

Folding of an Artificial β -Sheet in Competitive Solvents

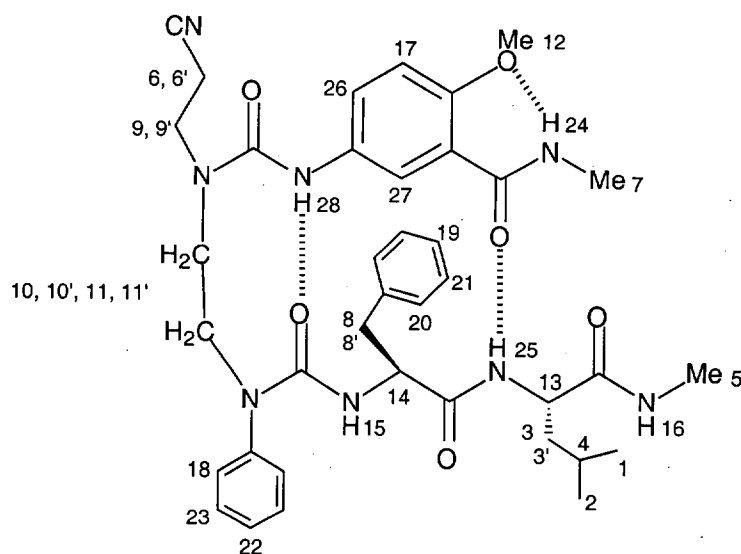
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University of California, Irvine
Irvine, CA 92697-2025

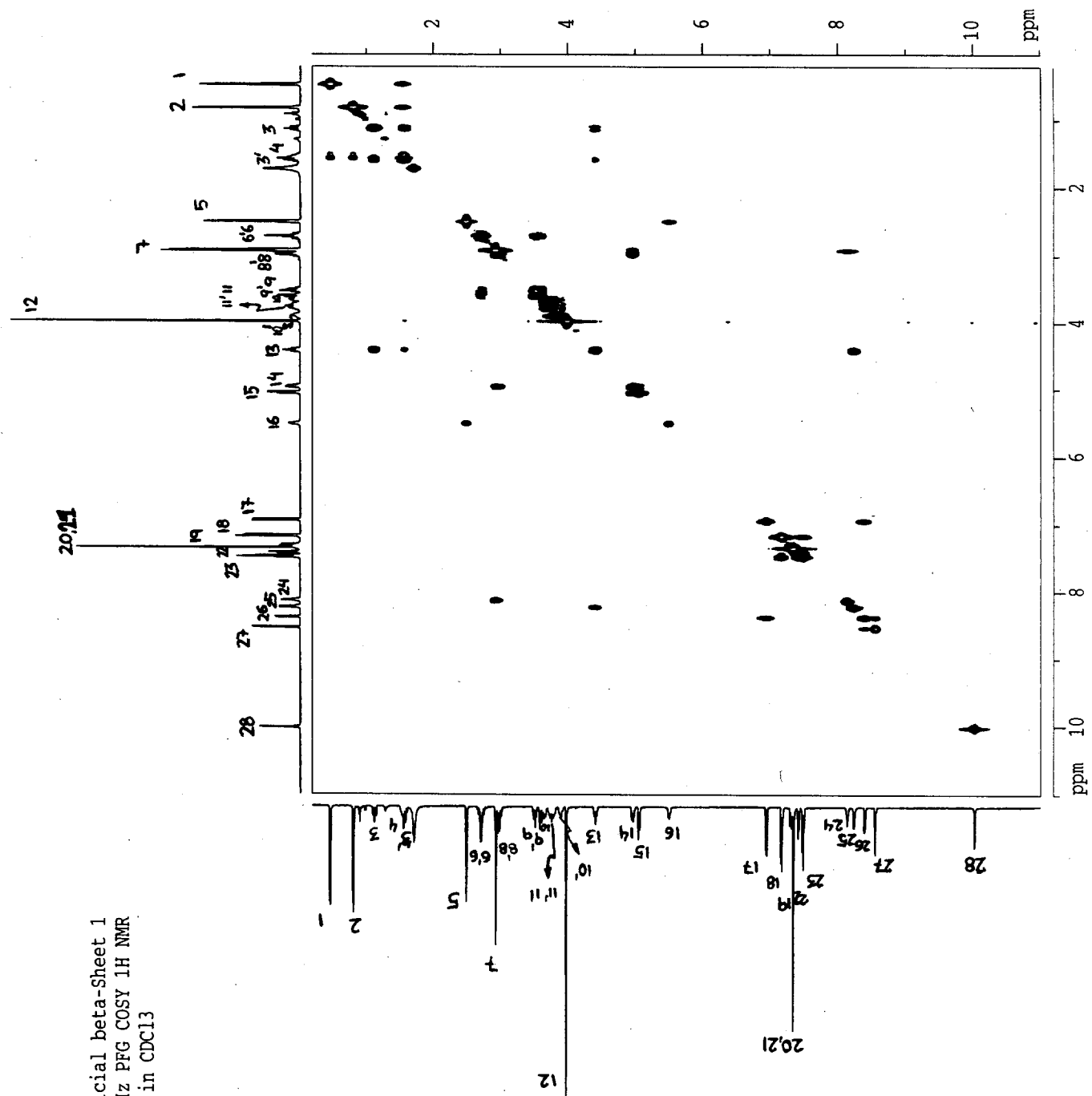
Supporting Information: PFG COSY and Tr-ROESY spectra of artificial β -sheet 1 in CDCl_3 , CD_3OD , CD_3OH , 50% v/v $\text{CD}_3\text{OD}-\text{D}_2\text{O}$, 50% v/v $\text{CD}_3\text{OH}-\text{H}_2\text{O}$, and CD_3SOCD_3 solution (59 pages).

Solvent	PFG COSY	Tr-ROESY
CDCl_3	pp 2-6	pp 29-33
CD_3OD	pp 7-9	pp 34-38
CD_3OH	pp 10-14	pp 39-44
$\text{CD}_3\text{OD}-\text{D}_2\text{O}$	pp 15-17	pp 45-49
$\text{CD}_3\text{OH}-\text{H}_2\text{O}$	pp 18-22	pp 50-54
CD_3SOCD_3	pp 23-28	pp 55-59

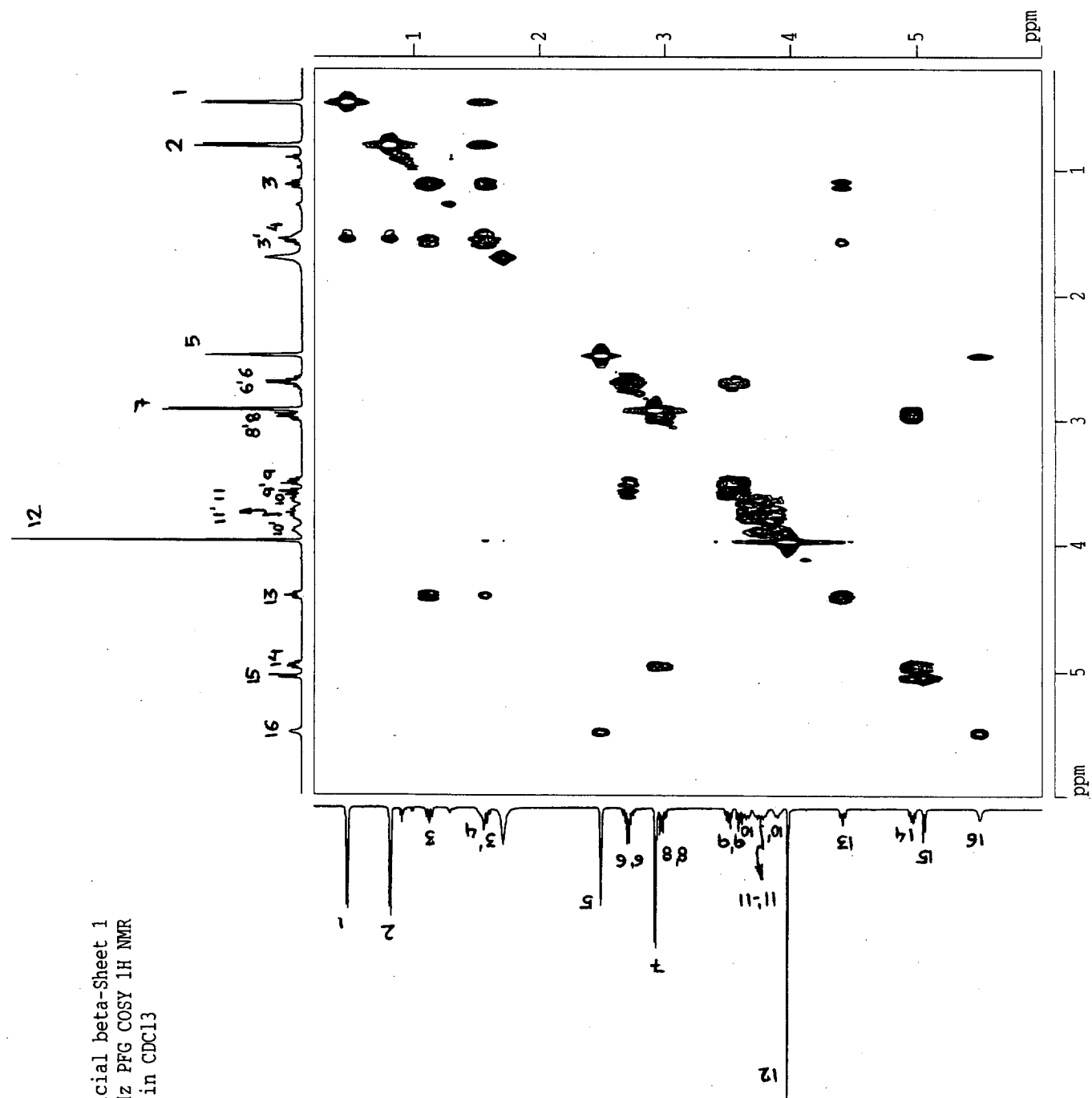
Spectra are numbered according to the following diagram:



2

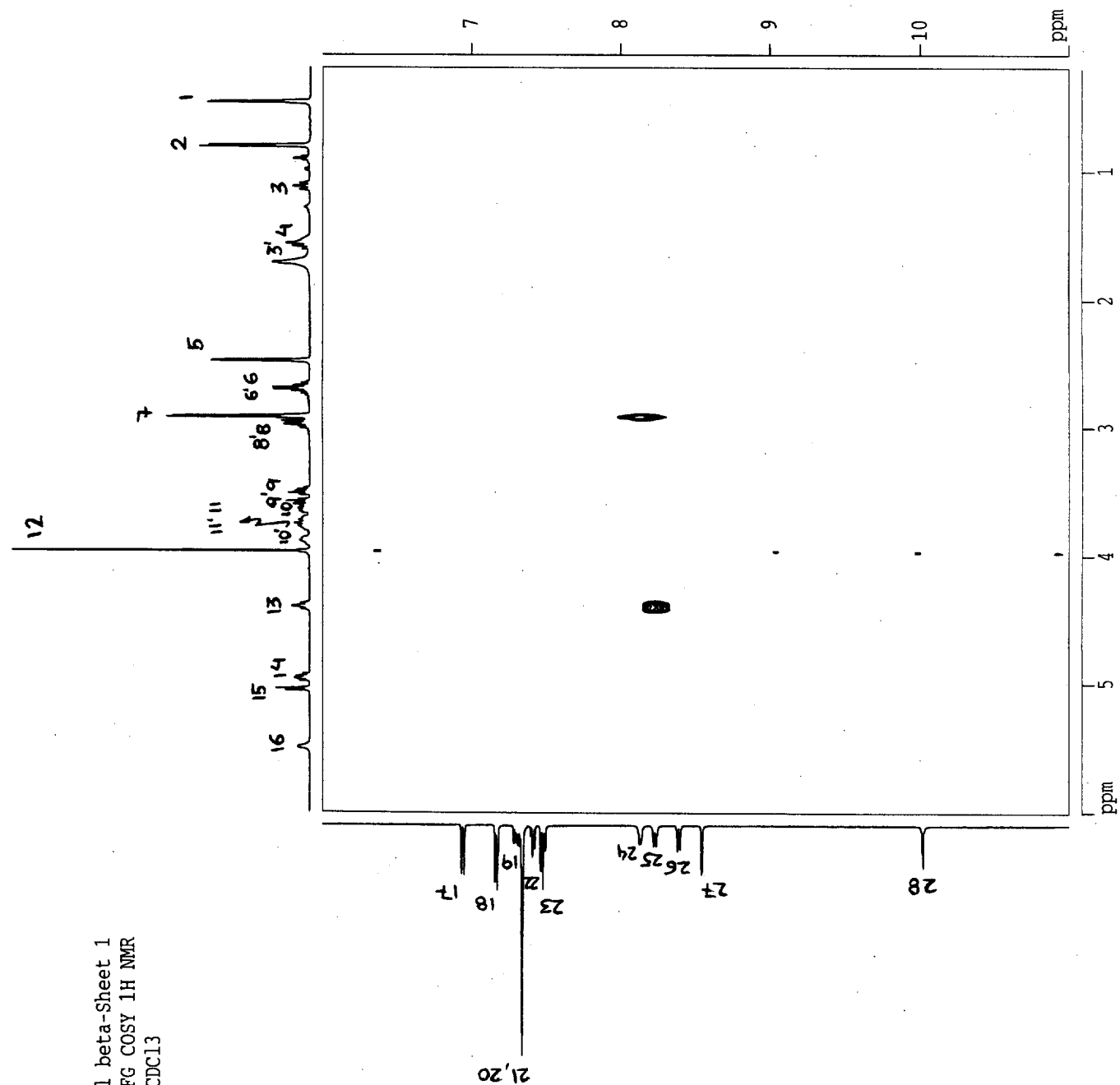


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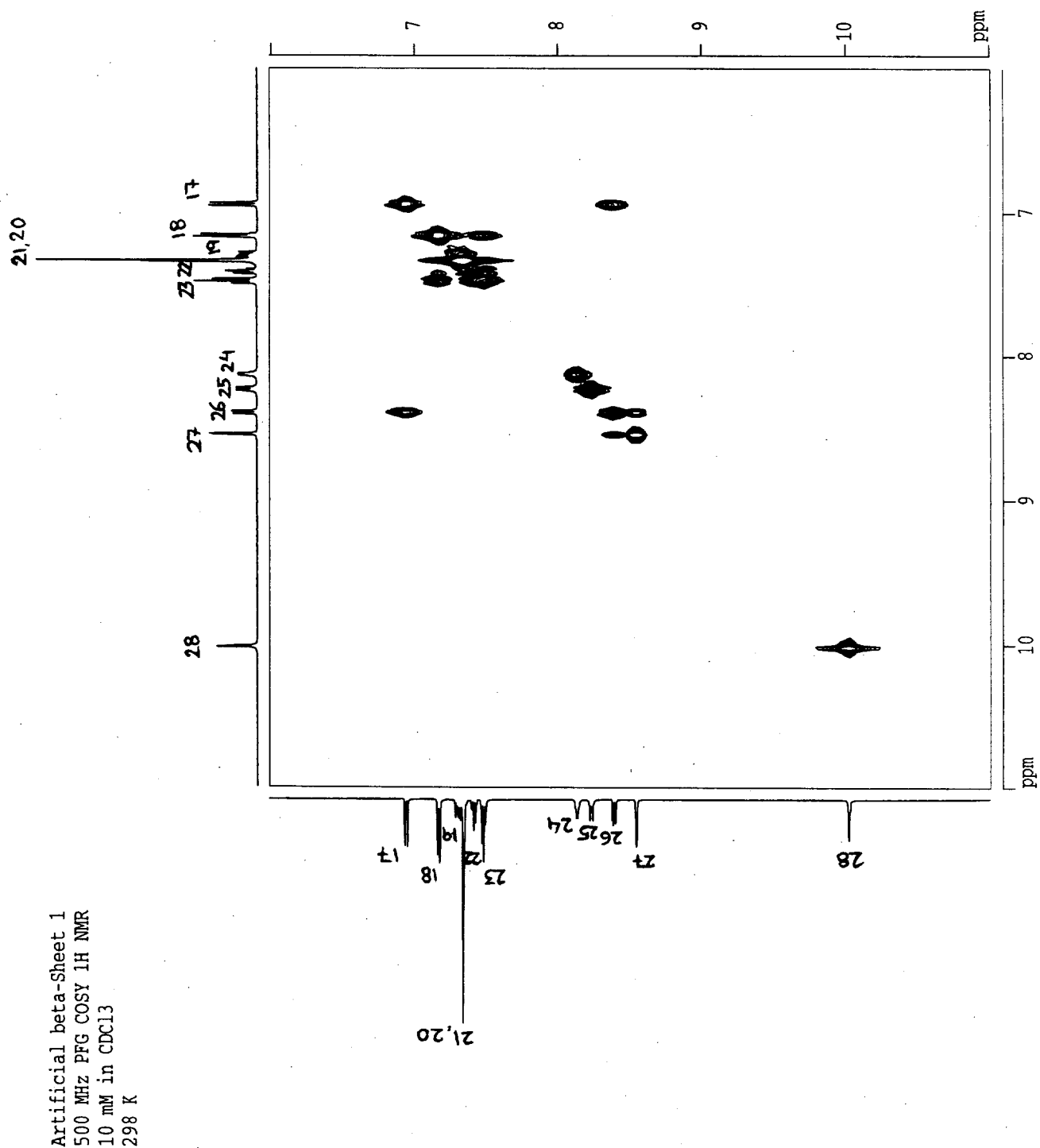


Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CDCl₃
298 K

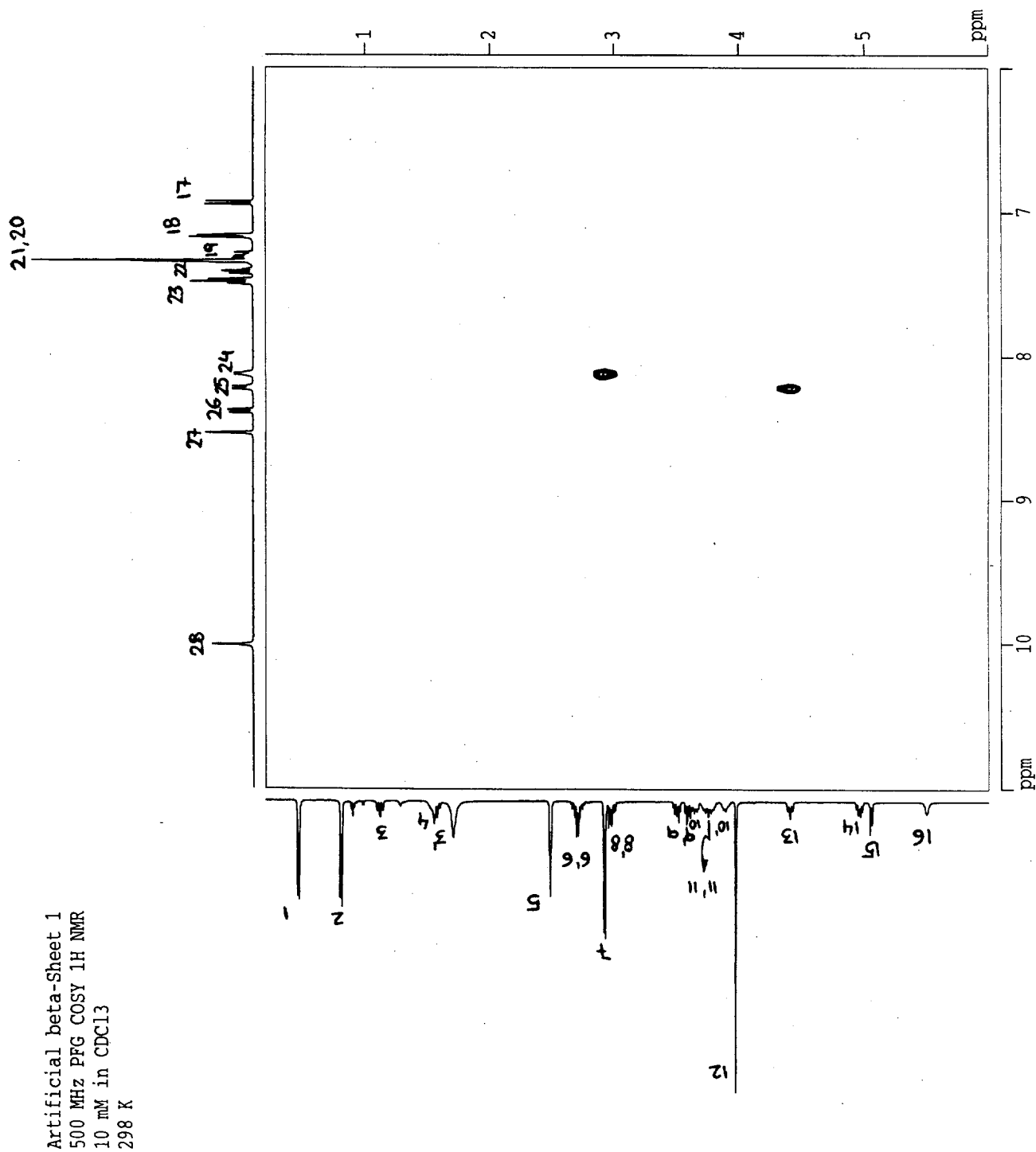
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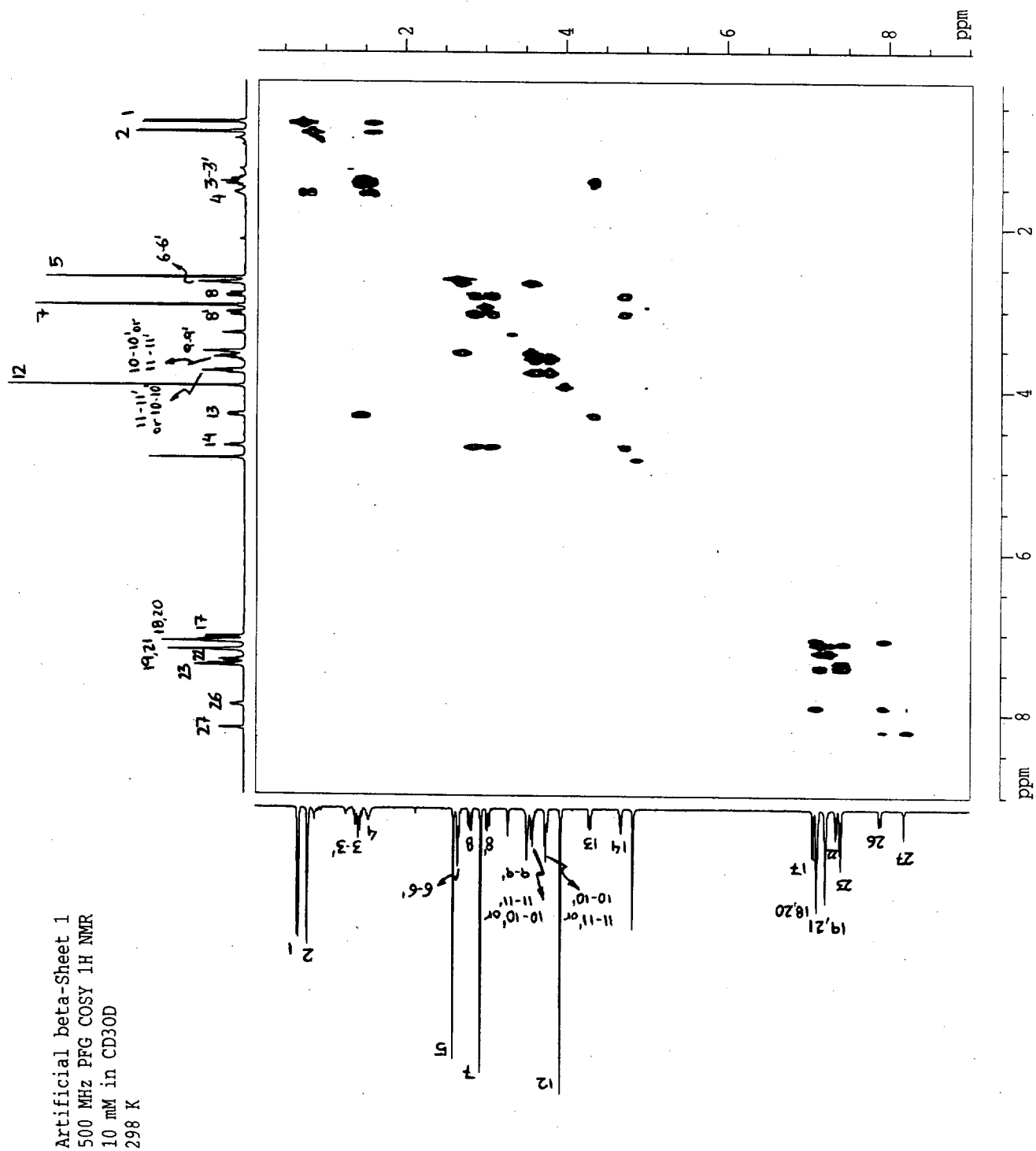
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6



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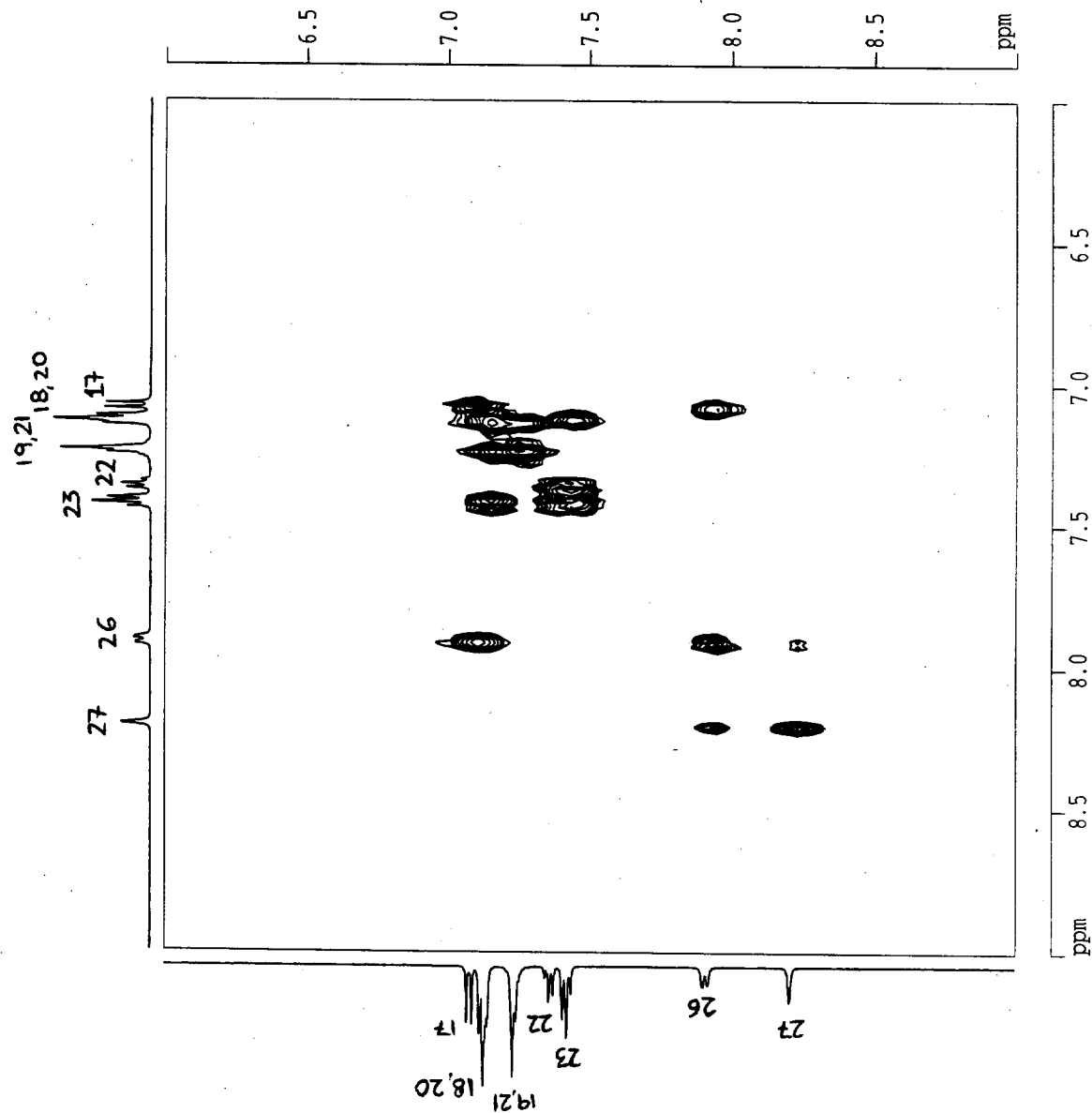


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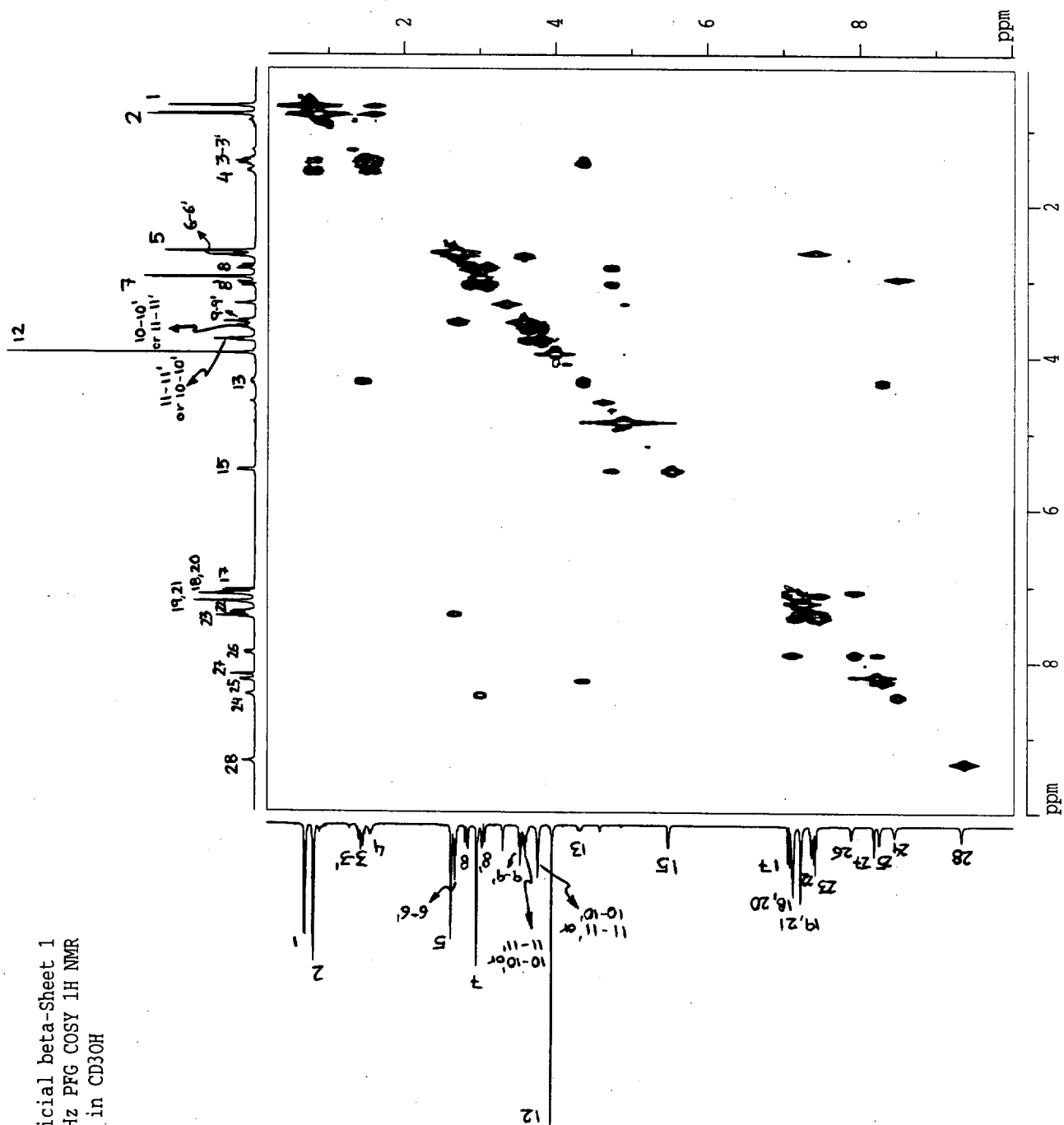


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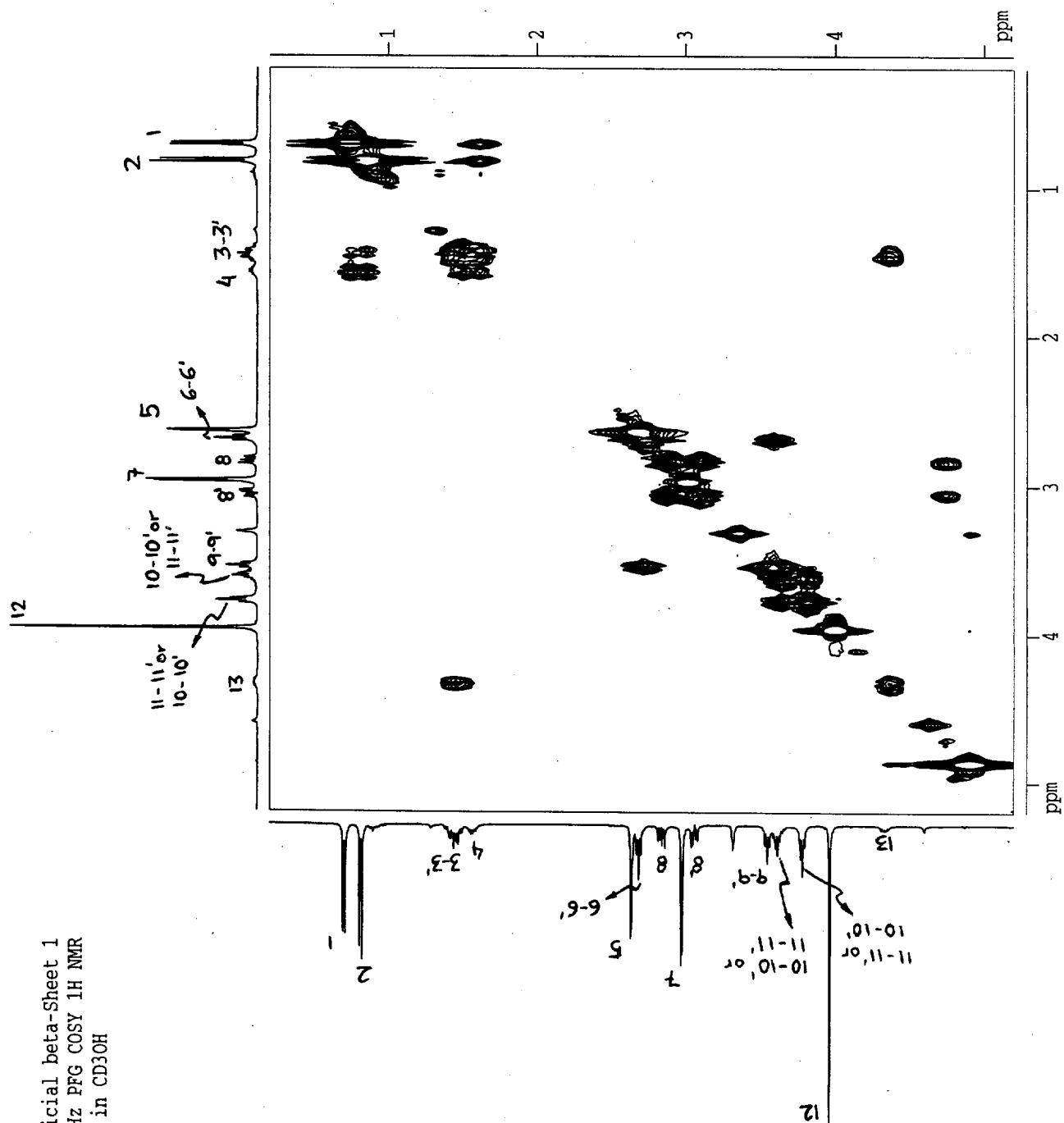
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OD
298 K



