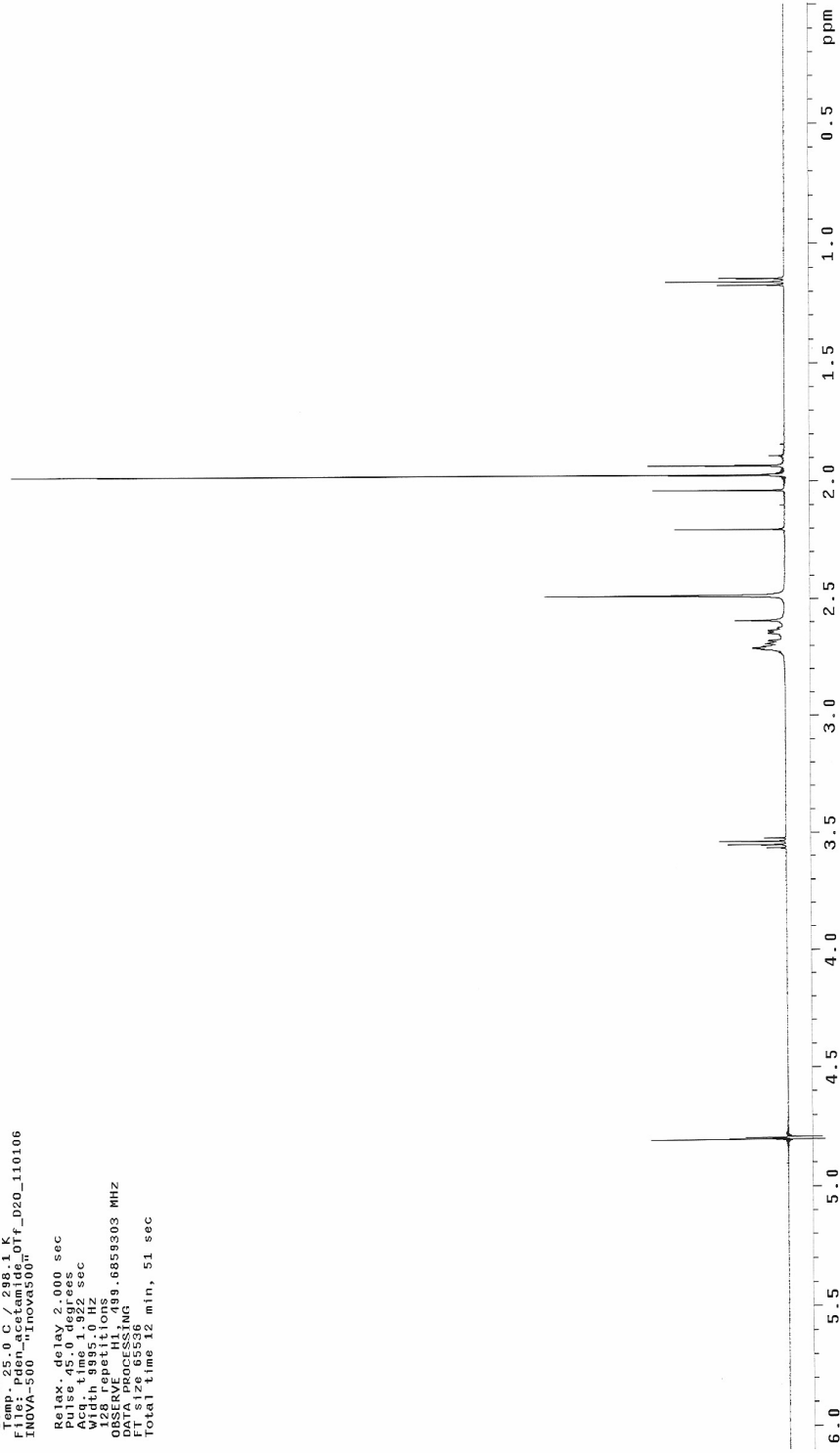


Figure S10

Acetamide\_D20\_060806  
Pulse Sequence: presat  
Solvent: d2o / 288.1 K  
File: Acetamide\_D20\_060806  
INOVA-500 "Inova500"  
Relax. delay 2.000 sec  
Acq. delay 1.000 sec  
Acq. time 1.922 sec  
Width 5718.8 Hz  
Observer: H1  
RESERVE H1: 499.6943949 MHZ  
DATA PROCESSING  
Total time 9 min, 21 sec

