Supporting Information

Coordination-Driven Face-Directed Self-Assembly of Trigonal Prisms. Face-Based Conformational Chirality

Douglas C. Caskey,[ξ] Takuya Yamamoto,[†] Chris Addicott,[†] Richard K. Shoemaker,[ξ] Jaroslav Vacek,[ξ,¶] Adam M. Hawkridge,[‡] David C. Muddiman,[‡] Gregg S. Kottas, [ξ] Josef Michl[*,ξ,¶] and Peter J. Stang[*,†]

[†] *Department of Chemistry, University of Utah, 315 South 1400 East, Rm. 2020, Salt Lake City, Utah 84112*

[‡] *W. M. Keck FT-ICR Mass Spectrometry Laboratory, Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695*

[ξ] *Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado 80309-0215*

[¶] *Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, 166 10 Prague 6, Czech Republic*

stang@chem.utah.edu, michl@eefus.colorado.edu

Figure S1 ^{31}P NMR spectrum of **3a**. Page S2
Figure S2 ^{1}H NMR spectrum of **3a**. Page S3
Figure S3 Infrared spectrum of **3a** in KBr. Page S4
Figure S4 ^{31}P NMR spectrum of **3b**. Page S5
Figure S5 ^{1}H NMR spectrum of **3b**. Page S6
Figure S6 Infrared spectrum of **3b** in KBr. Page S7
Figure S7 ^{31}P NMR spectrum of **3c**. Page S8
Figure S8 ^{1}H NMR spectrum of **3c**. Page S9
Figure S9 Infrared spectrum of **3c** in KBr. Page S10
Figure S10 ^{31}P NMR spectrum of **3d**. Page S11
Figure S11 ^{1}H NMR spectrum of **3d**. Page S12
Figure S12 Infrared spectrum of **3d** in KBr. Page S13
Figure S13 DNMR of **3a**. Page S14
Figure S14 DNMR of **3b**. Page S15
Figure S15 DNMR of **3c**. Page S16
Figure S16 DNMR of **3d**. Page S17
Figure S17 1D EXCHSY (DPFGSE) chemical exchange of **3b**. Page S18
Figure S18 2D-EXCHSY/ROESY of **3b**. Page S19

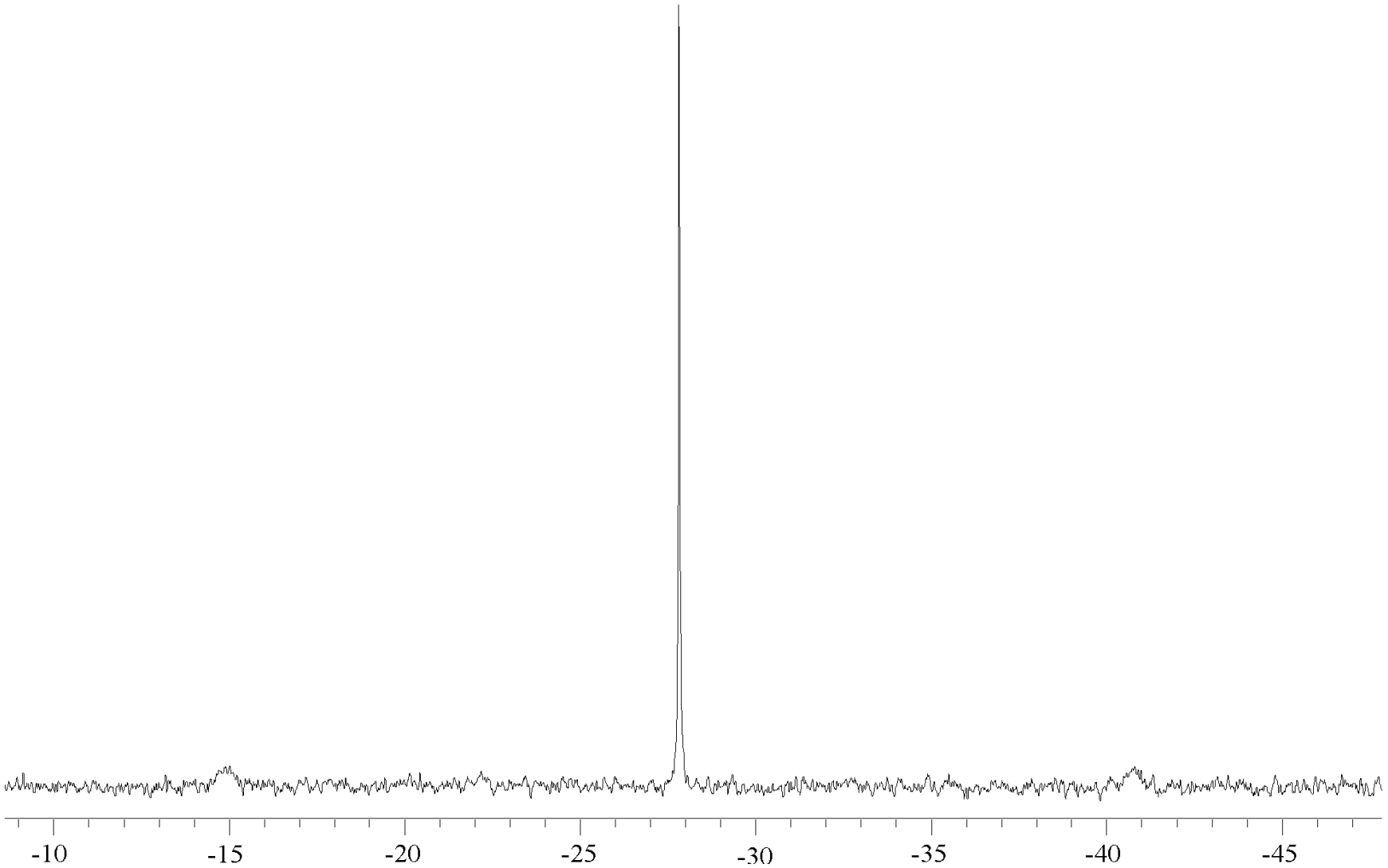

Figure S1. ^{31}P NMR spectrum of **3a**.