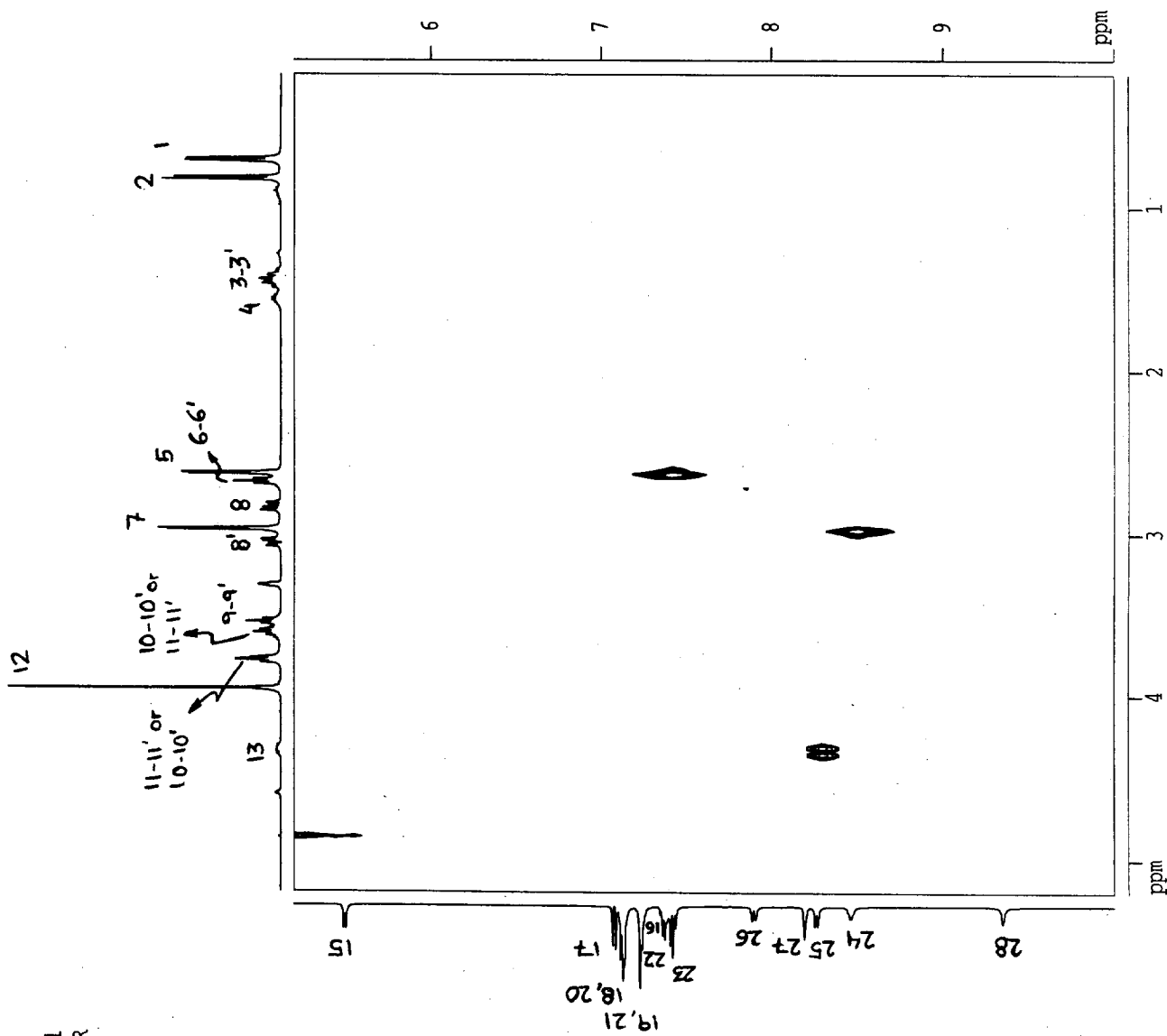
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Artificial beta-Sheet 1
 500 MHz PFG COSY 1H NMR
 10 mM in CD3OH
 298 K



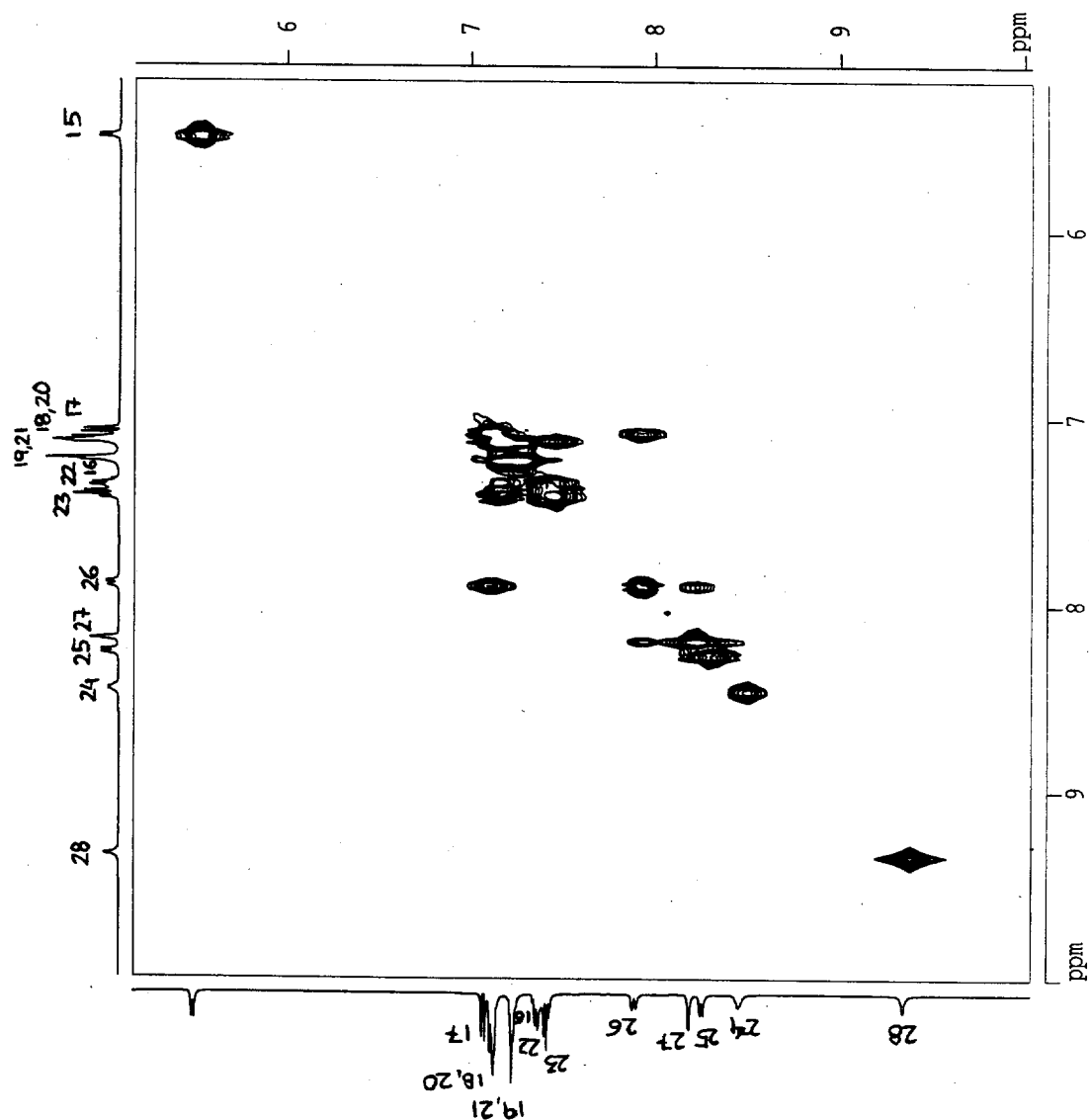
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Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OH
298 K

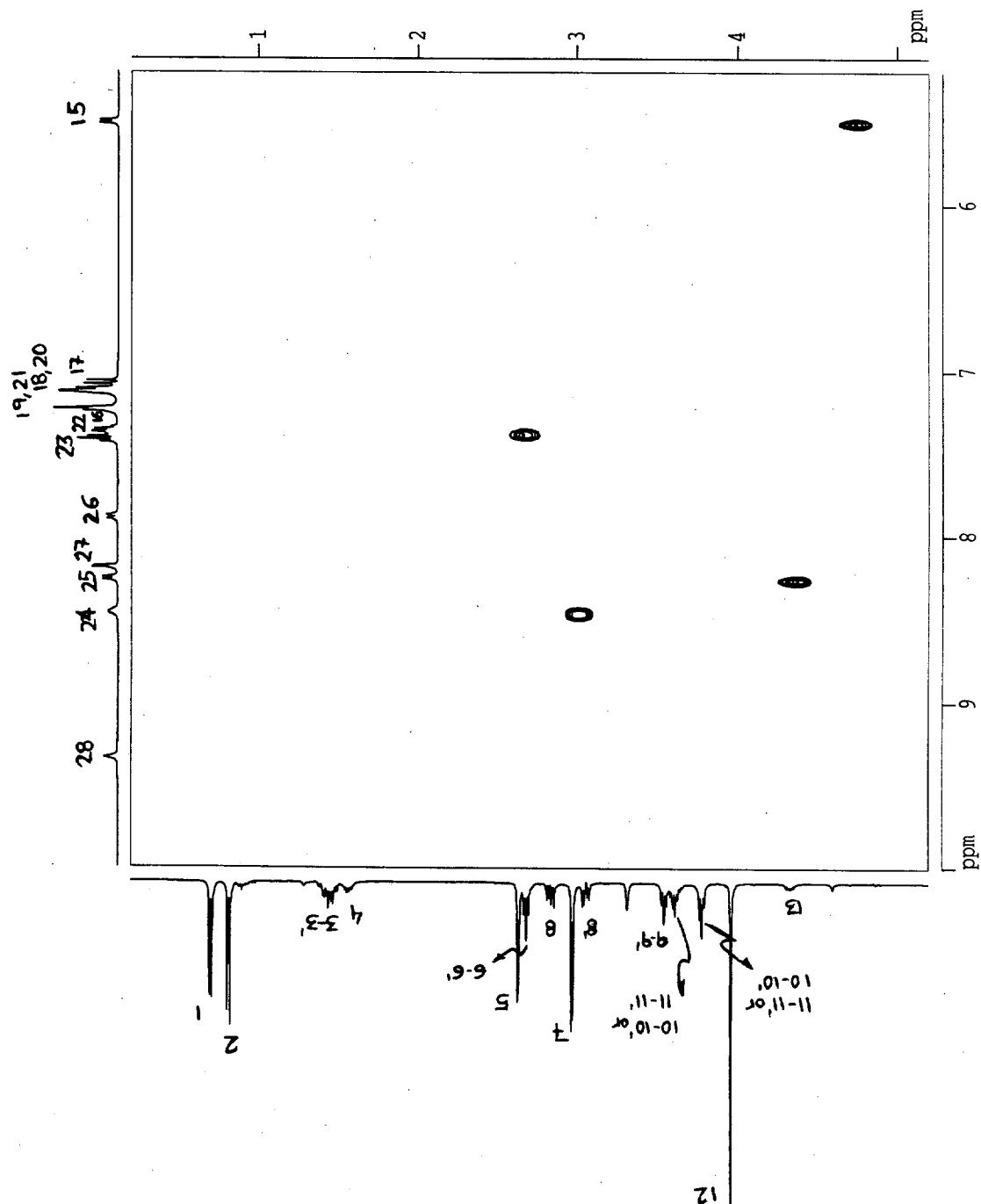
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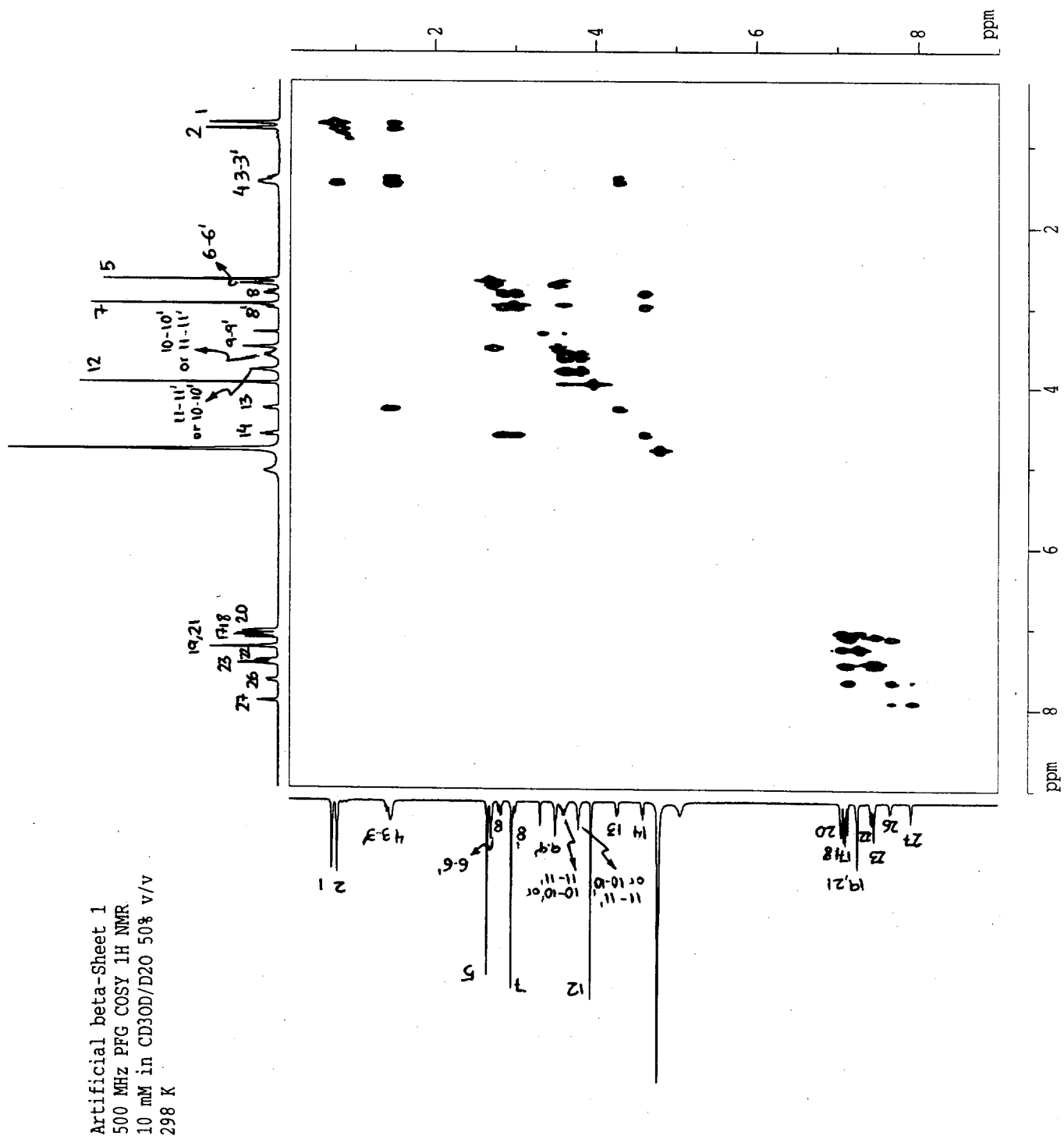
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OH
298 K