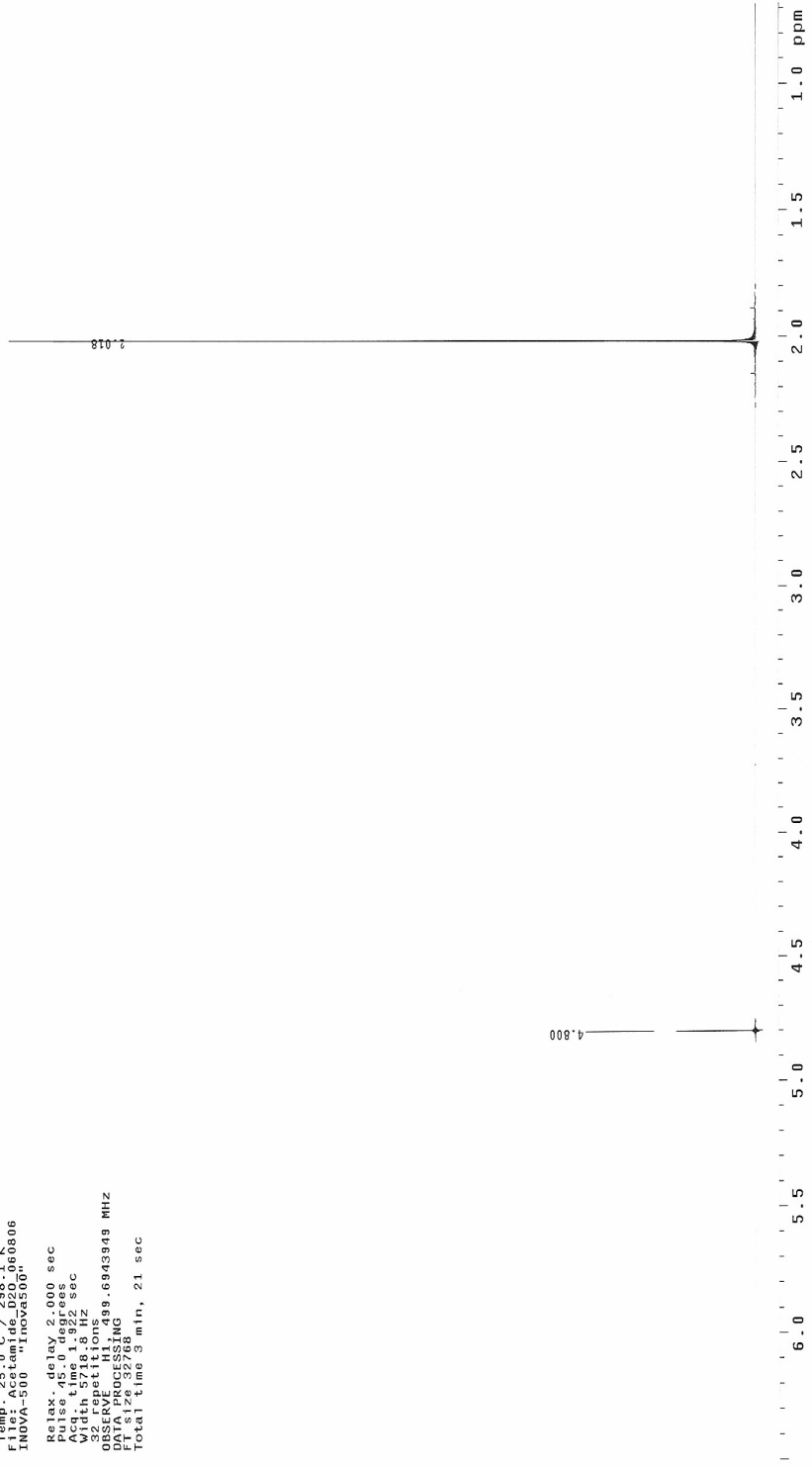


Figure S11