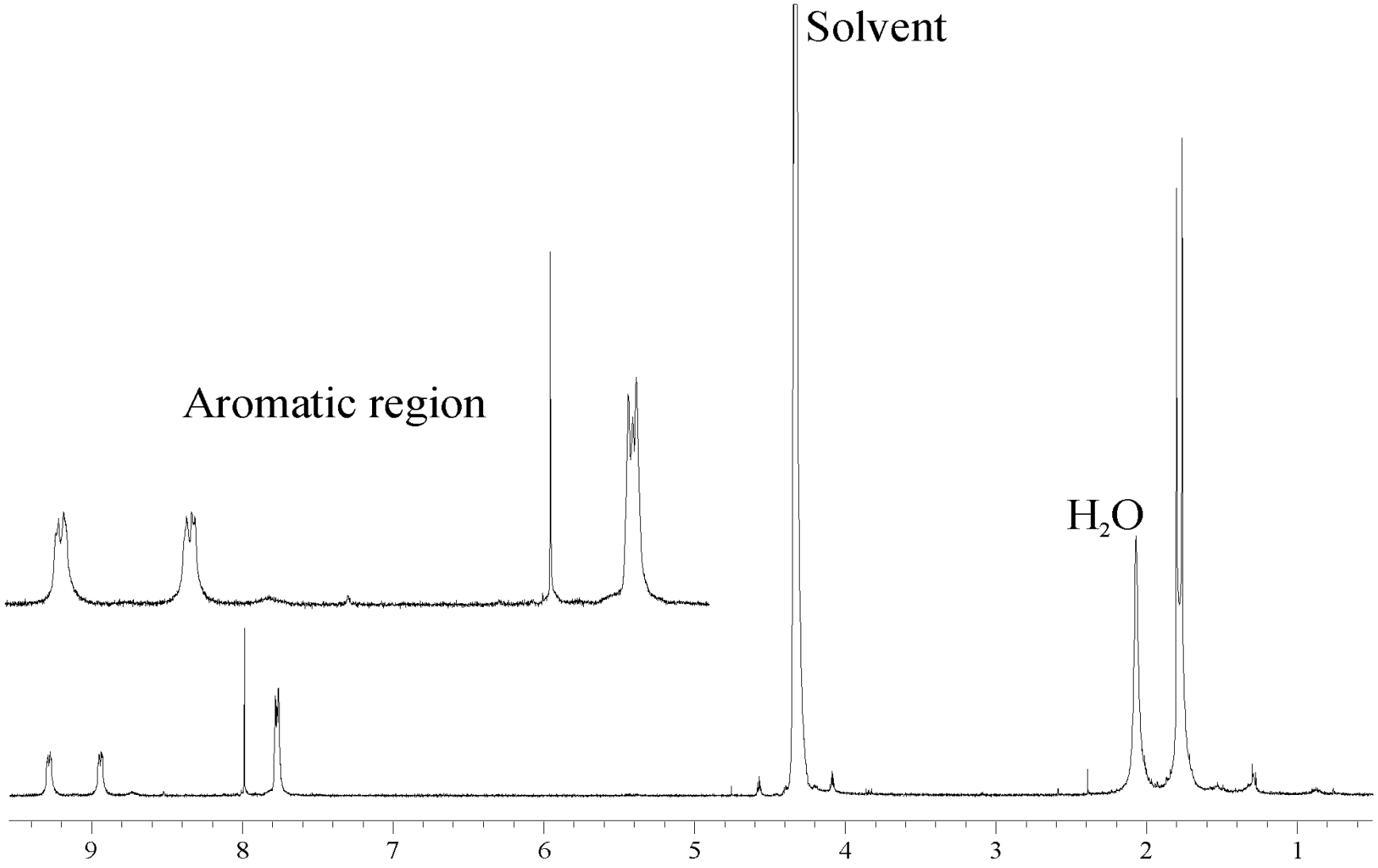

Figure S2. ^{1}H NMR spectrum of **3a**.

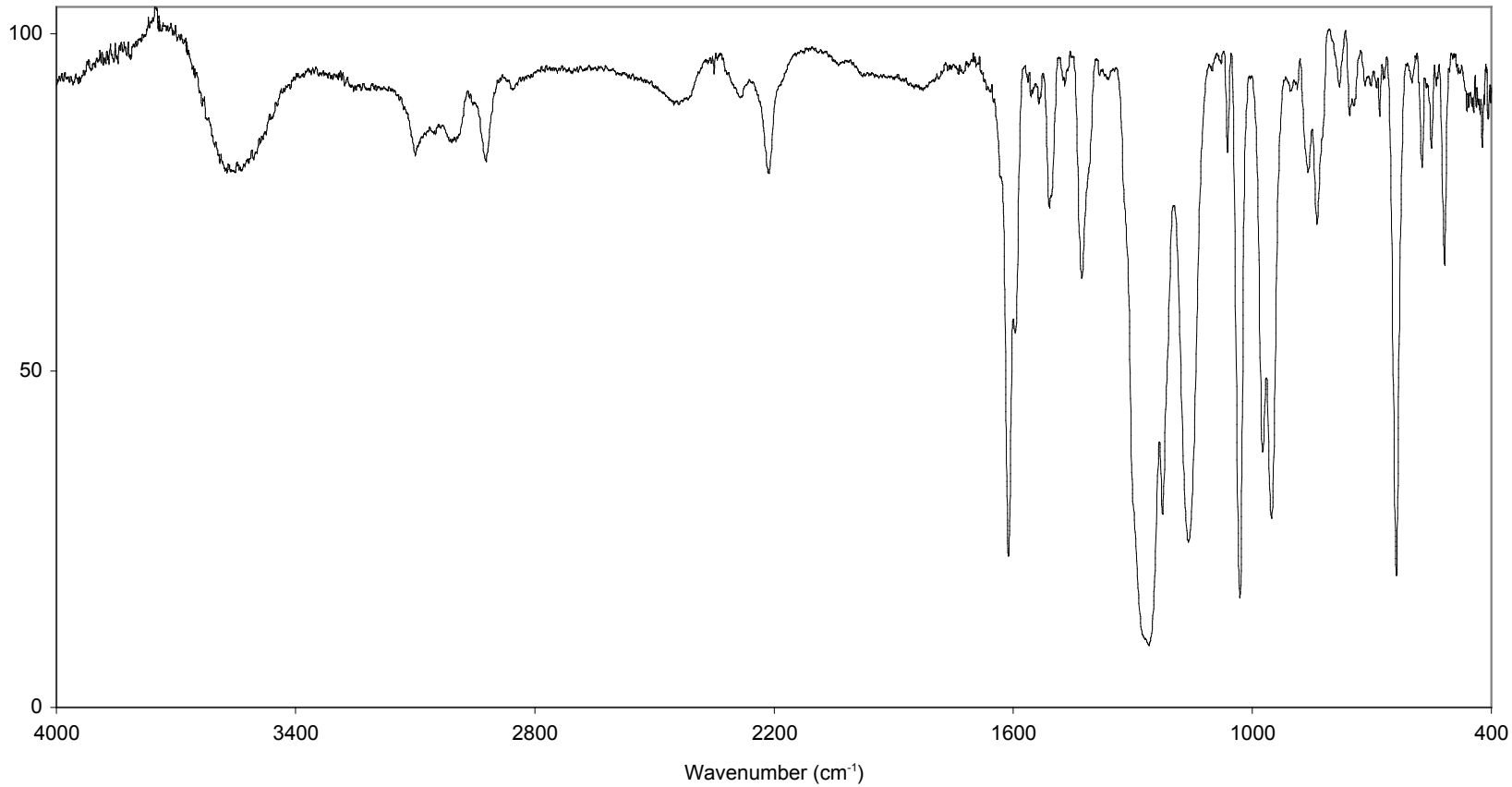

Figure S3. Infrared spectrum of **3a** in KBr.

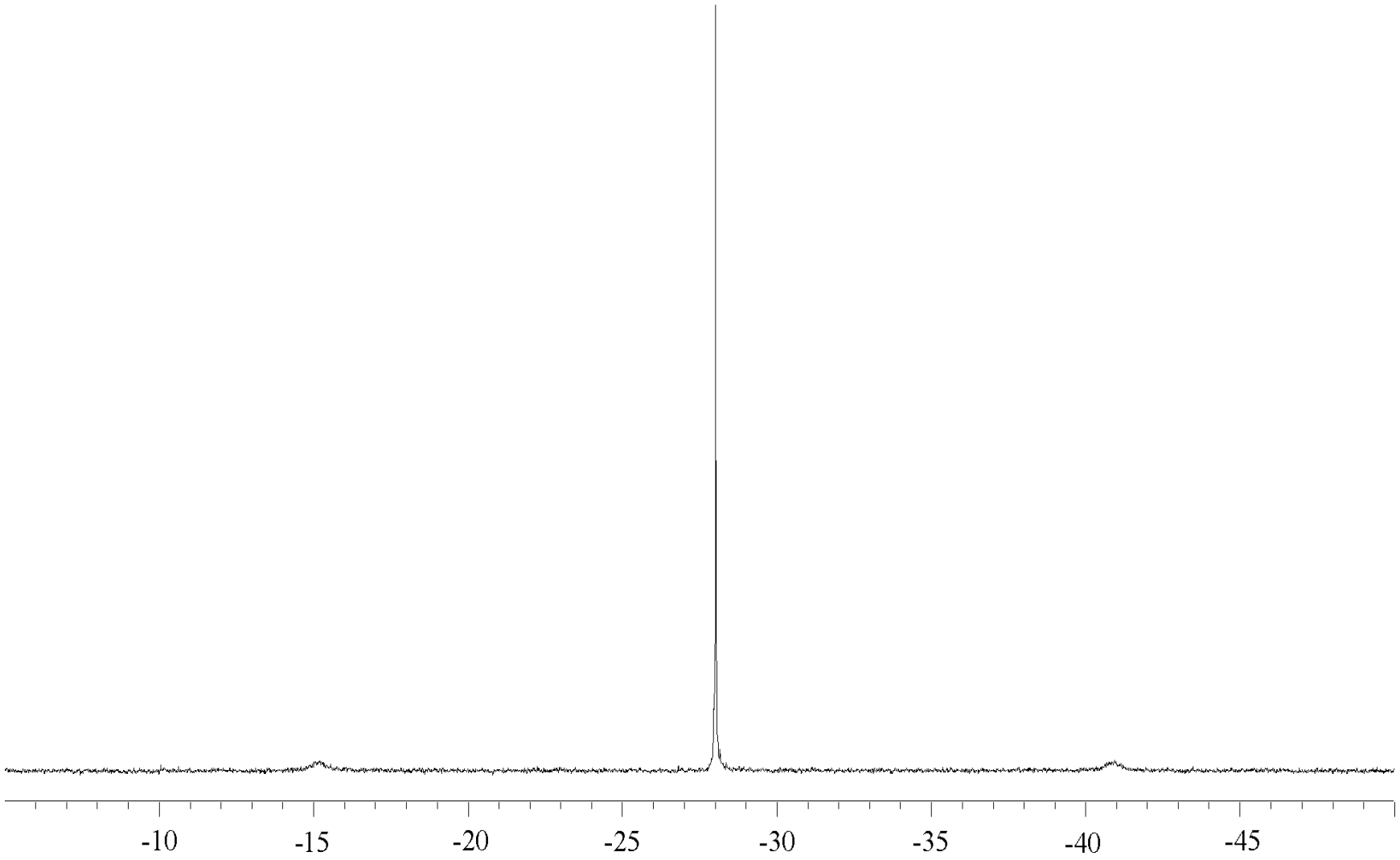

Figure S4. ^{31}P NMR spectrum of **3b**.