14

Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OH
298 K



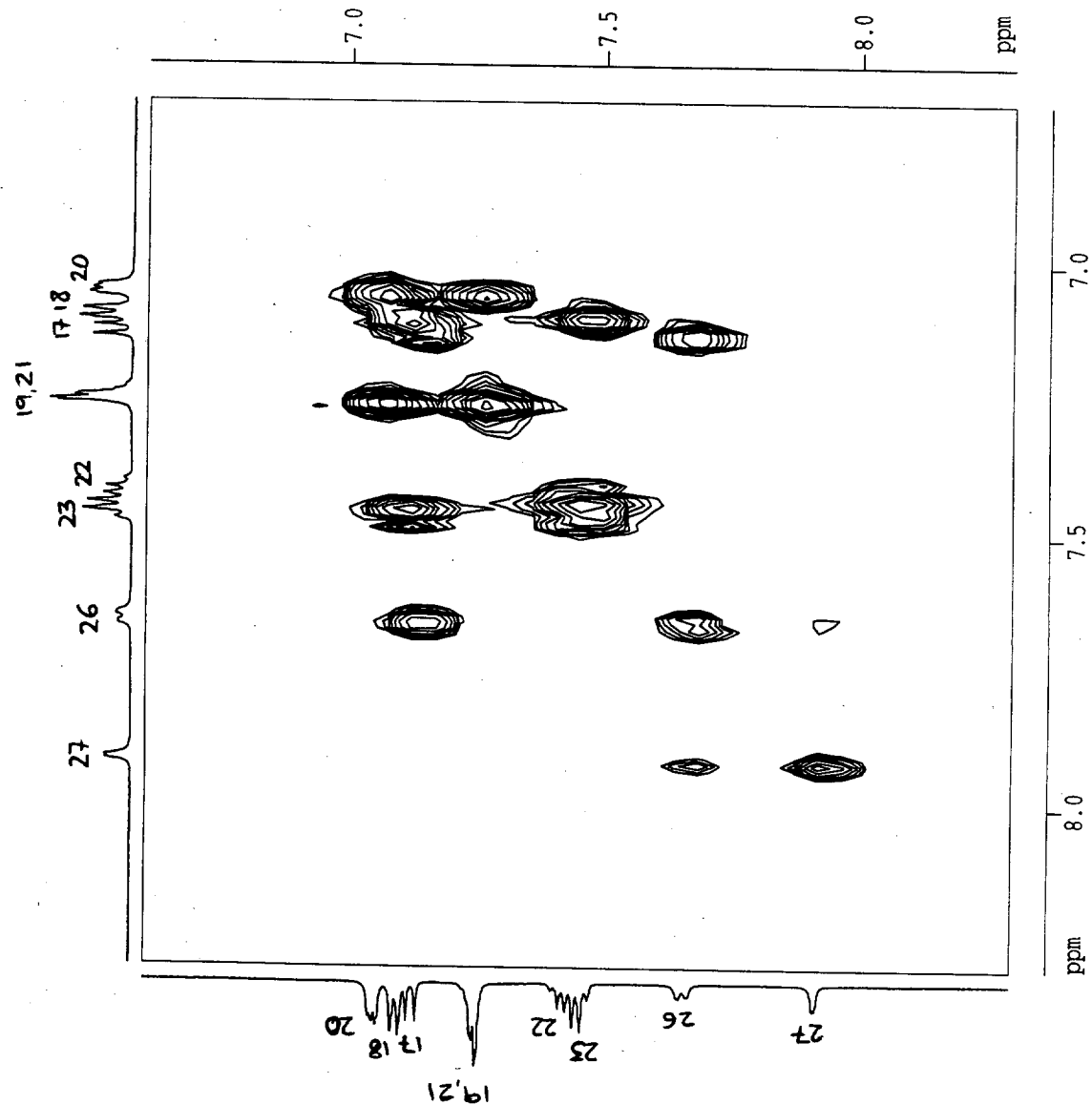


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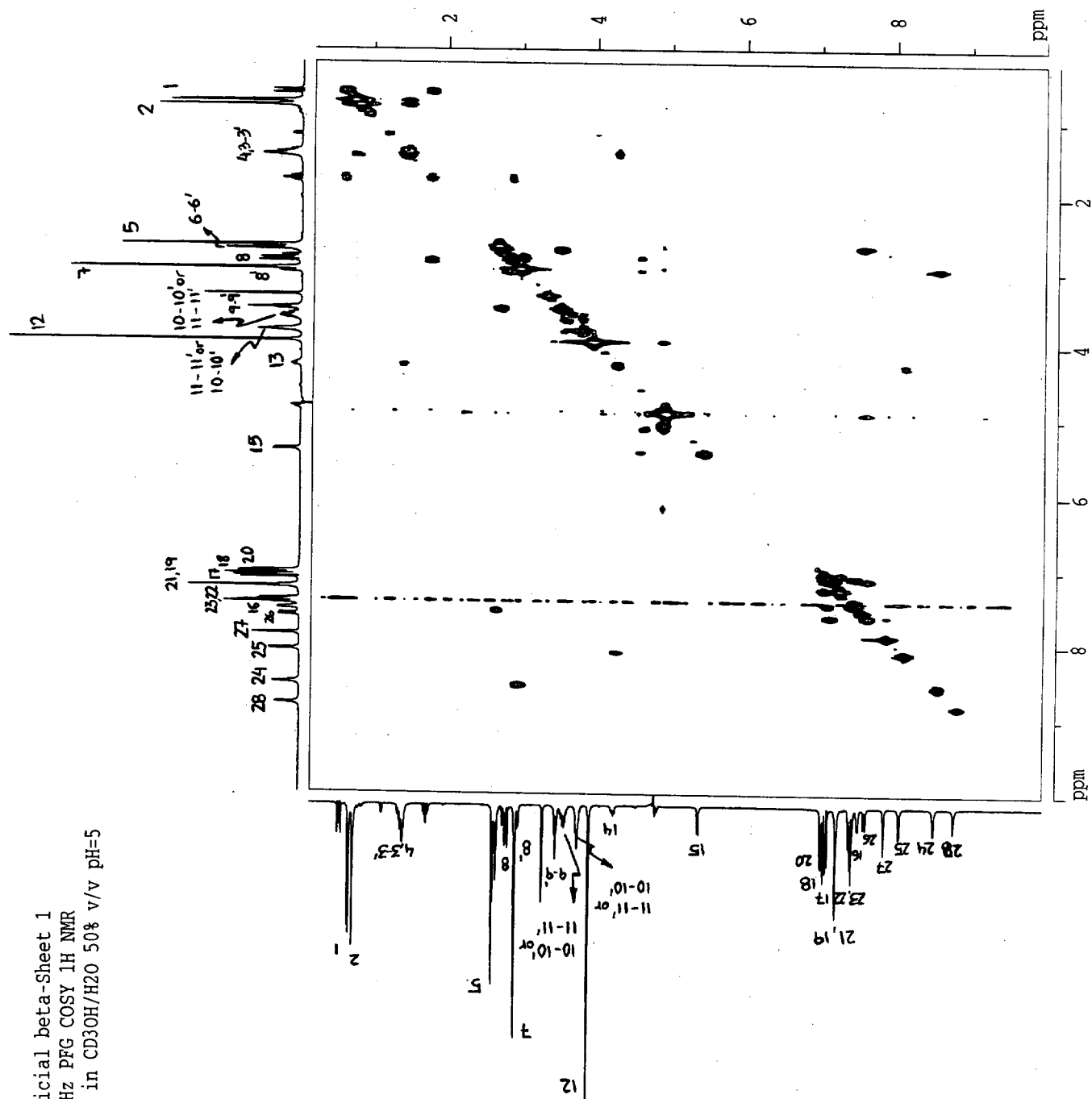


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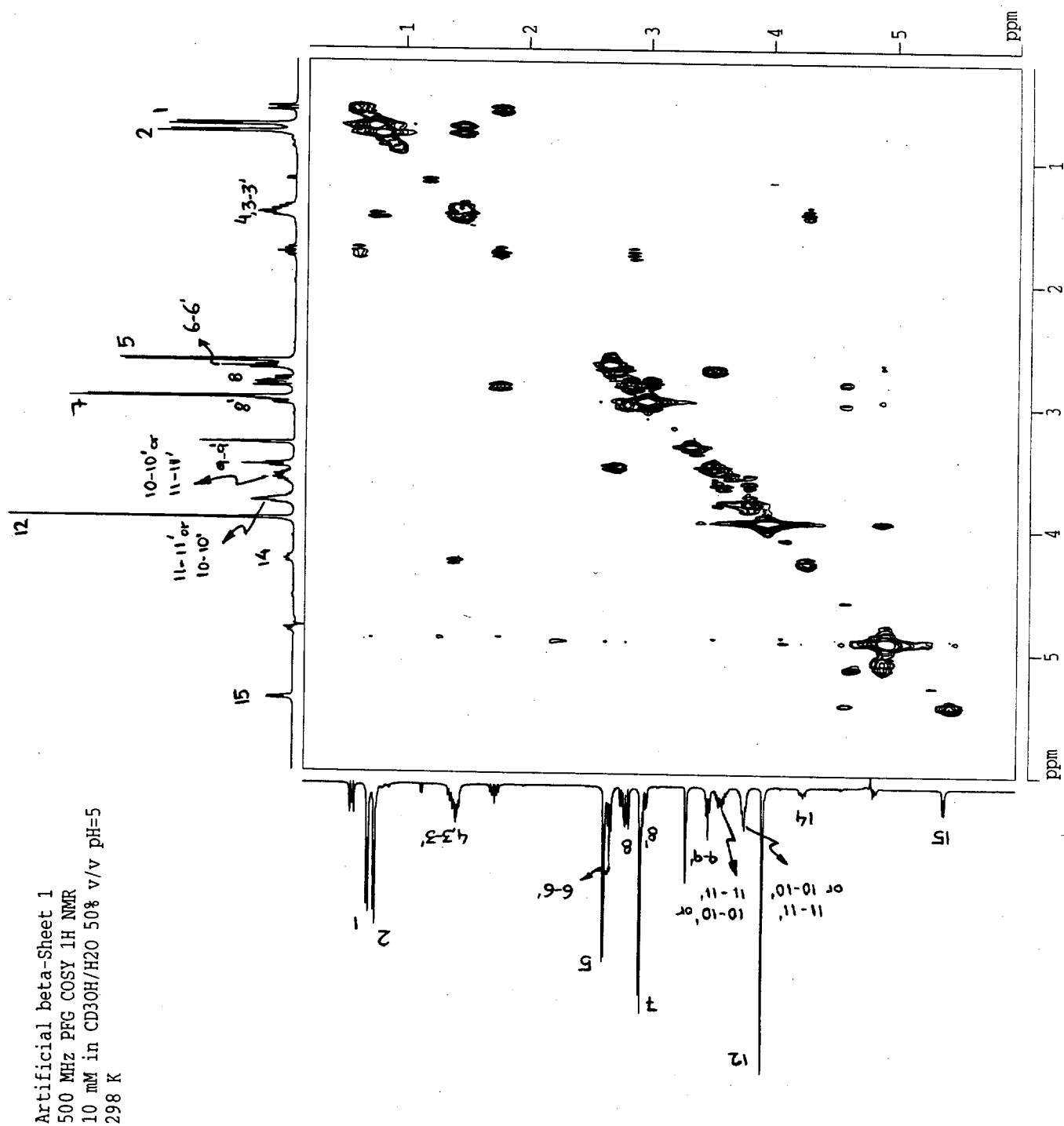
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OD/D2O 50% v/v
298 K



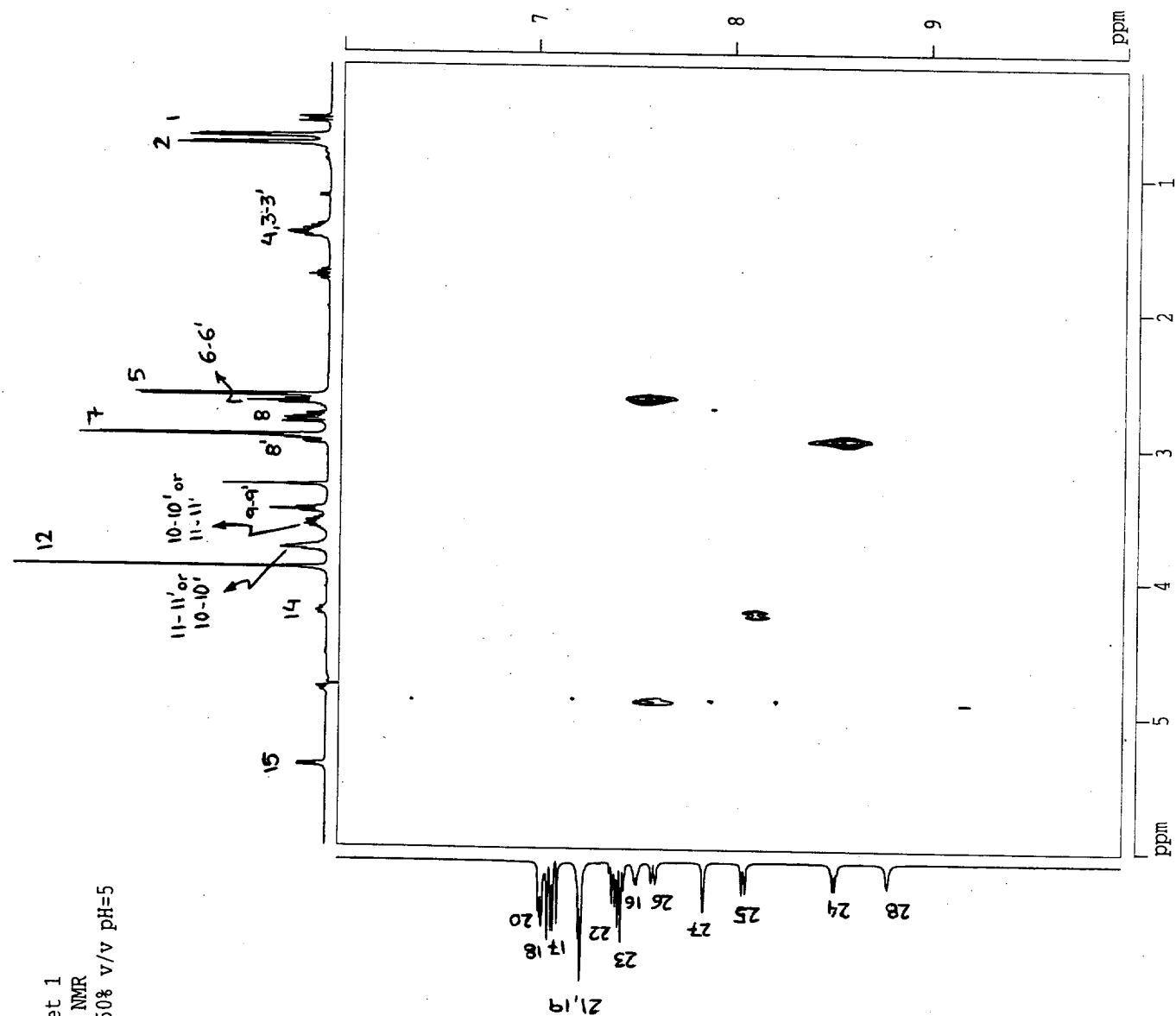
Artificial beta-Sheet 1
 500 MHz PFG COSY 1H NMR
 10 mM in CD3OH/H2O 50% v/v pH=5
 298 K



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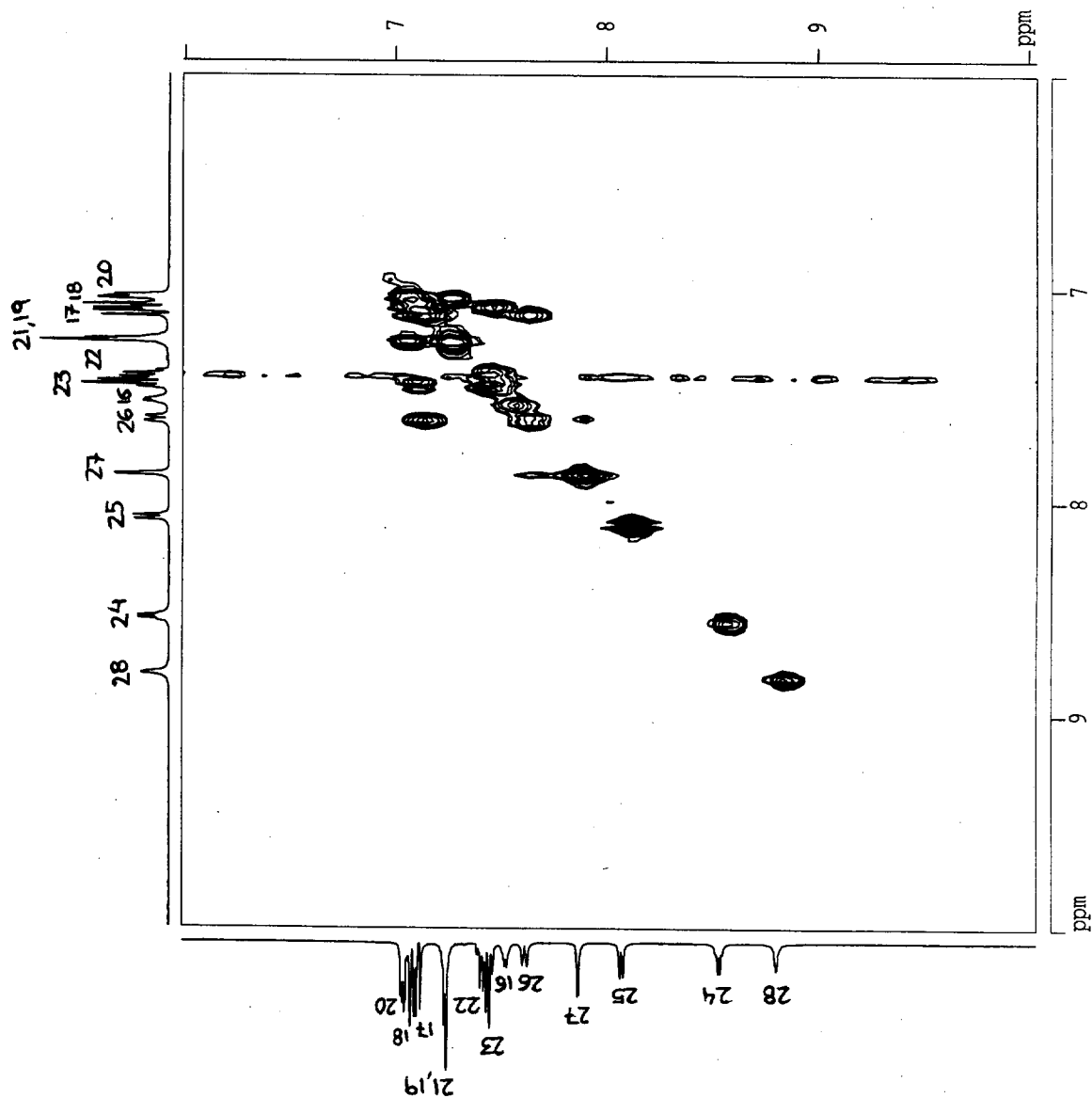


