

SUPPLEMENTARY MATERIAL

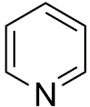
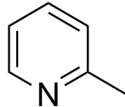
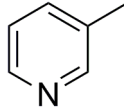
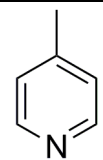
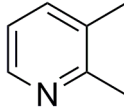
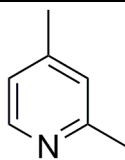
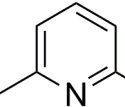
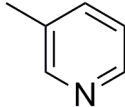
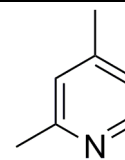
Synthesis of ^{15}N labelled 3,5-dimethylpyridine

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Content:

Supplementary Table 1	page 2
^1H spectrum of 2-ethoxy-3,4-dihydro-3,5-dimethyl-2 <i>H</i> -pyrane 13	page 3
^{13}C spectrum of 2-ethoxy-3,4-dihydro-3,5-dimethyl-2 <i>H</i> -pyrane 13	page 4
^1H spectrum of 3,5-dimethylpyridine 3	page 5
^{13}C spectrum of 3,5-dimethylpyridine 3	page 6
^{15}N spectrum of 3,5-dimethylpyridine 3	page 7

Supplementary Table 1: Comparison of ^{15}N chemical shifts of pyridine derivatives measured in CDCl_3 at 298 K and referenced to external CH_3NO_2 .

									
pyridine	2-picoline	3-picoline	4-picoline	2,3-lutidine	2,4-lutidine	2,6-lutidine	3,5-lutidine	2,4,6-collidine	References
							-69.7 ppm		This work
							-69.8 ppm ^a		(1)
-70.1 ppm ^b	-71.6 ppm ^b	-75.8 ppm ^b	-84.1 ppm ^b			-72.2 ppm ^b			(2)
				-71.4 ppm ^c	-80.0 ppm ^c	-72.0 ppm ^c	-71.0 ppm ^c	-80.1 ppm ^c	(3)
-67.7 ppm ^d	-68.8 ppm ^d	-68.4 ppm ^d	-76.7 ppm ^d						(4)

^a ^{15}N measurements at natural abundance in different solvents, among them CDCl_3 ; data were measured at 302 K and referenced to external CH_3NO_2

^b Dodalik et al. reported ^{15}N data in CDCl_3 as well as DMSO-d_6 at 300K, at natural abundance, referenced to external liquid NH_3 ; for this table we calculated the chemical shifts referenced to external CH_3NO_2 by subtracting 381.7 ppm according to Marek and Lycka 2002 (5) and Pazderski et al. 2009 (6).

^c data measured with CDCl_3 at 303 K, at natural abundance, referenced to external CH_3NO_2

^d data measured at with CDCl_3 at 298 K, at natural abundance, referenced to external CH_3NO_2

References:

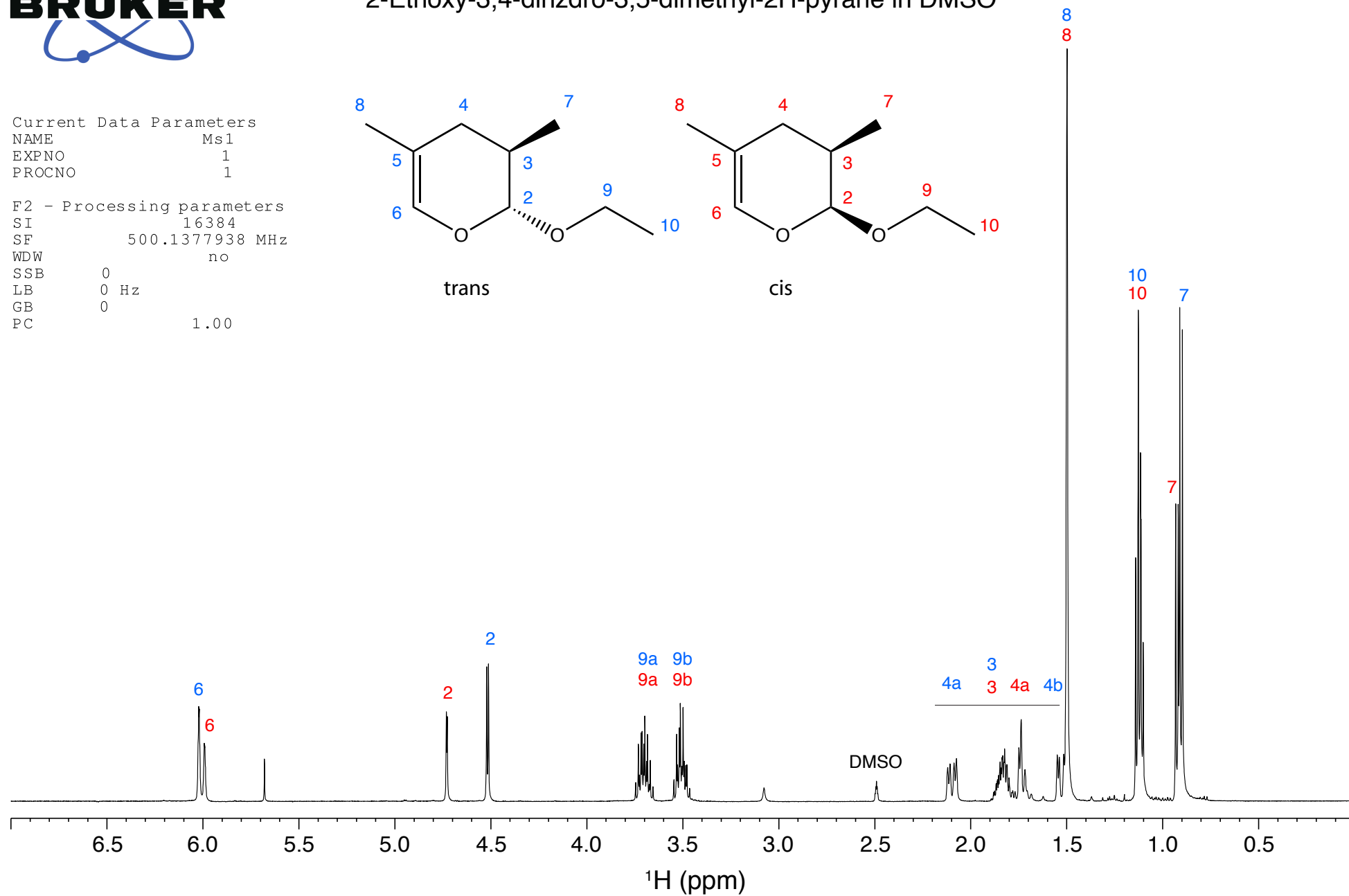
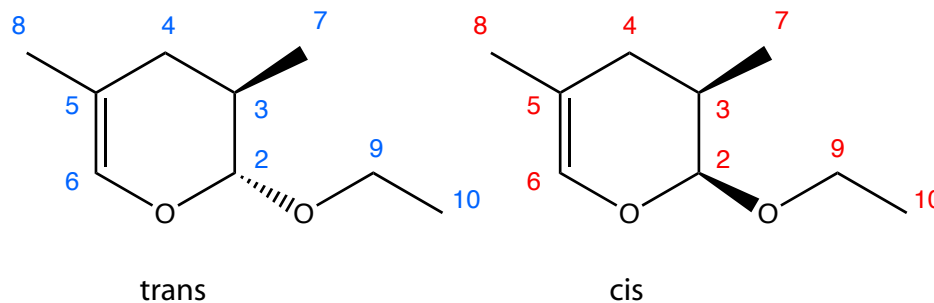
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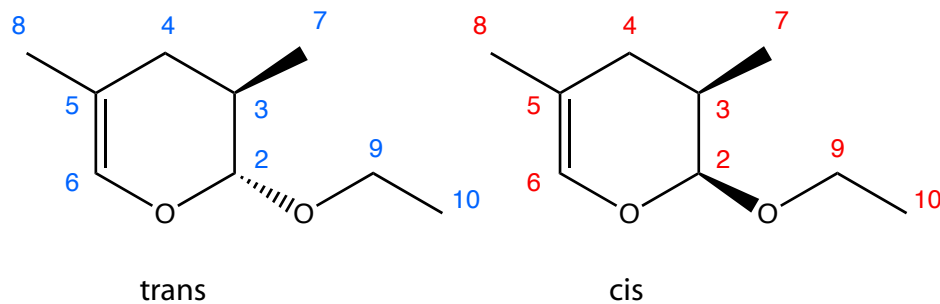
2-Ethoxy-3,4-dihydro-3,5-dimethyl-2H-pyran in DMSO