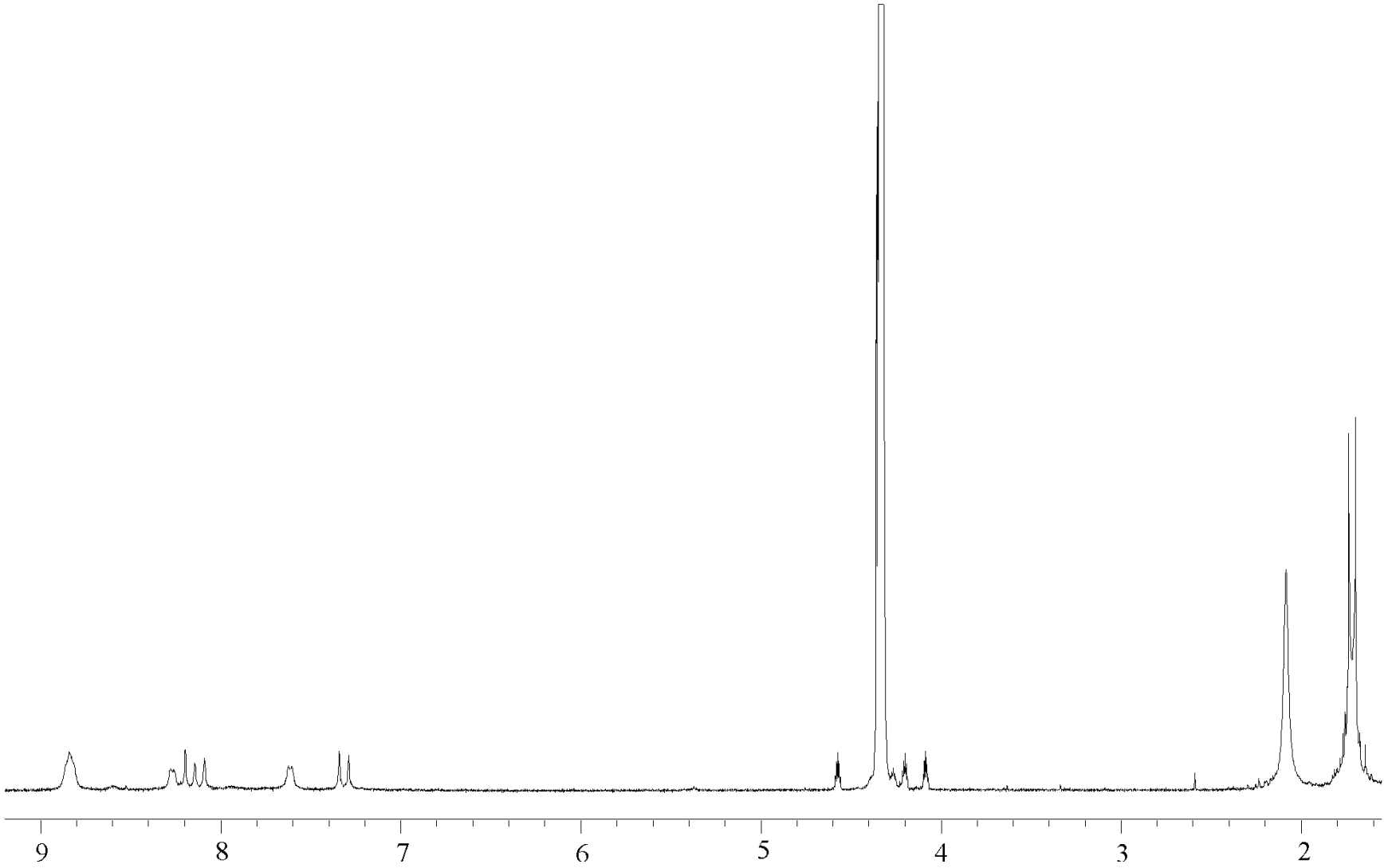

Figure S5. ^{1}H NMR spectrum of **3b**.

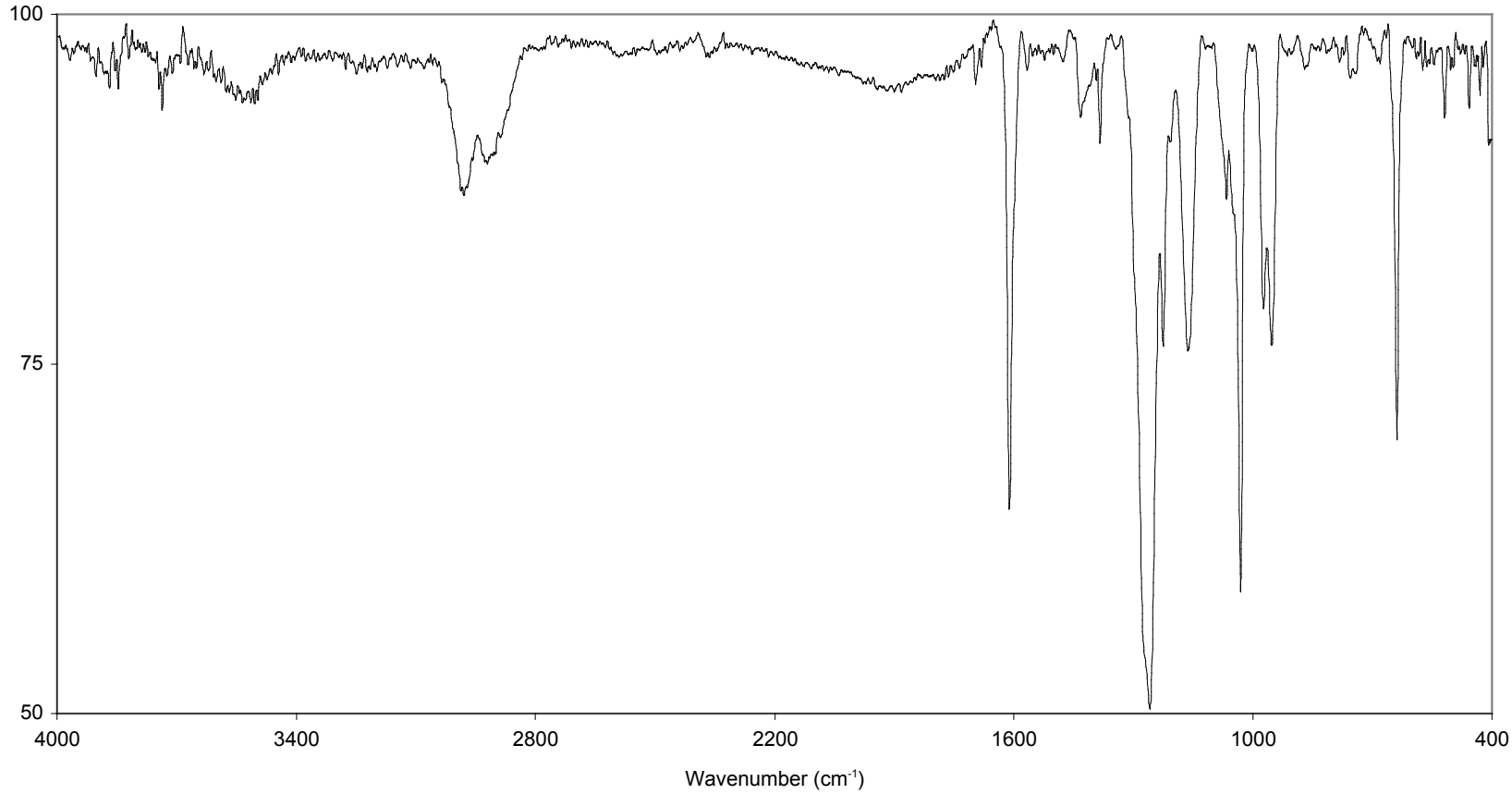

Figure S6. Infrared spectrum of **3b** in KBr.