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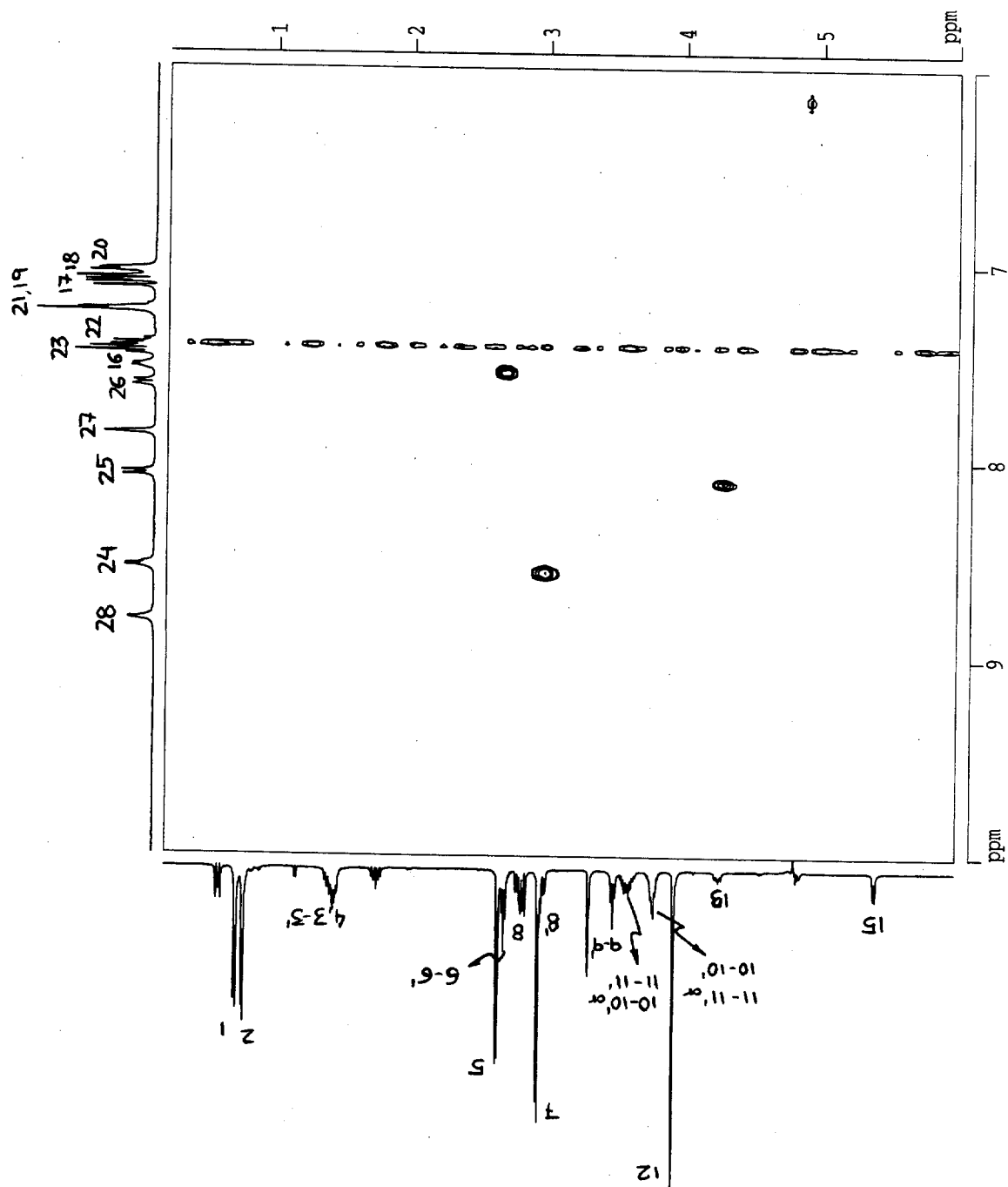
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Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OH/H2O 50% v/v pH=5
298 K

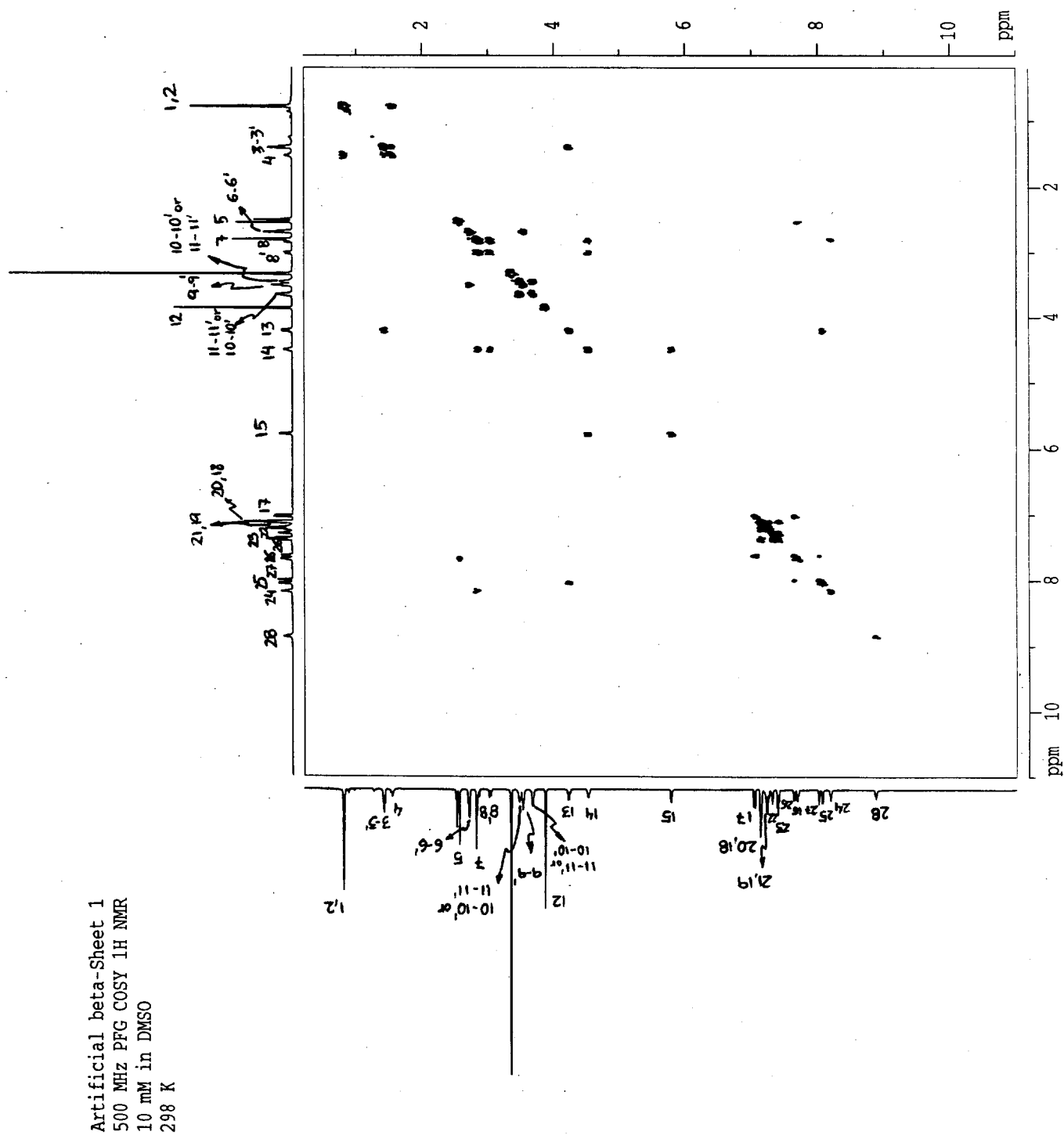


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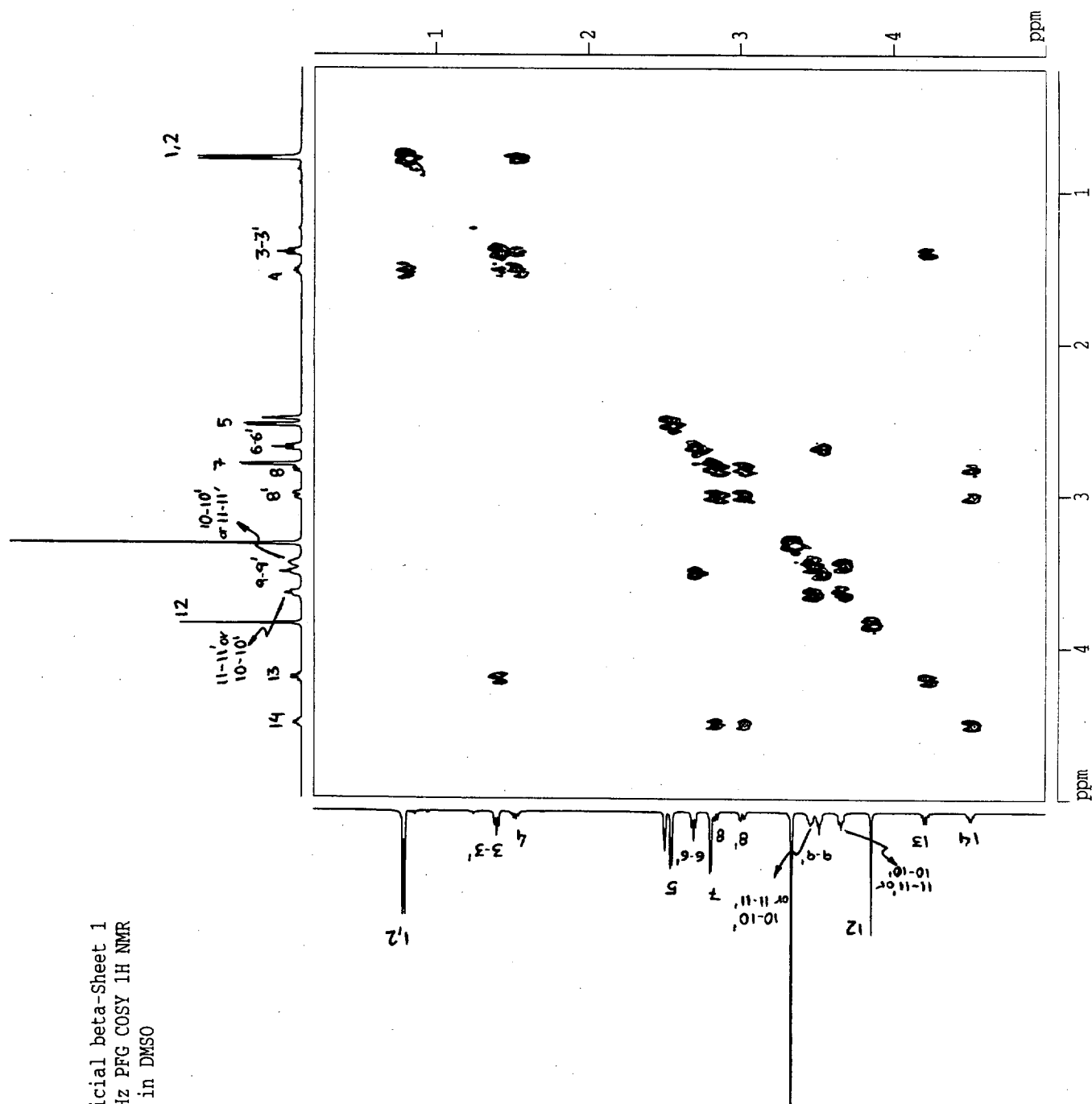
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in CD3OH/H2O 50% v/v pH=5
298 K



23

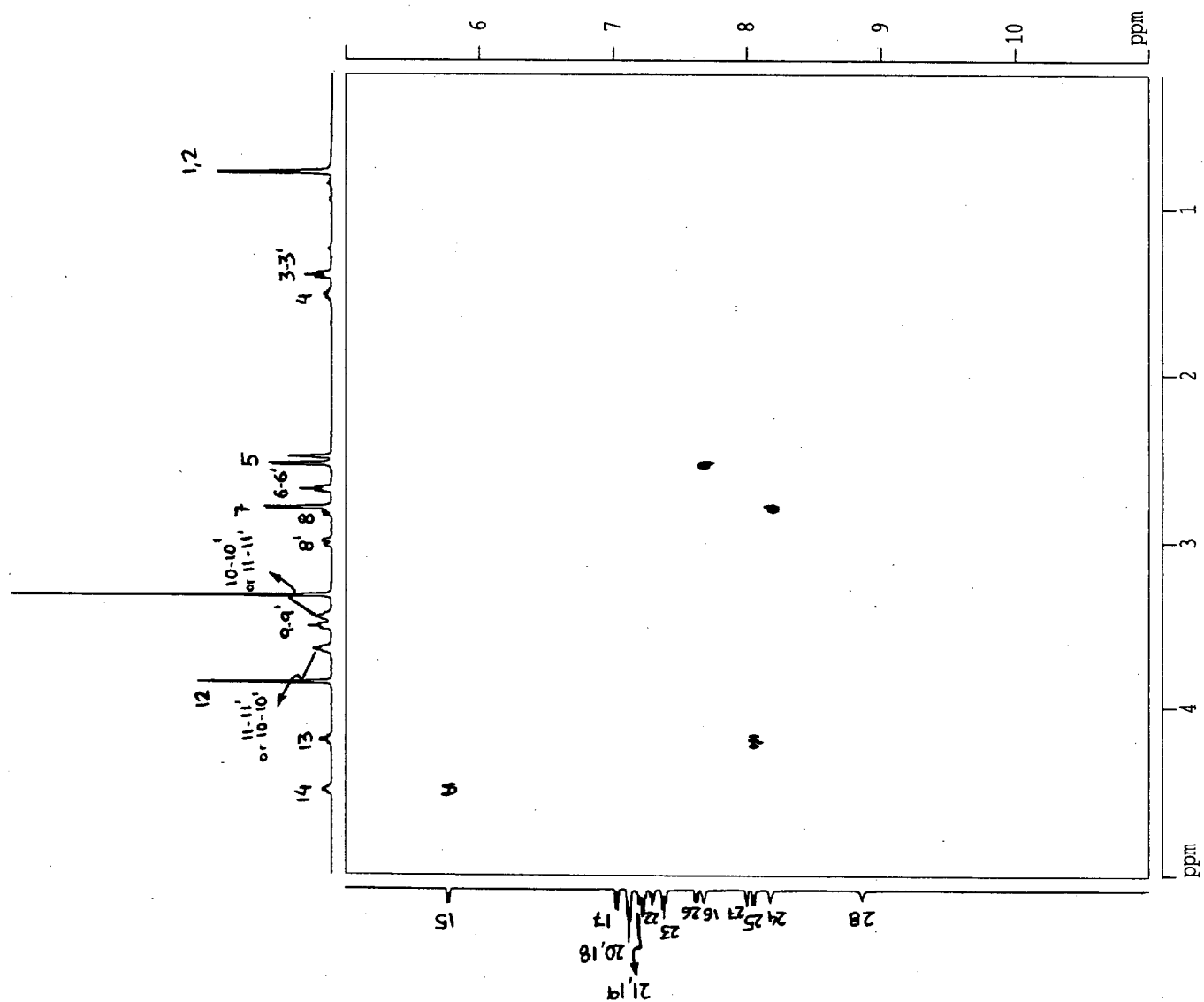


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Artificial beta-Sheet 1
 500 MHz PFG COSY 1H NMR
 10 mM in DMSO
 298 K

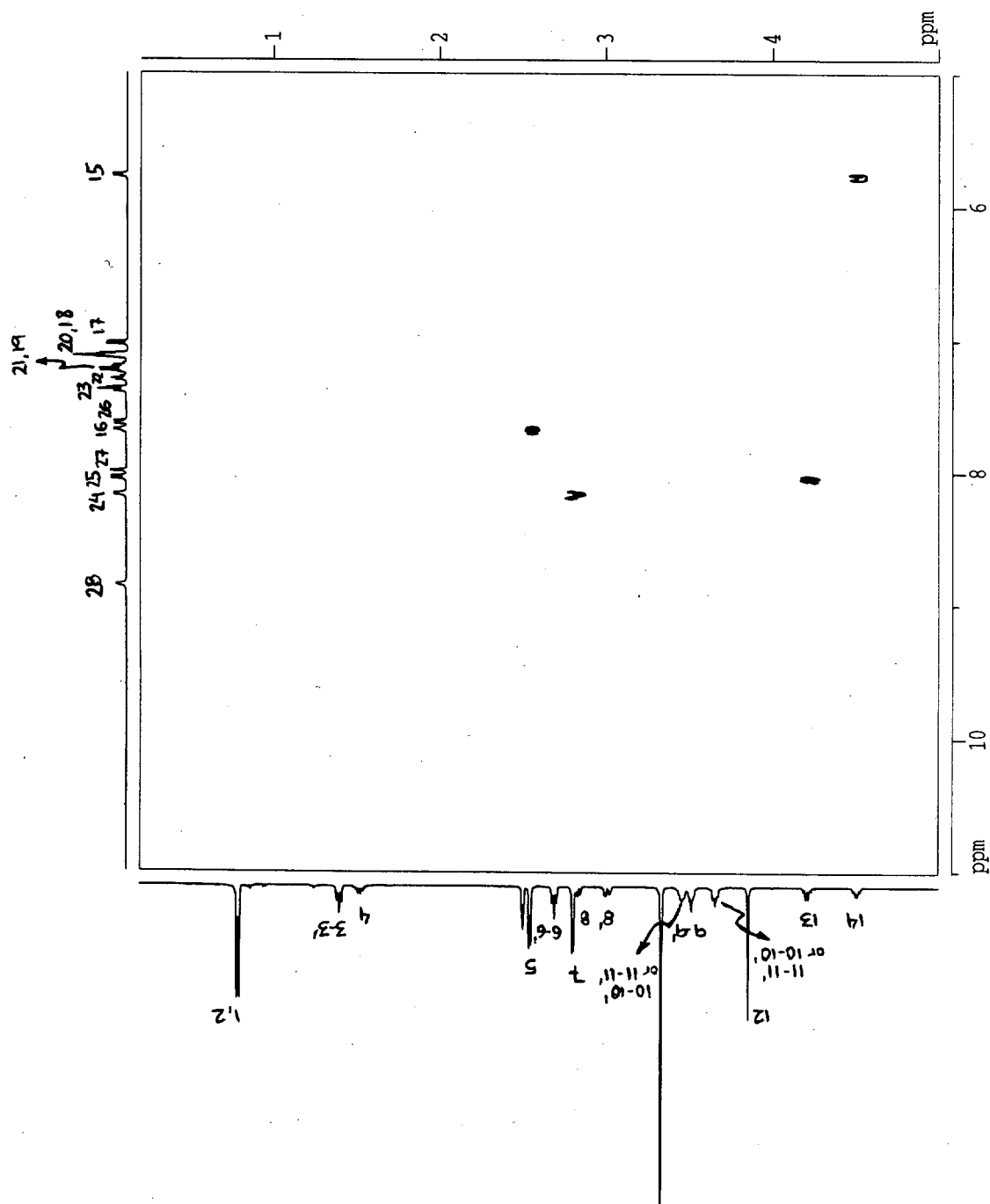
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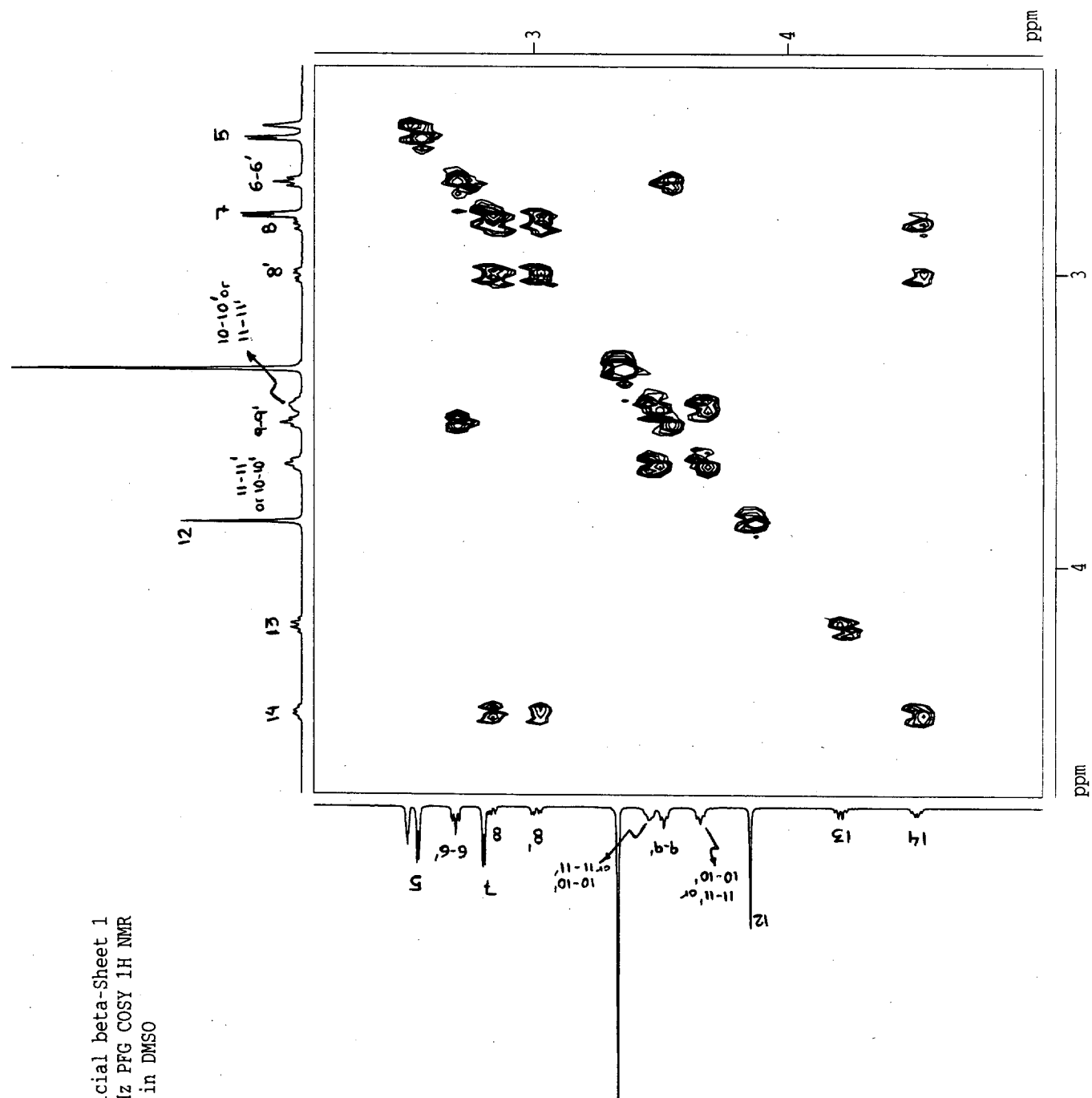
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in DMSO
298 K

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Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in DMSO
298 K



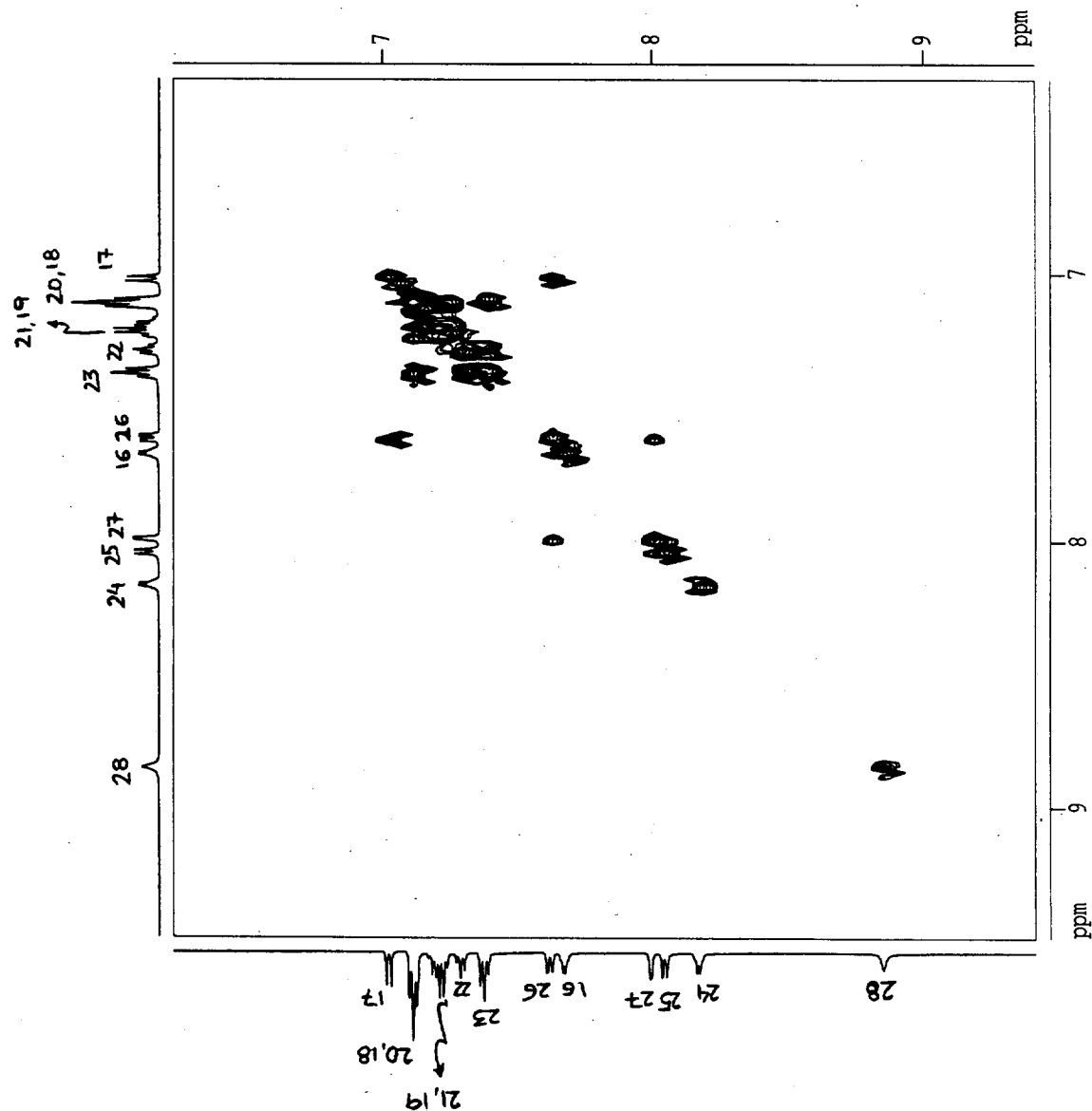
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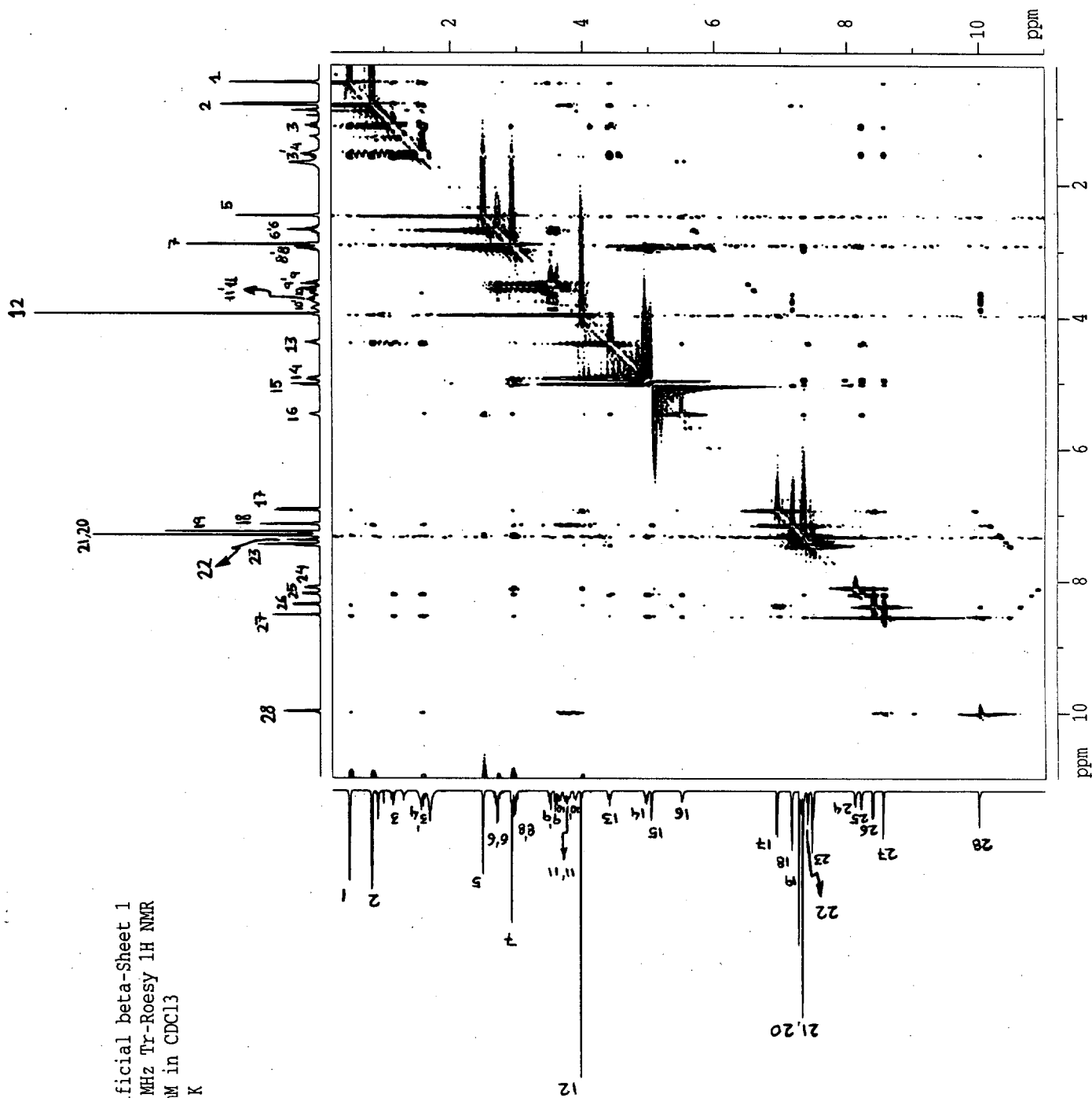
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in DMSO
298 K

28

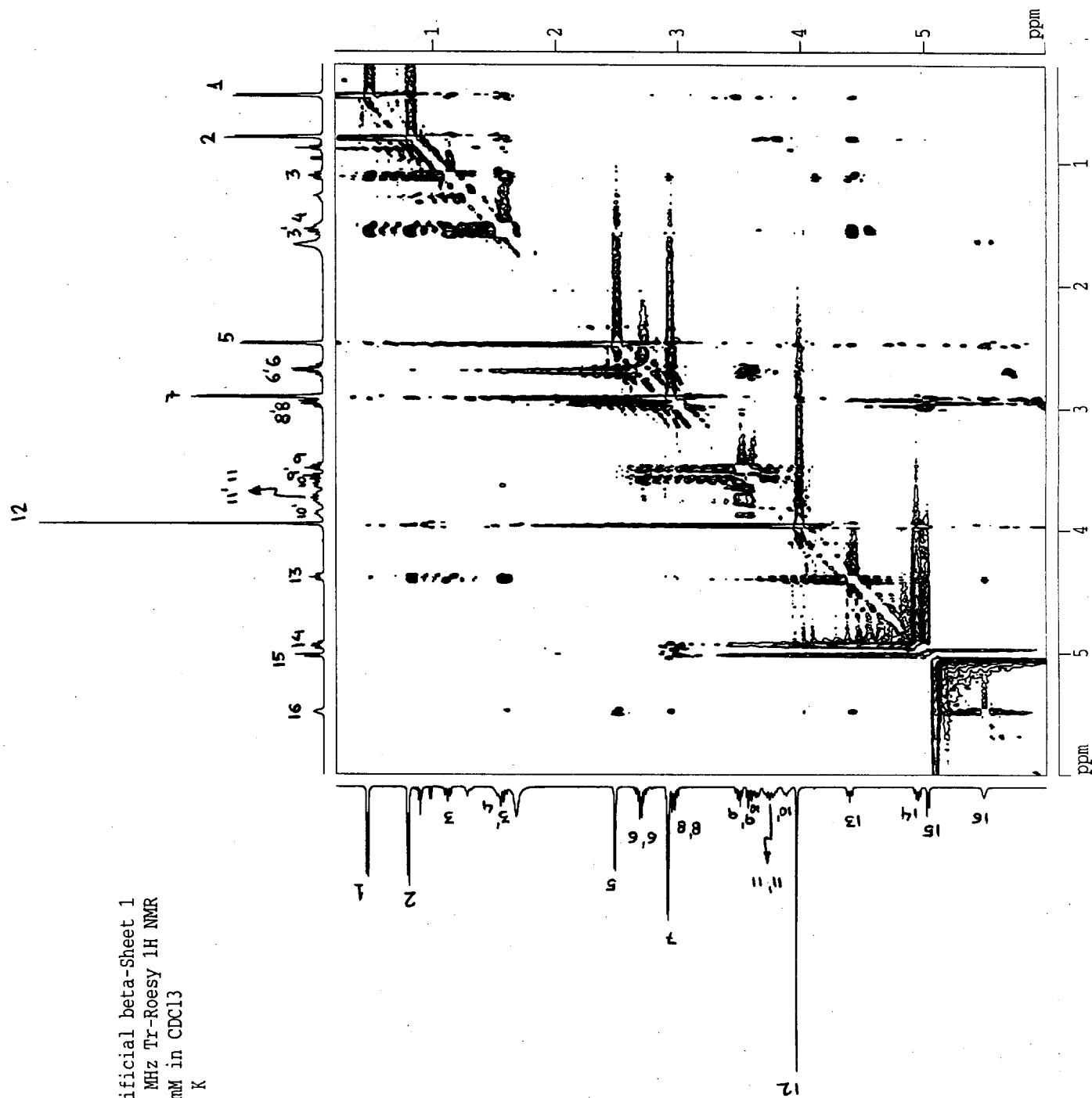
Artificial beta-Sheet 1
500 MHz PFG COSY 1H NMR
10 mM in DMSO
298 K