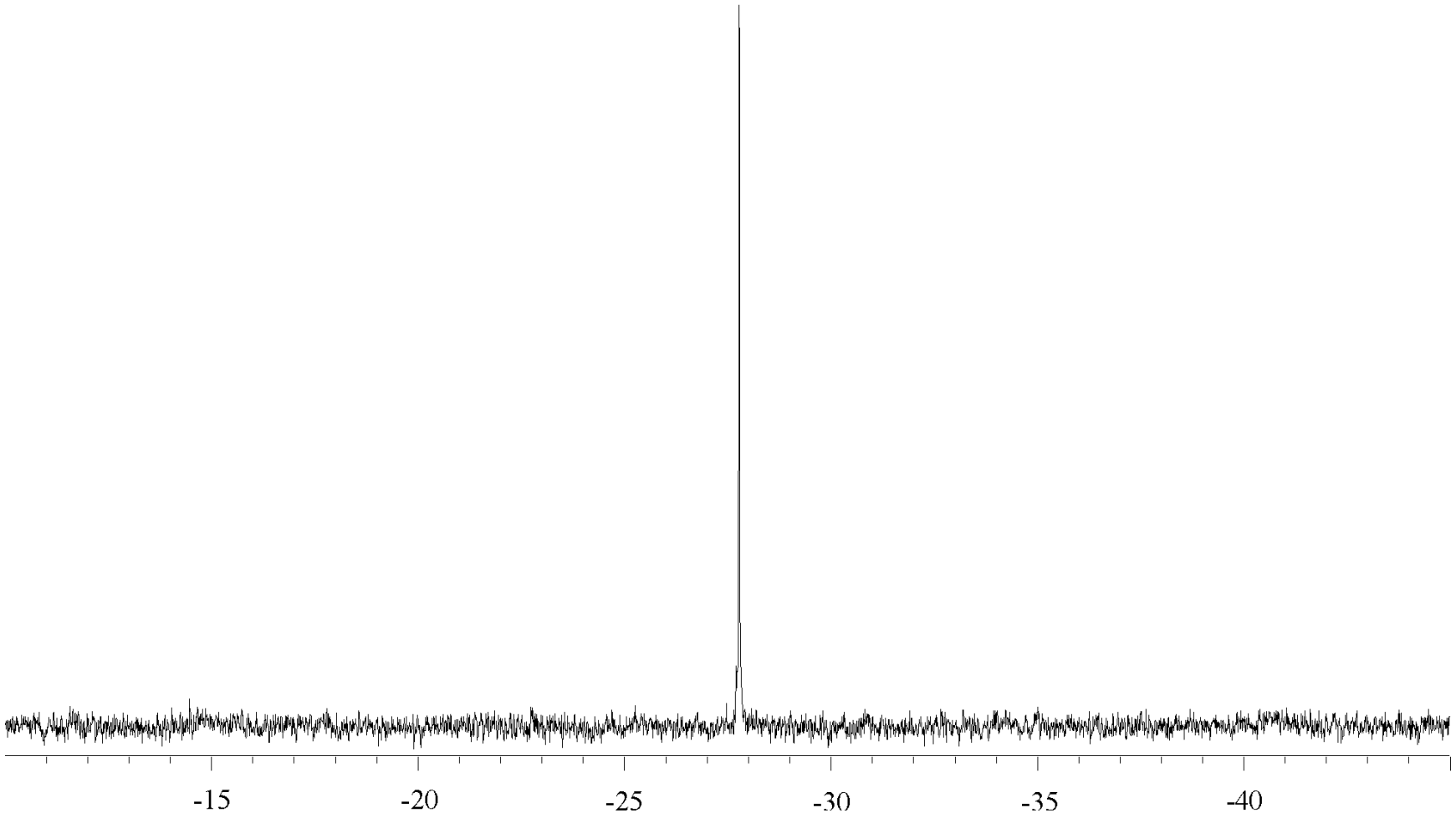

Figure S7. ^{31}P NMR spectrum of **3c**.

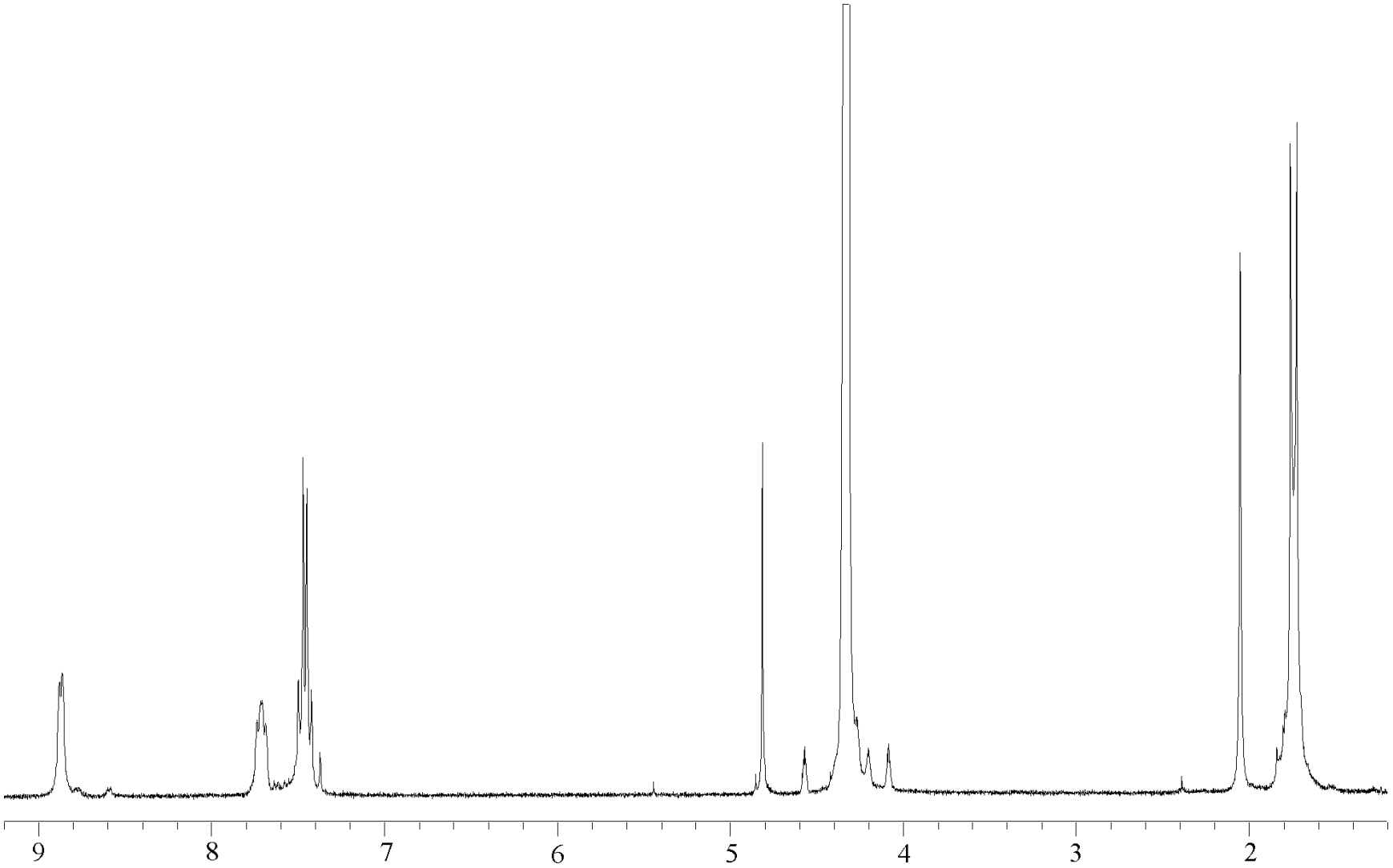

Figure S8. ^{1}H NMR spectrum of **3c**.

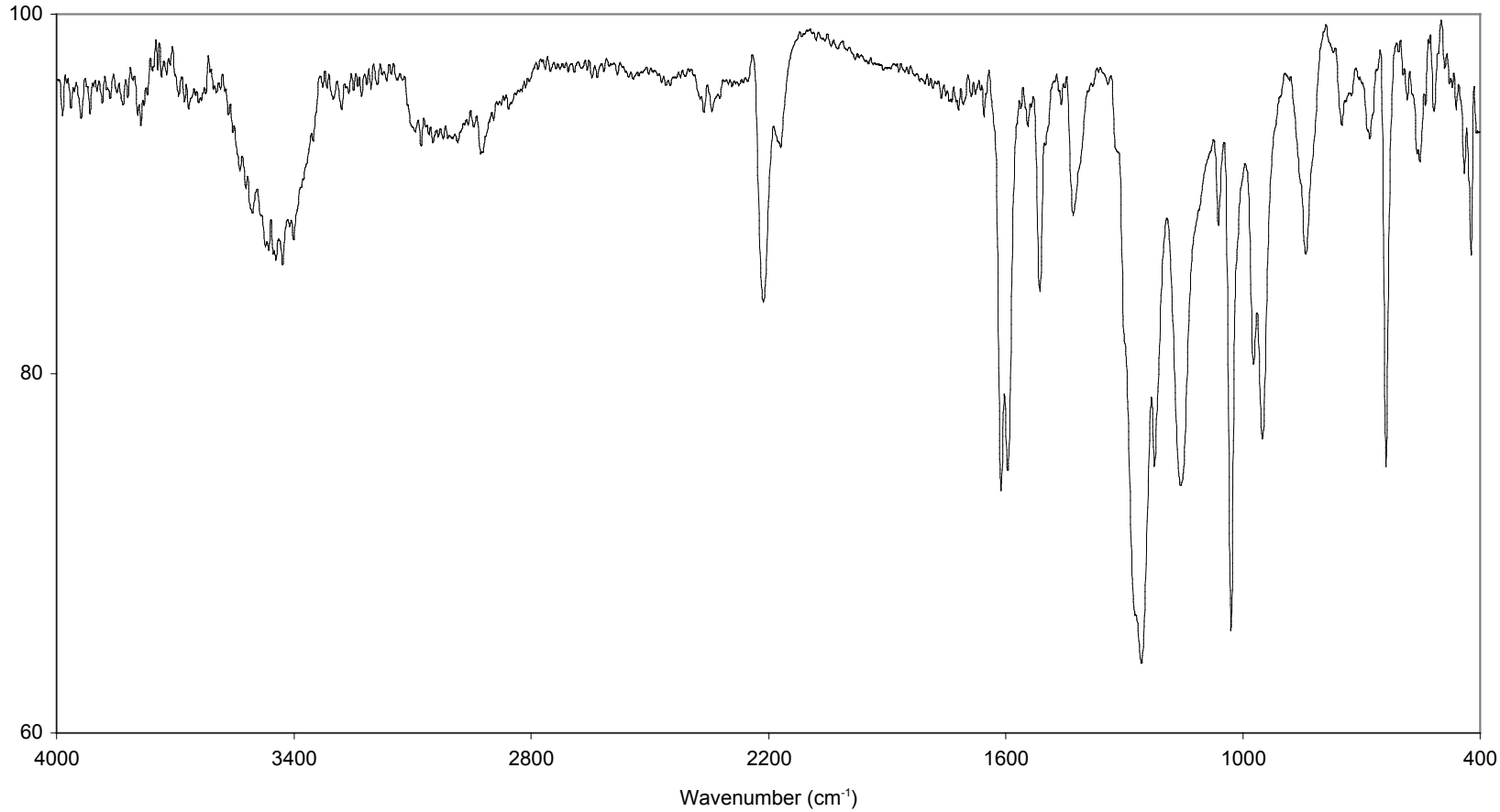

Figure S9. Infrared spectrum of **3c** in KBr.

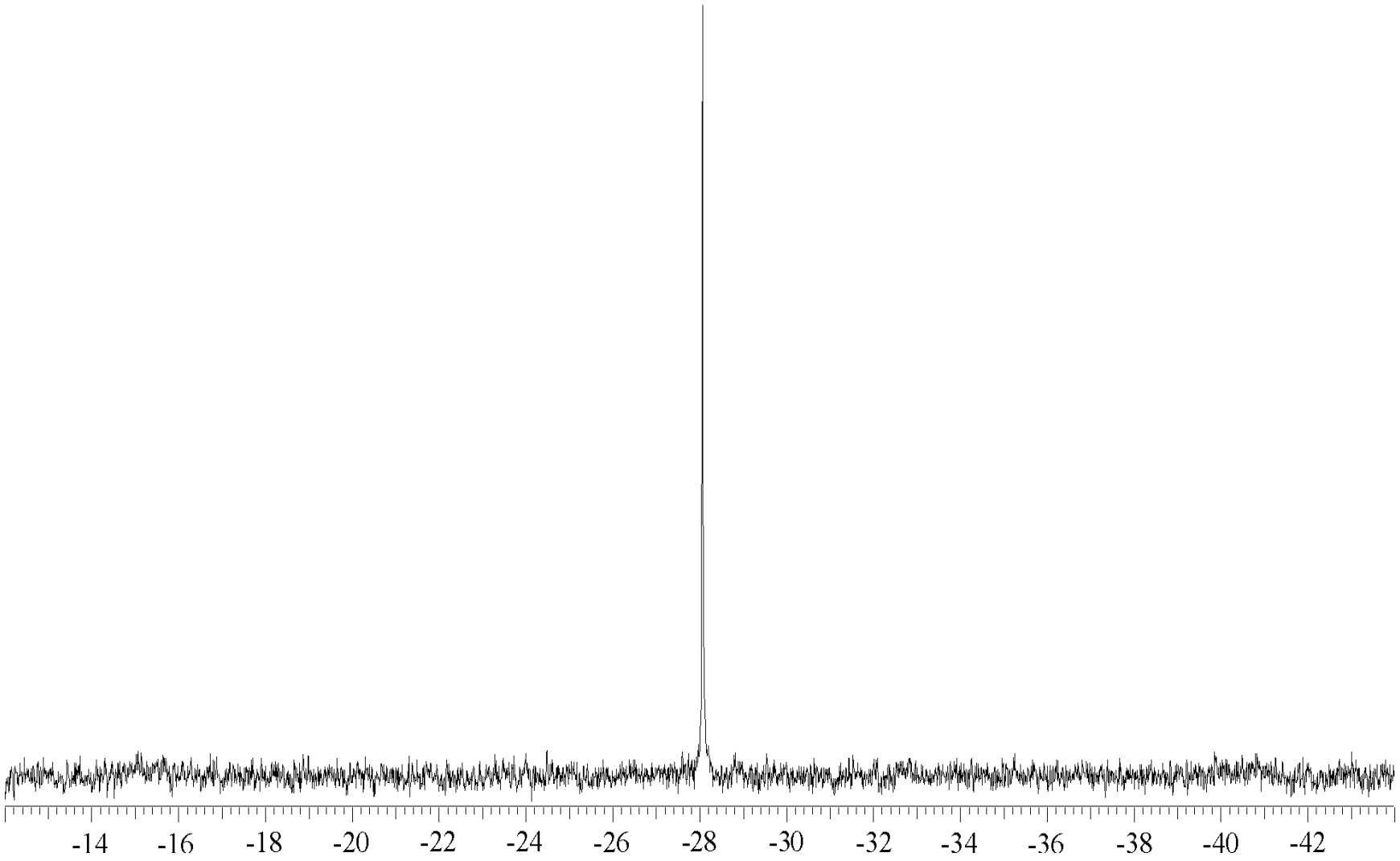

Figure S10. ^{31}P NMR spectrum of **3d**.