29

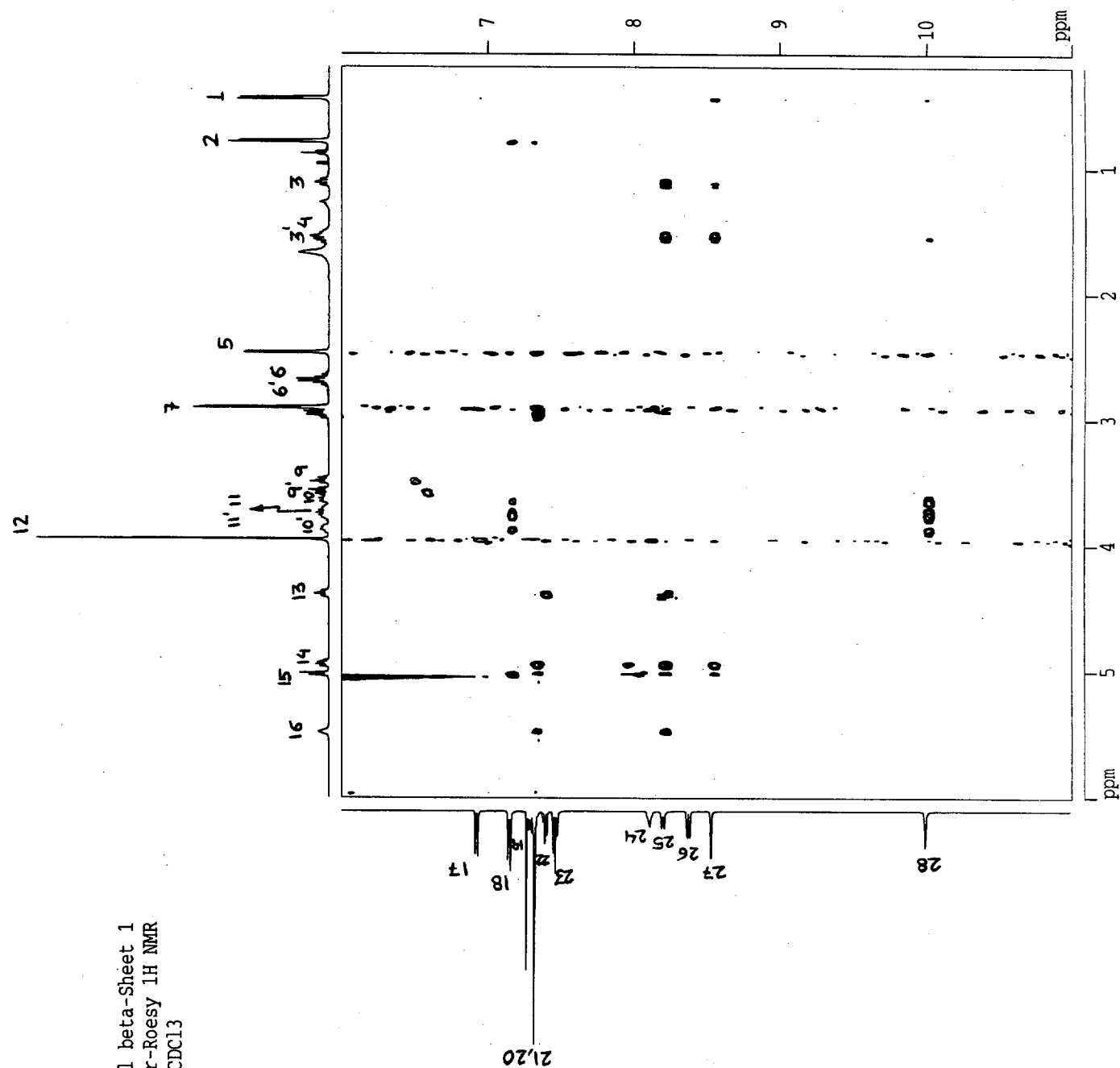


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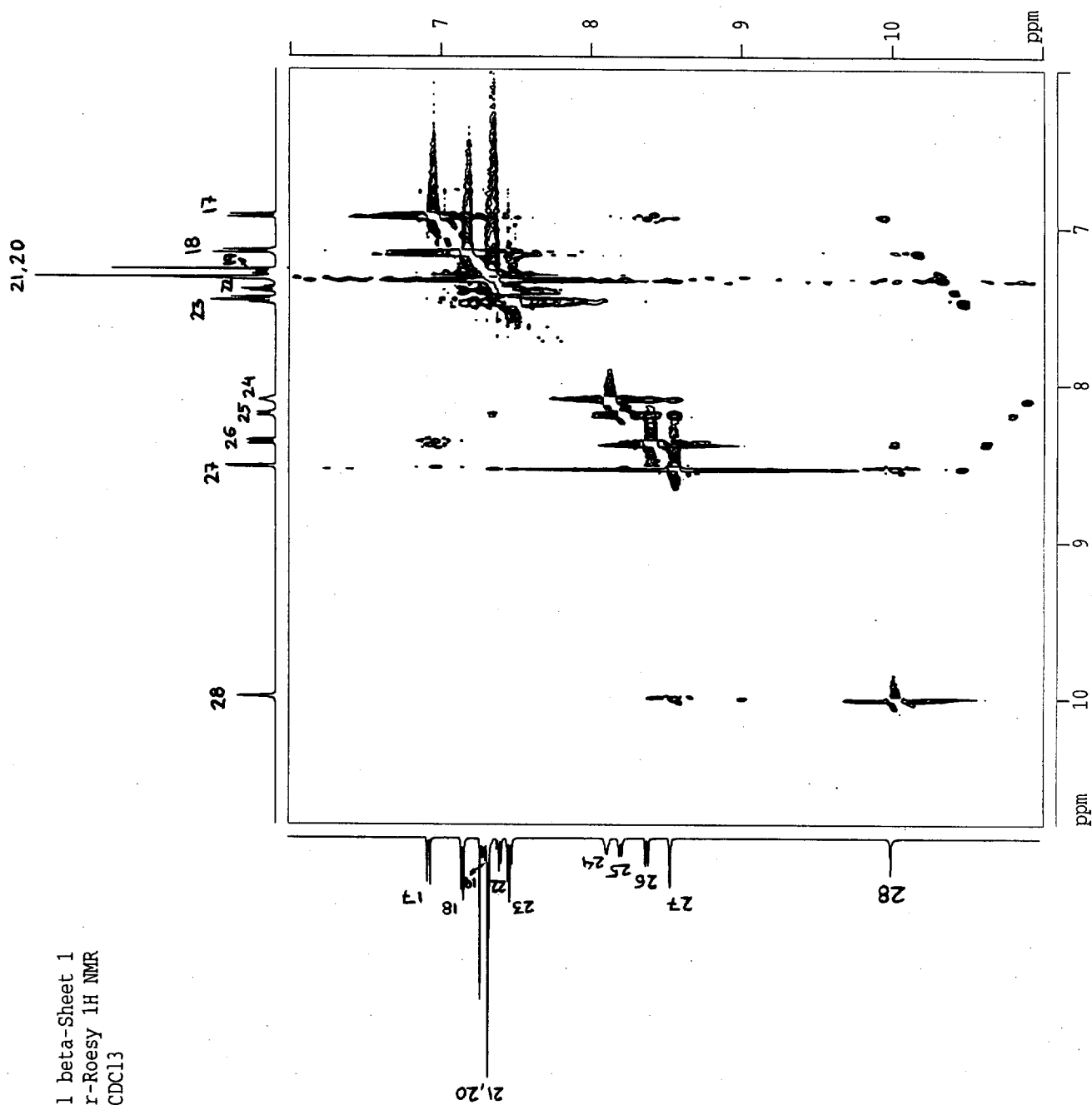