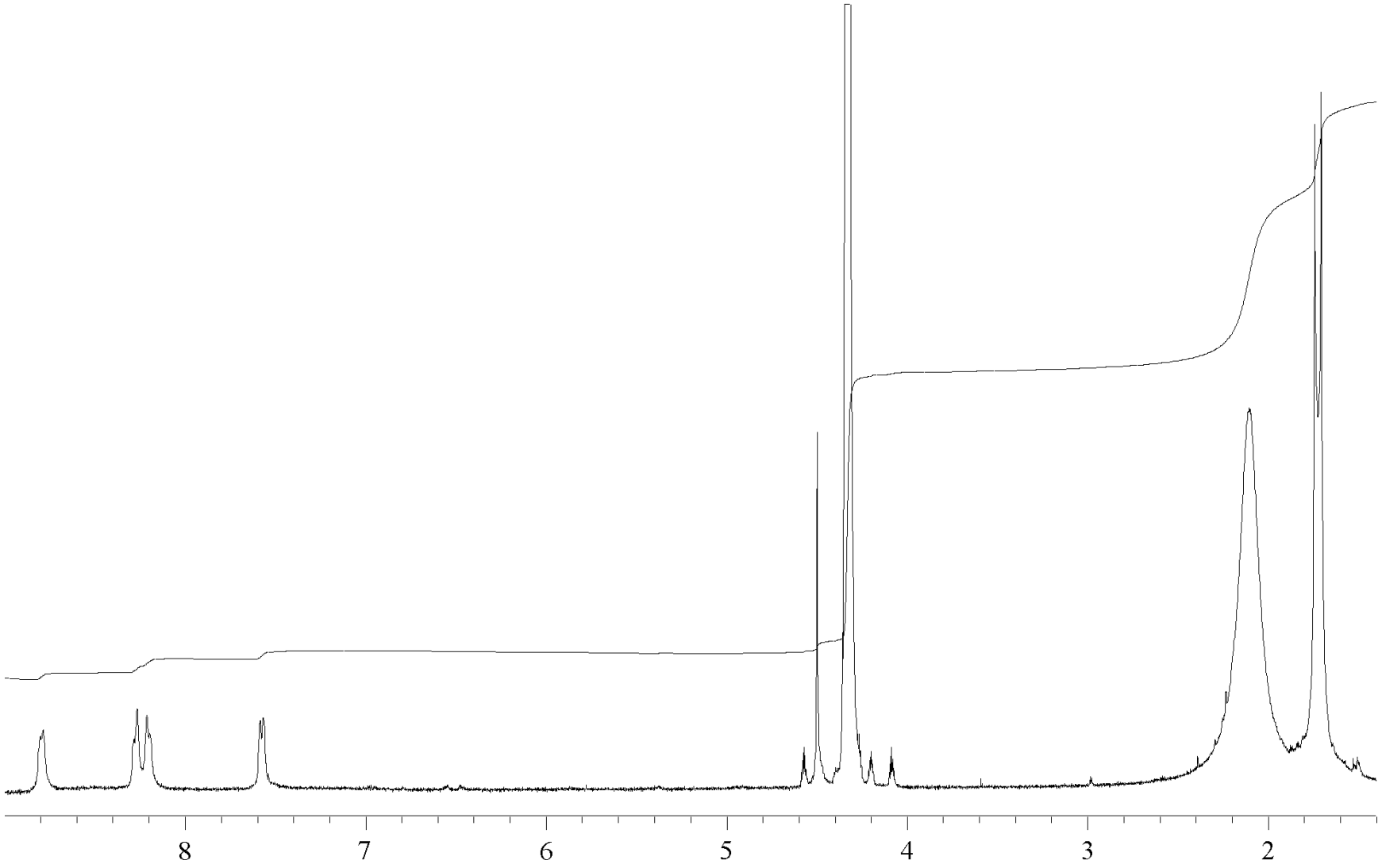

Figure S11. ^{1}H NMR spectrum of **3d**.

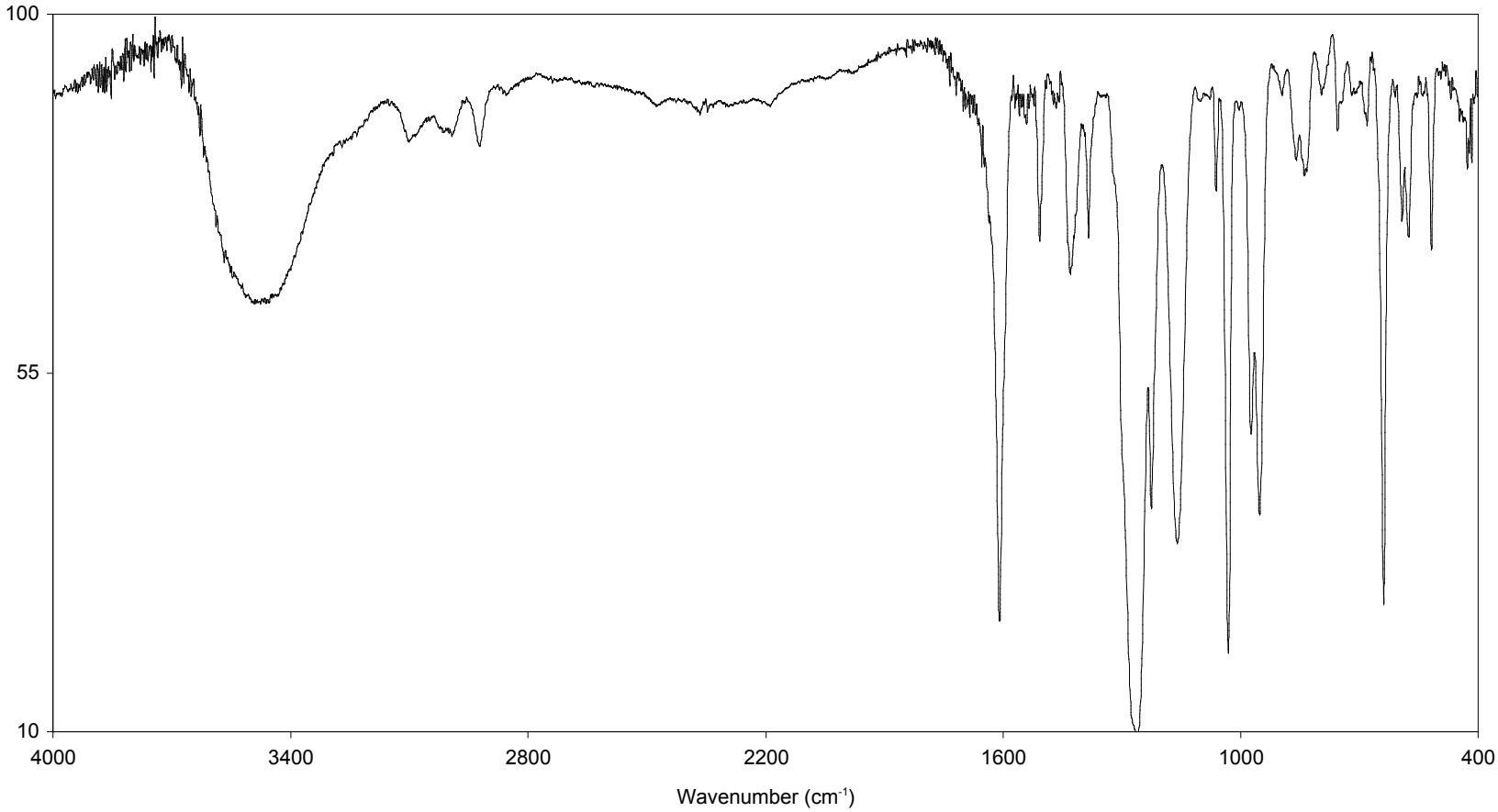

Figure S12. Infrared spectrum of **3d** in KBr.