Artificial beta-Sheet 1
500 MHz Tr-Rosy 1H NMR
10 mM in CDCl₃
298 K

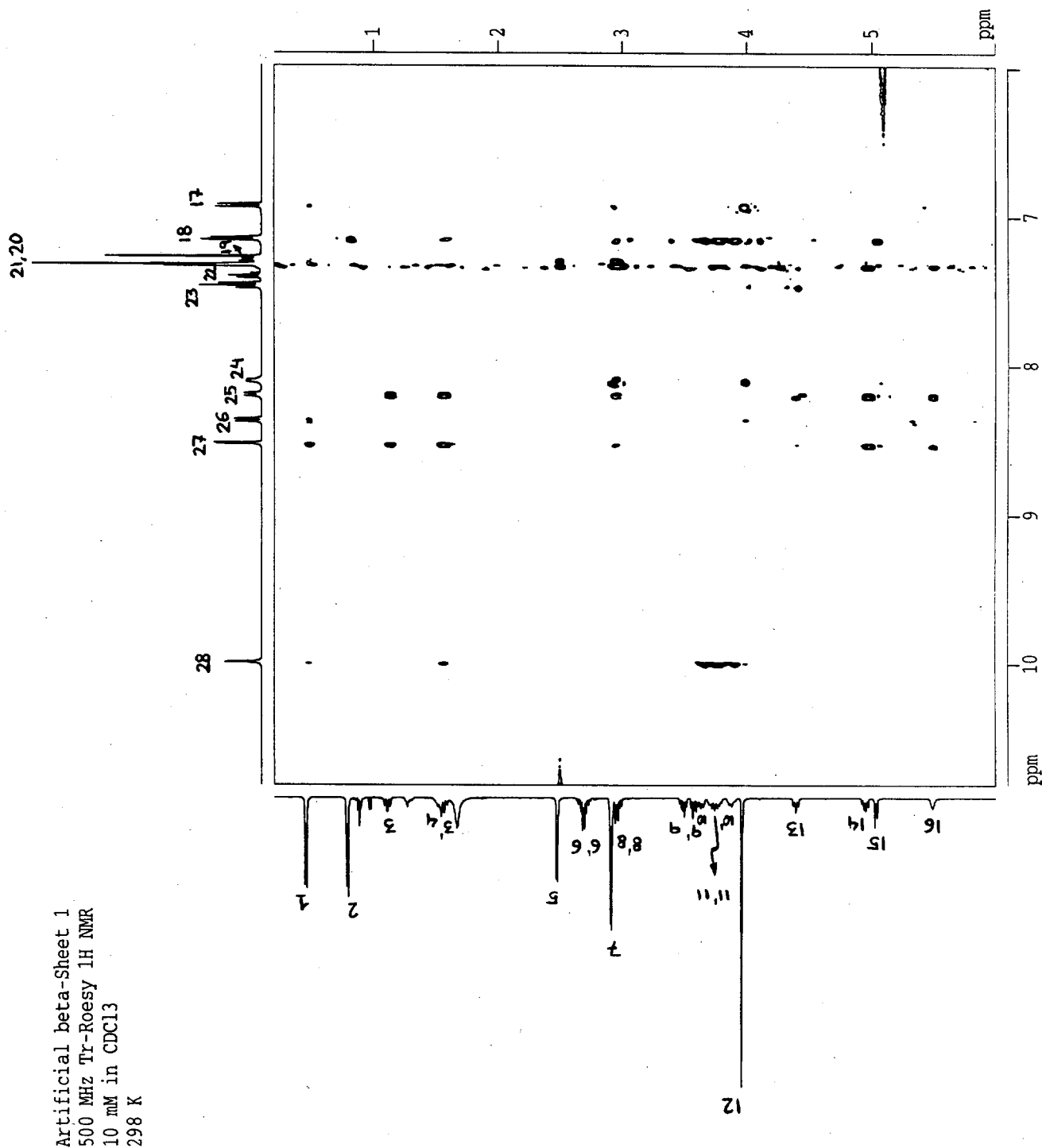
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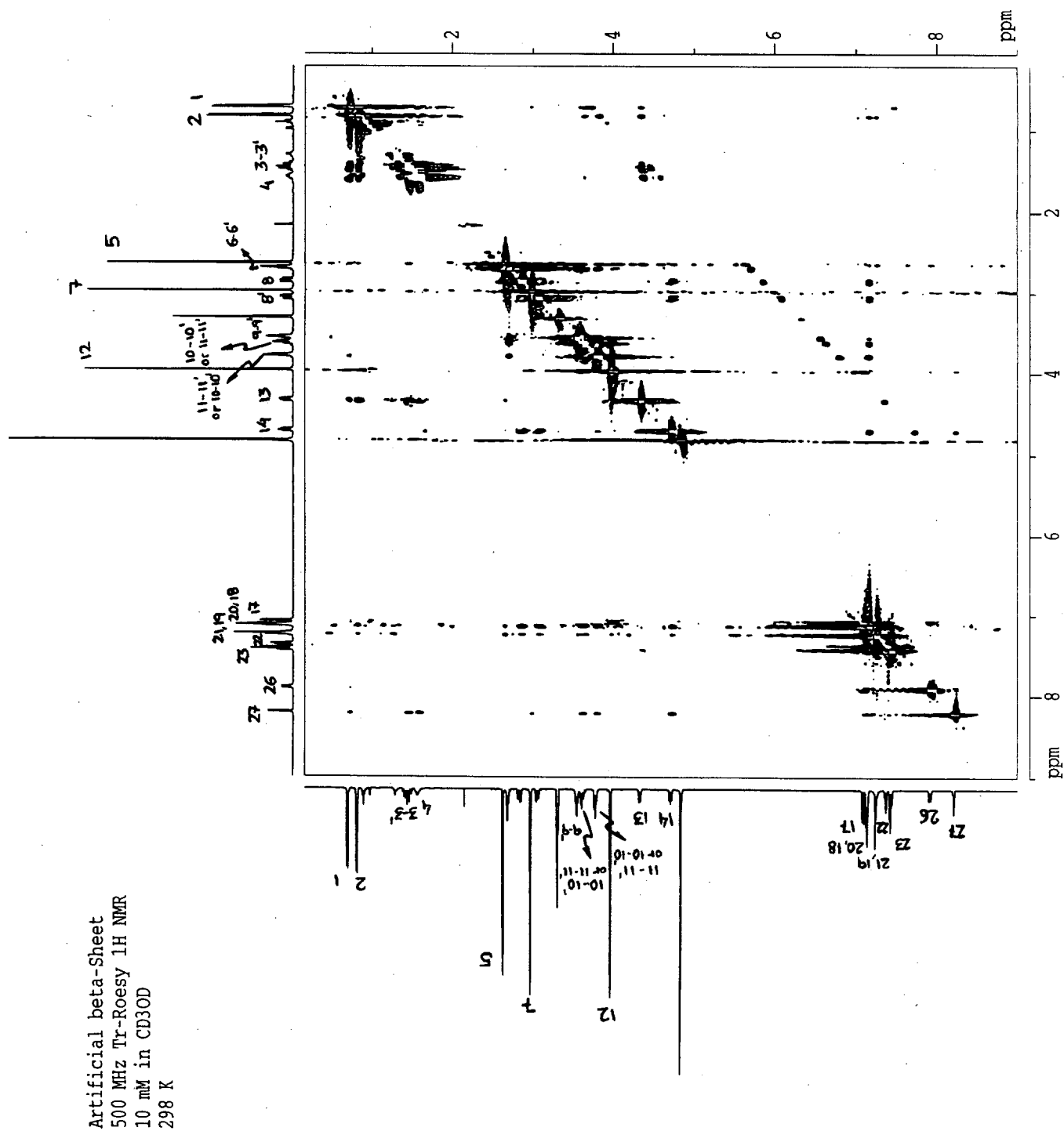
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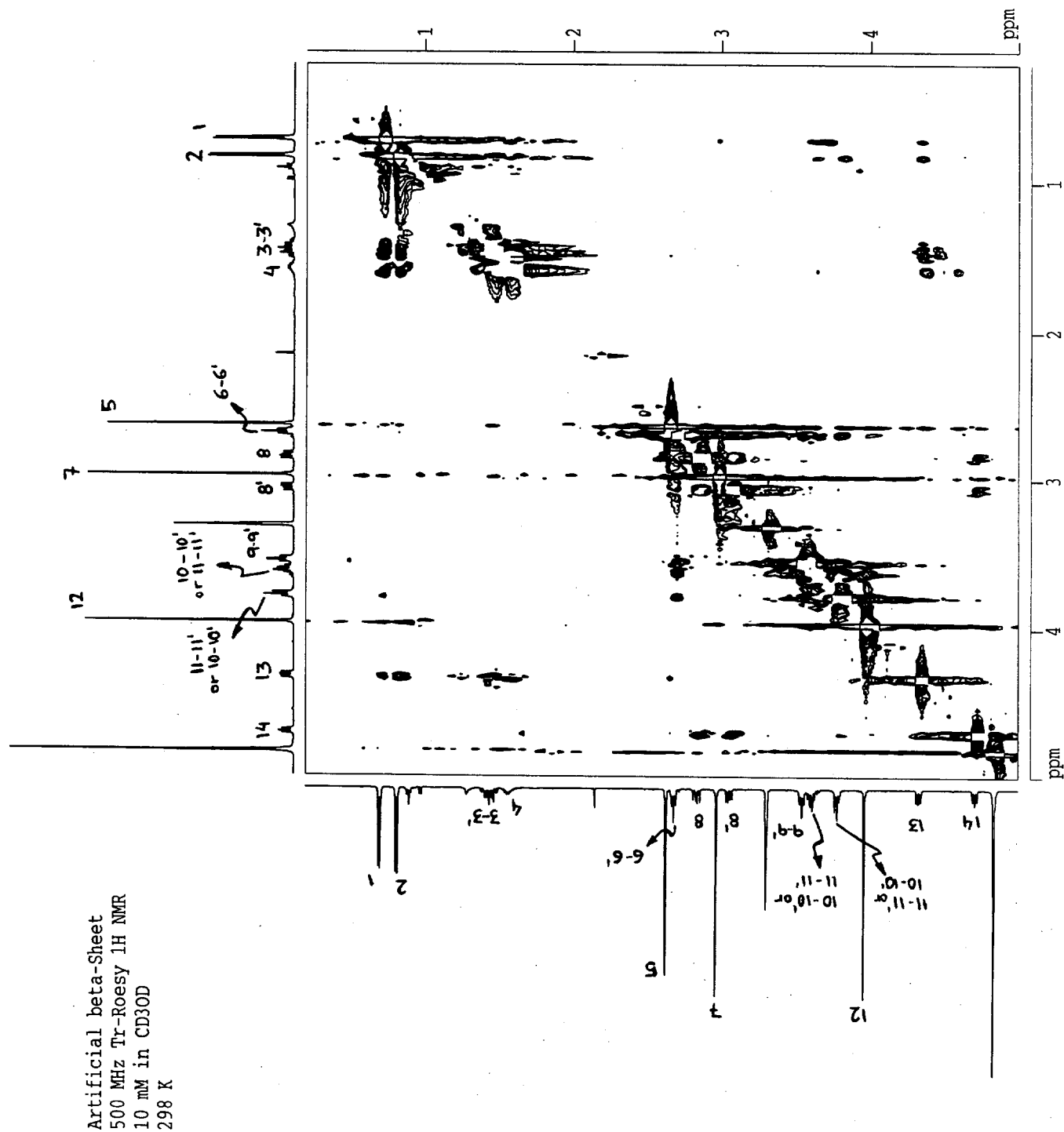
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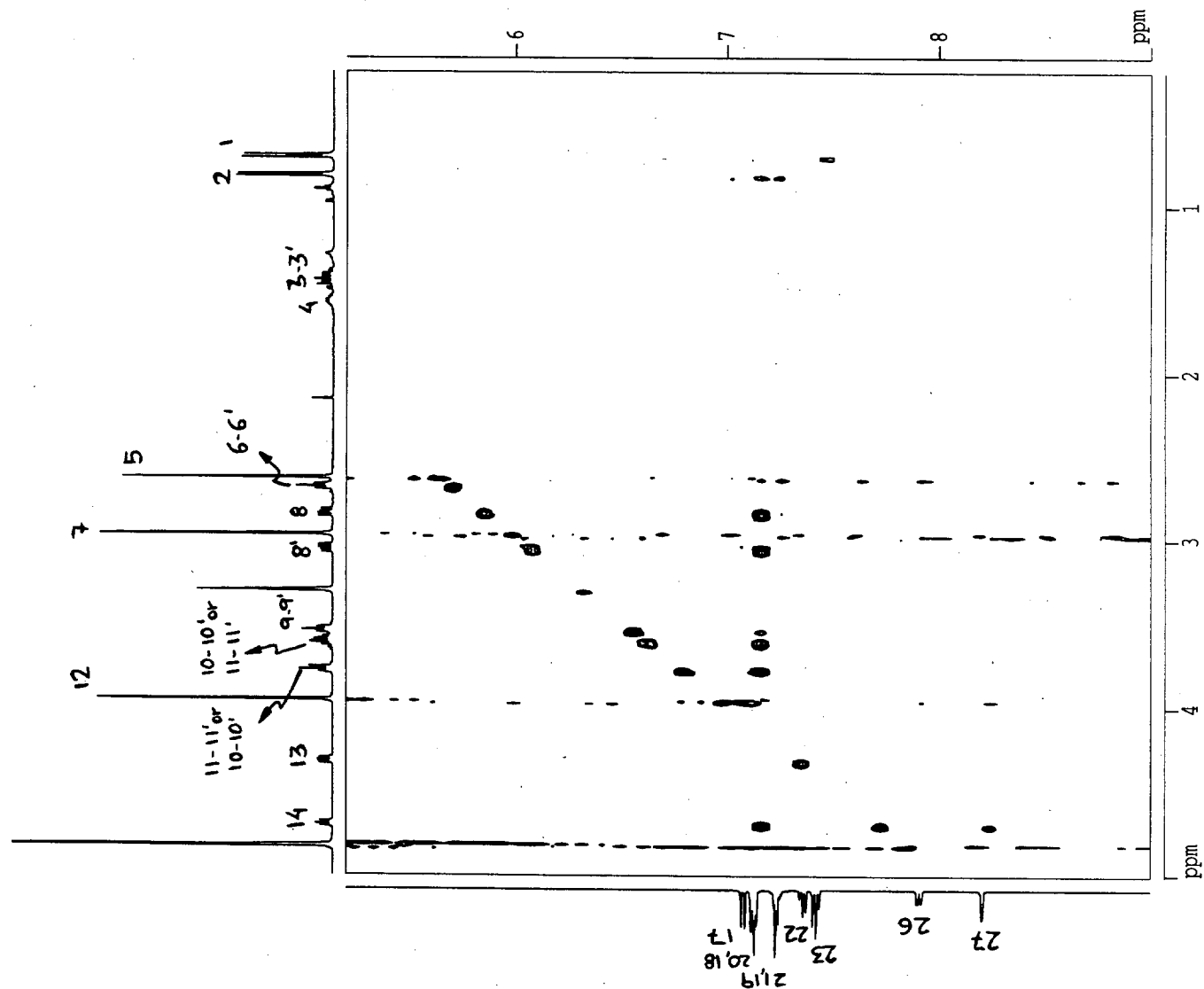
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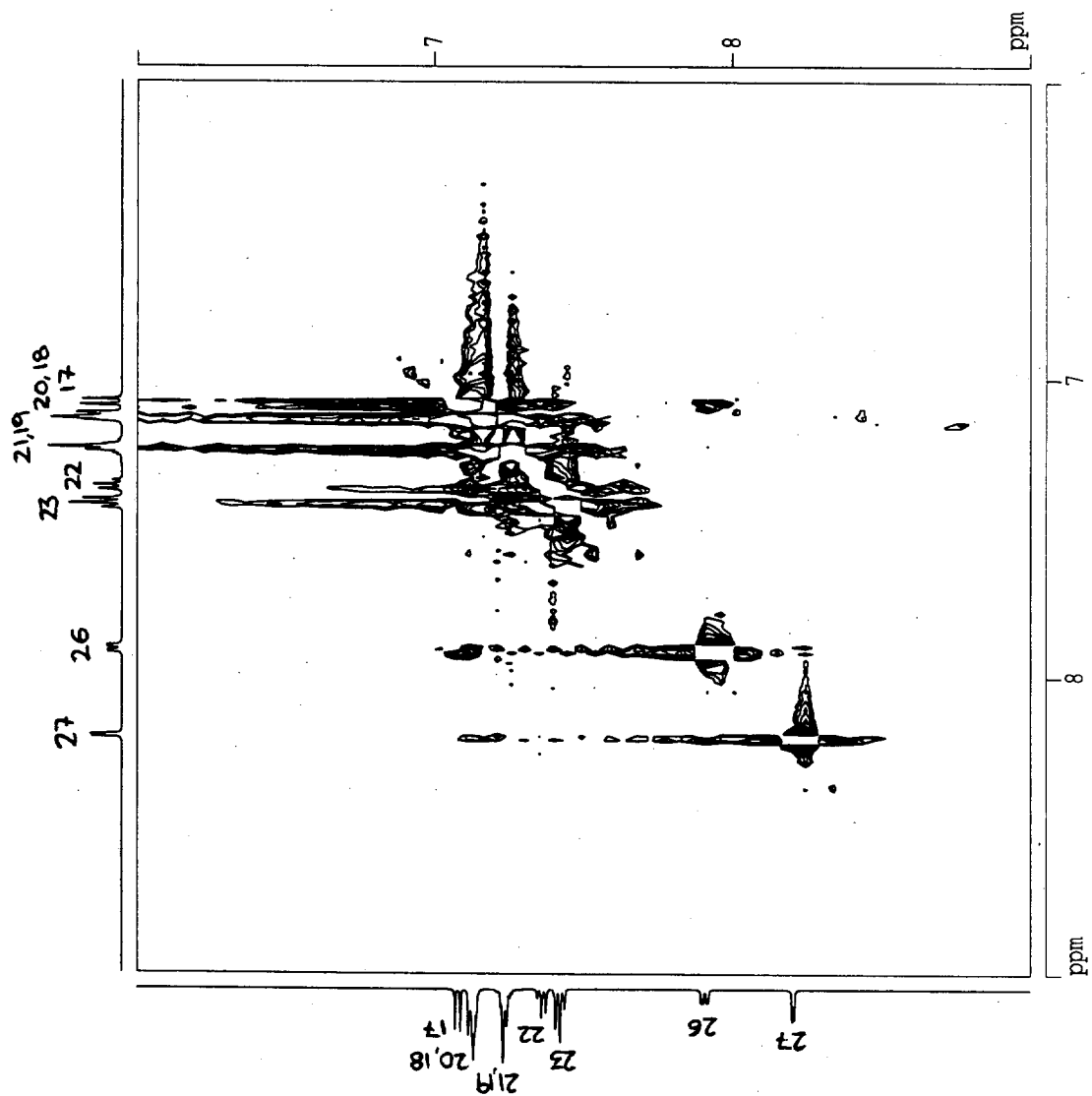


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Artificial beta-Sheet
500 MHz Tr-Rosy 1H NMR
10 mM in CD₃OD
298 K

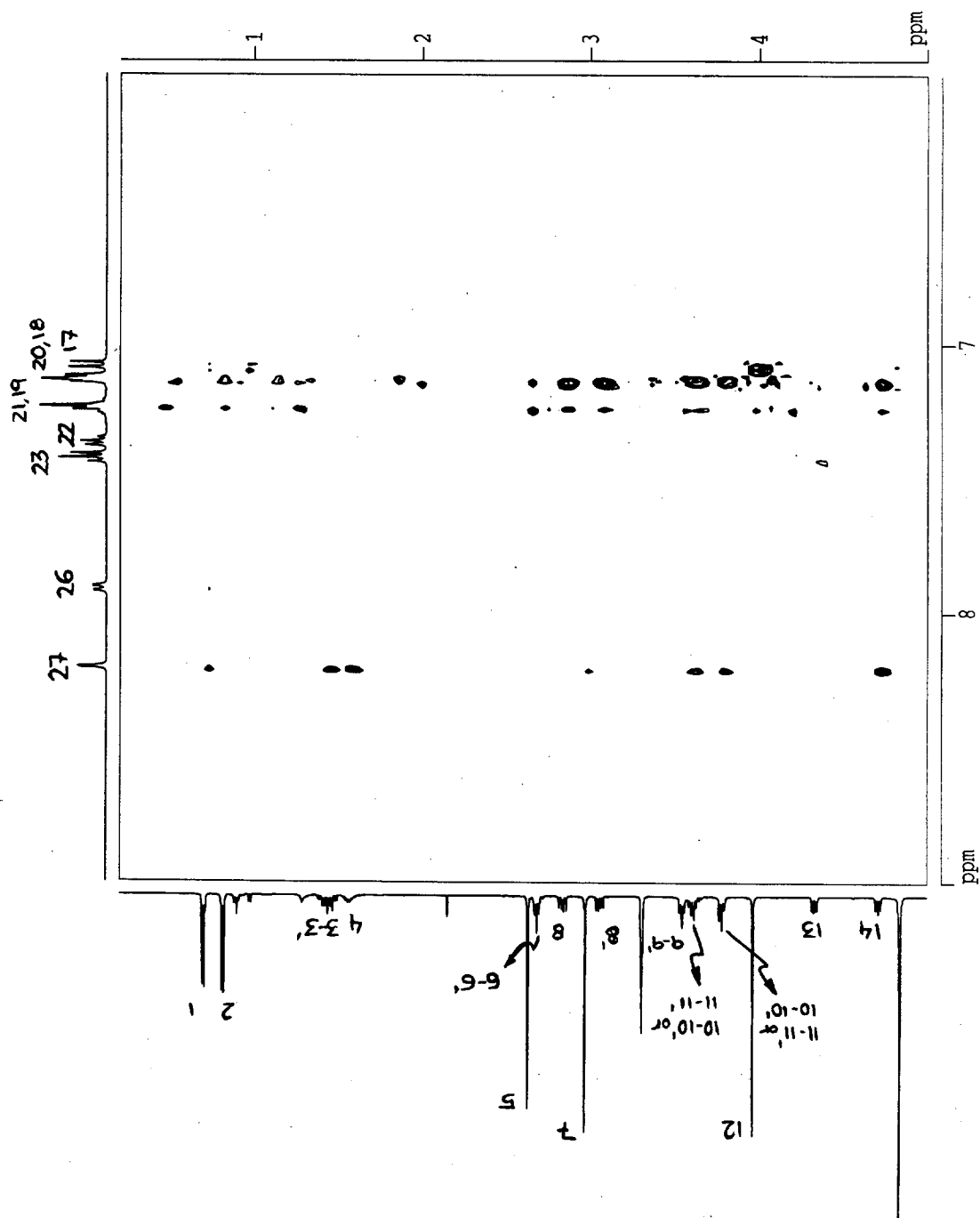
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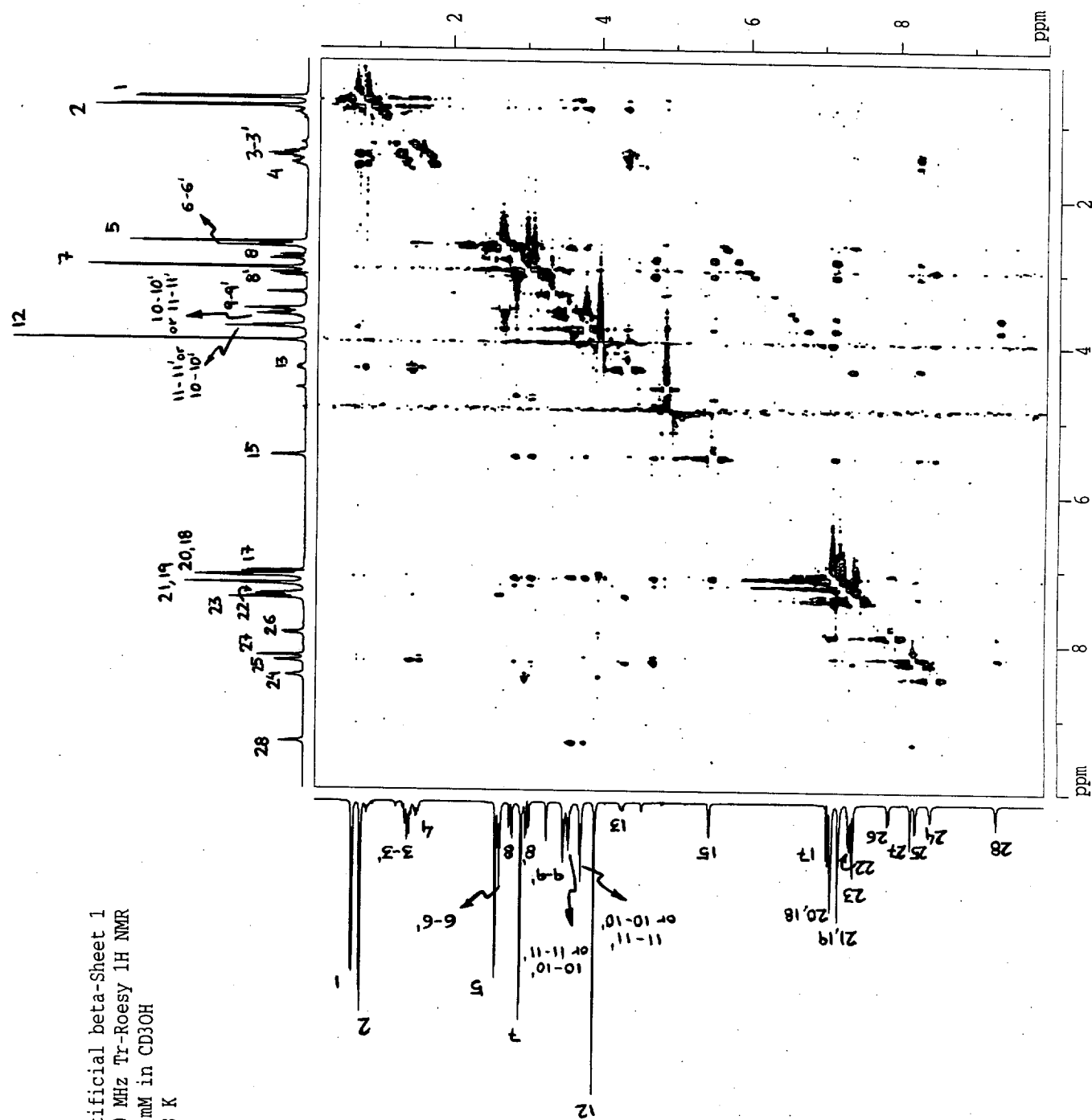
Artificial beta-Sheet
 500 MHz Tr-Rosy 1H NMR
 10 mM in CD3OD
 298 K

38

Artificial beta-Sheet
500 MHz Tr-Rosy 1H NMR
10 mM in CD3OD
298 K



39



40