Figure S13. DNMR of **3a**

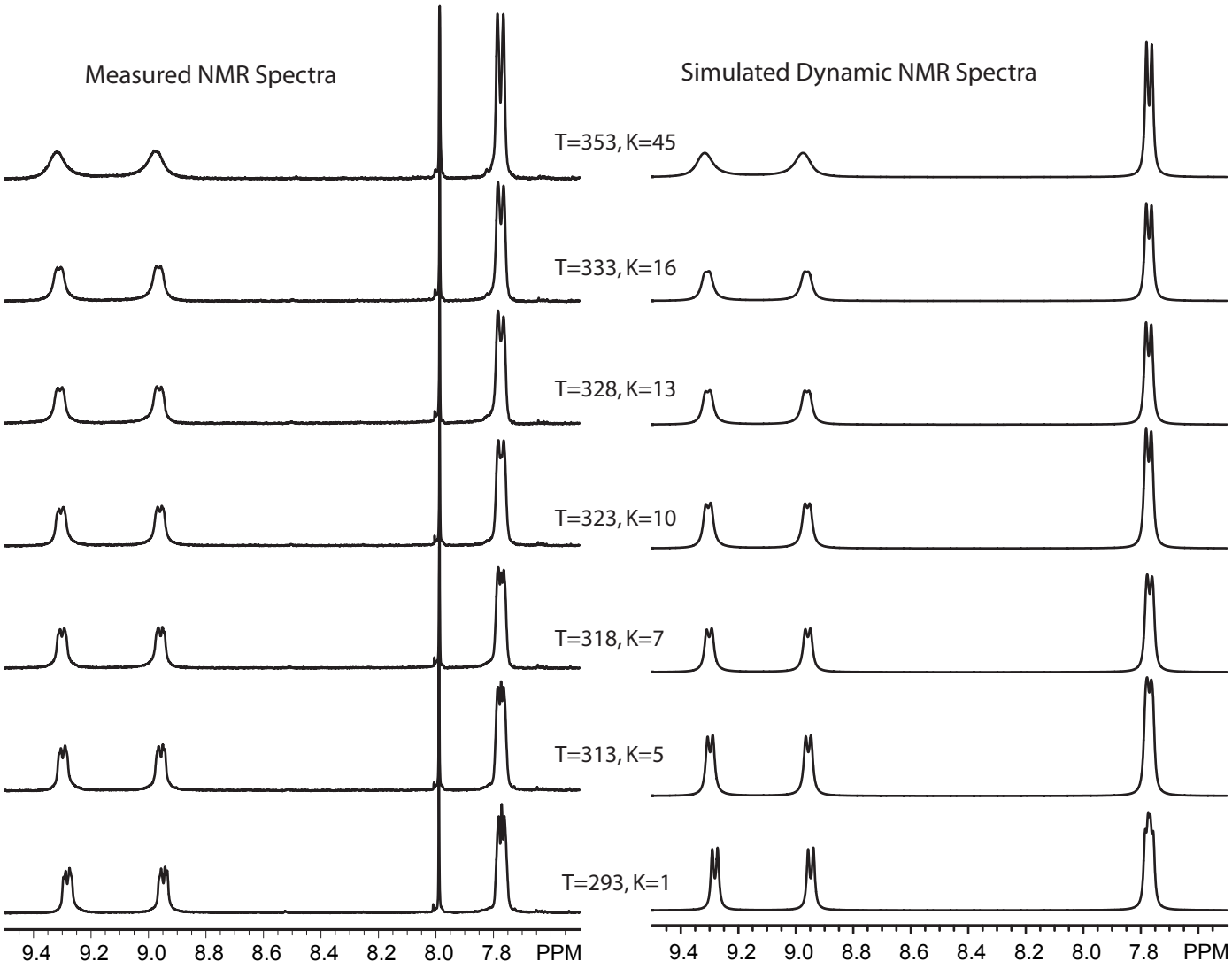

Figure S14. DNMR of **3b**

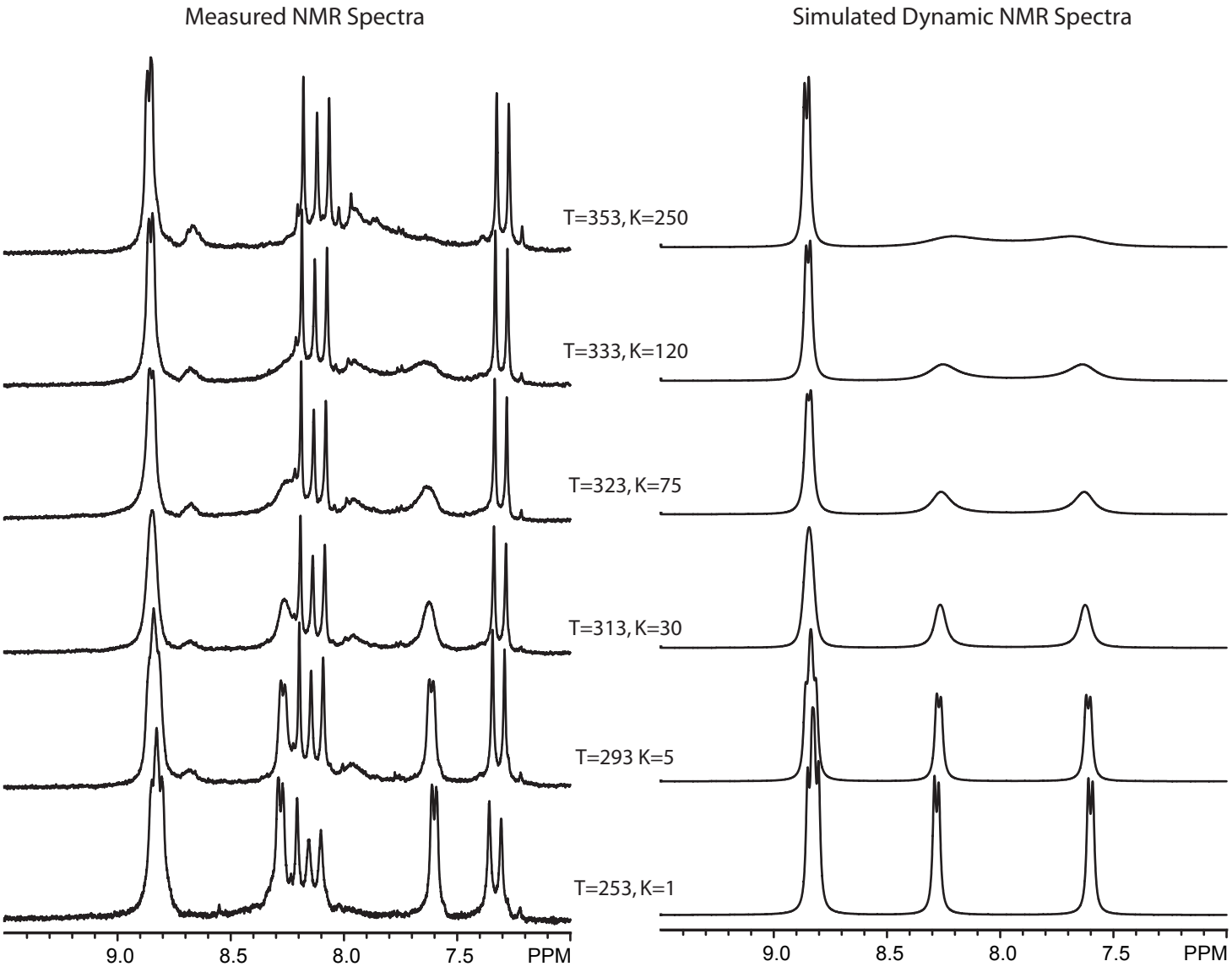

Figure S15. DNMR of **3c**

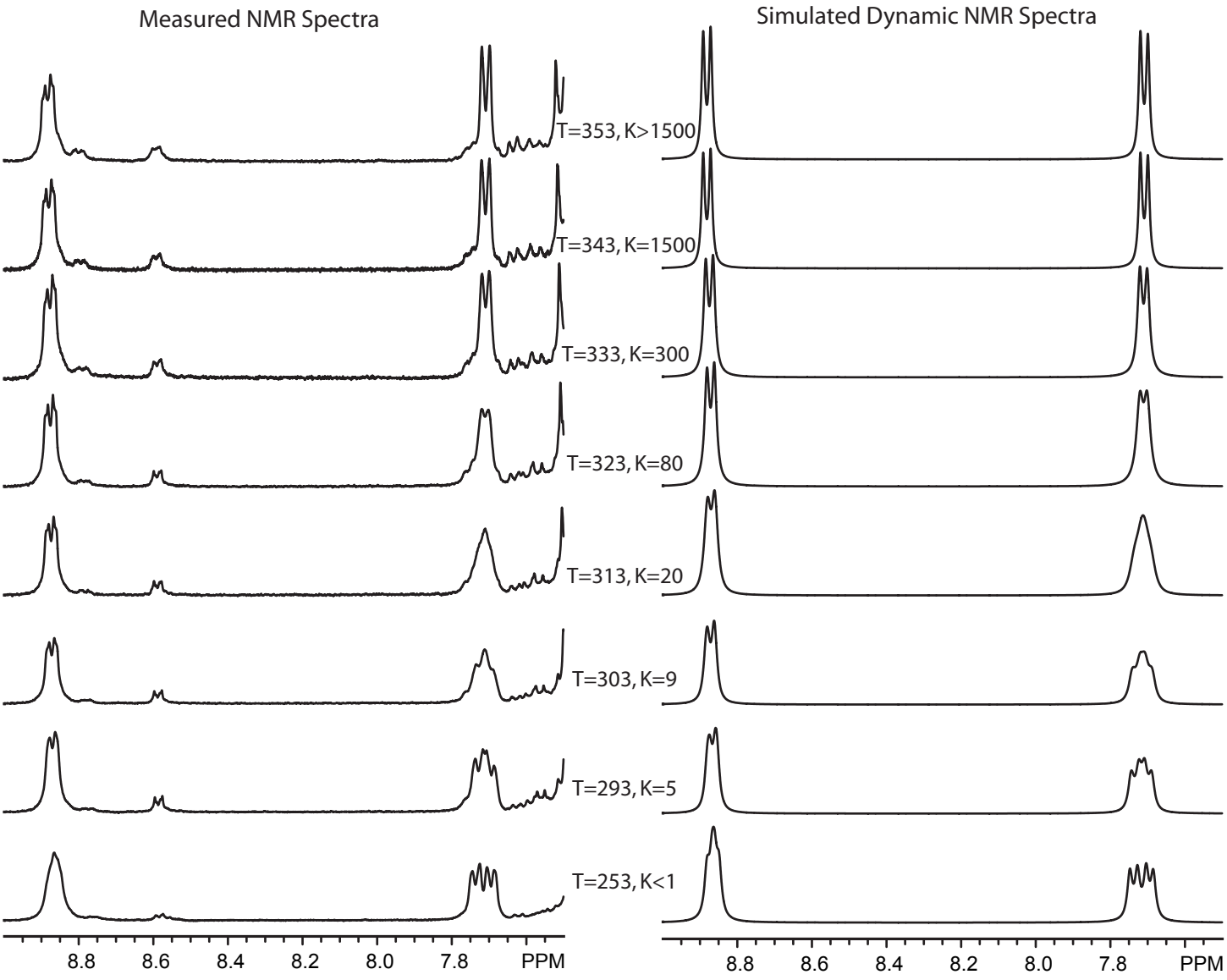

Figure 16. DNMR of **3d**

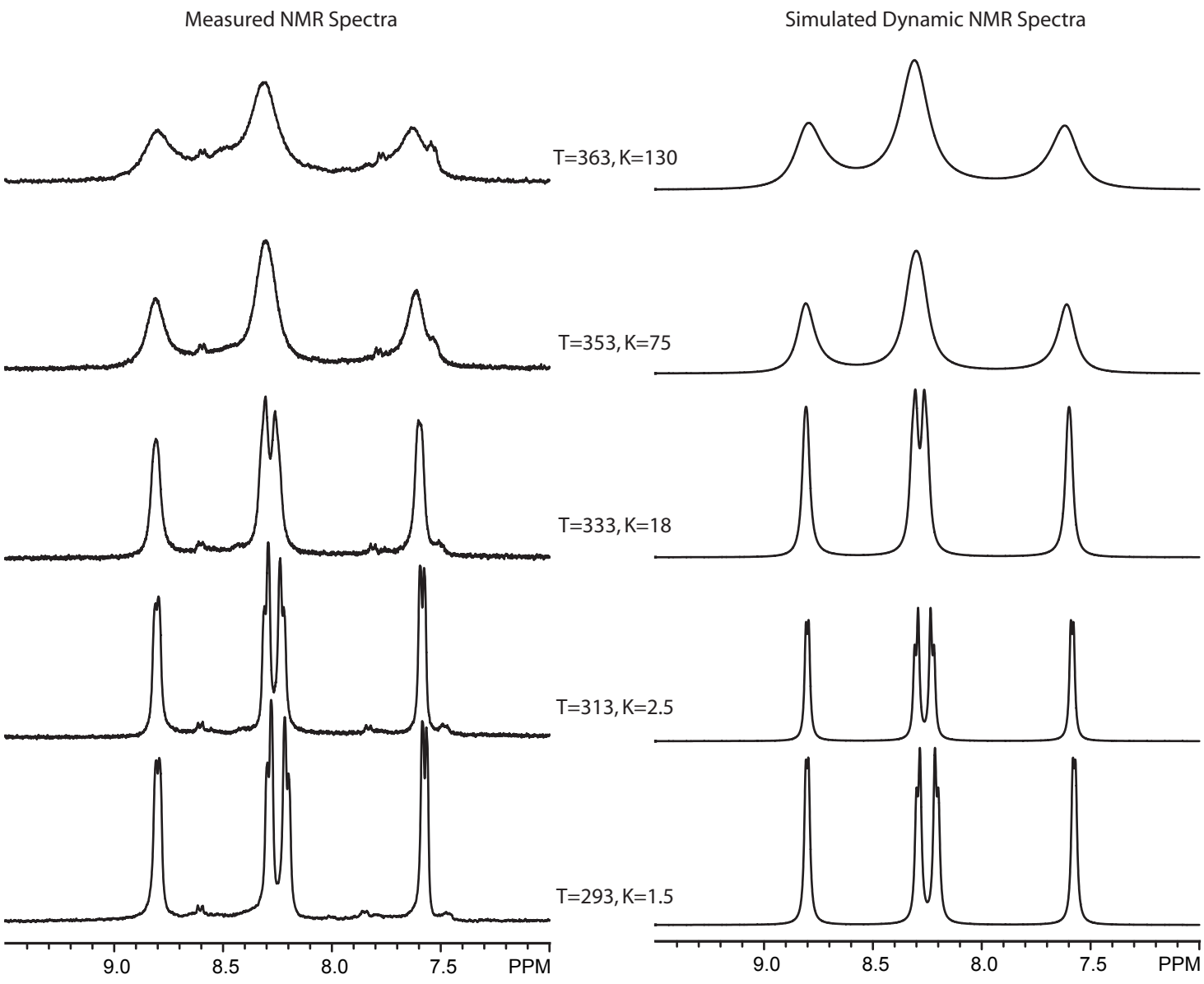

Figure S17. 1D EXCHSY (DPFGSE) chemical exchange of **3b**:

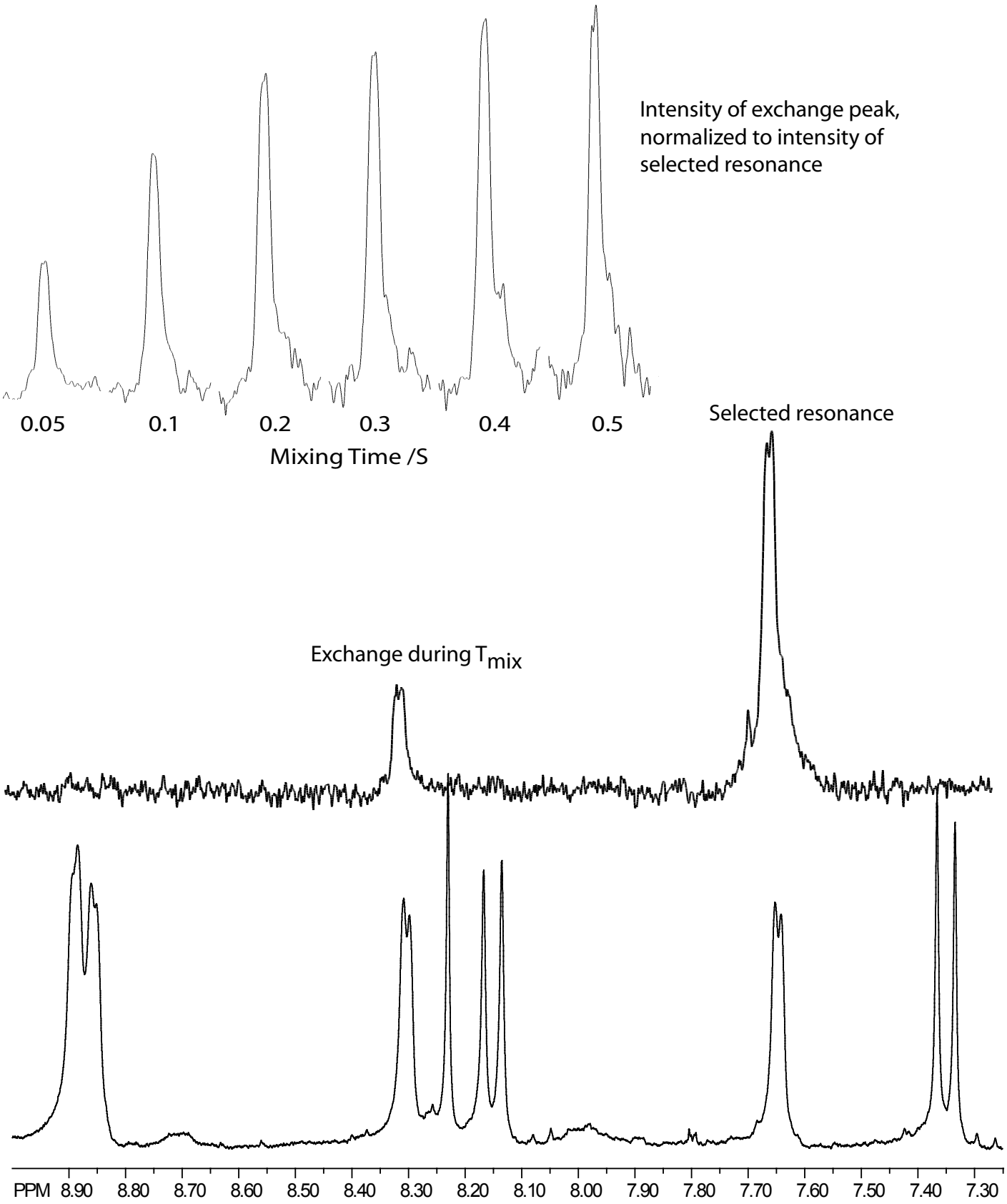

Figure S18. 2D-EXCHSY/ROESY of **3b**

UCB Varian Inova-500

Pulse Sequence: ROESY
Solvent: Nitromethane

File: 3b-1H_T20-ROESY

Relax. delay 1.000 sec
Mixing 0.200 sec
Acq. time 0.112 sec
Width 4567.3 Hz
2D Width 4567.3 Hz
8 repetitions
2 x 64 increments
OBSERVE H1, 500.3688803 MH
DATA PROCESSING
Gauss apodization 0.052 sec
F1 DATA PROCESSIN
Gauss apodization 0.008 sec
FT size 2048 x 2048

2D-EXCHSY / ROESY
Black cross peaks from exchange
Red cross peaks are NOE correlations