Current Data Parameters
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PROCNO 1

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WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

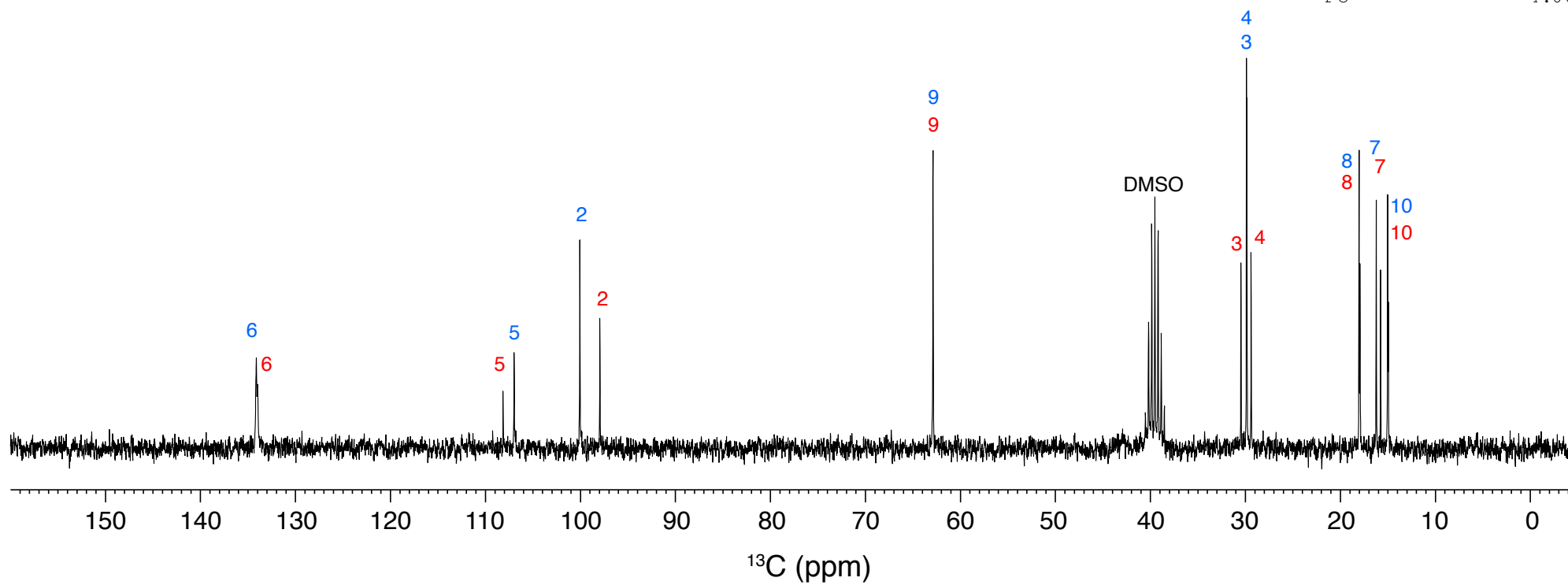


2-Ethoxy-3,4-dihydro-3,5-dimethyl-2H-pyran in DMSO

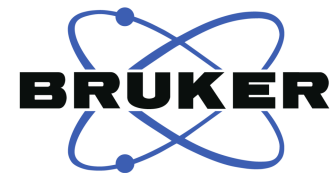
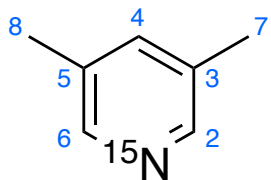


Current Data Parameters
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EXPNO 3
PROCNO 1

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LB 1.20 H
GB 0
PC 4.00



^{15}N -labeled 3,5-Dimethylpyridine in CDCl_3

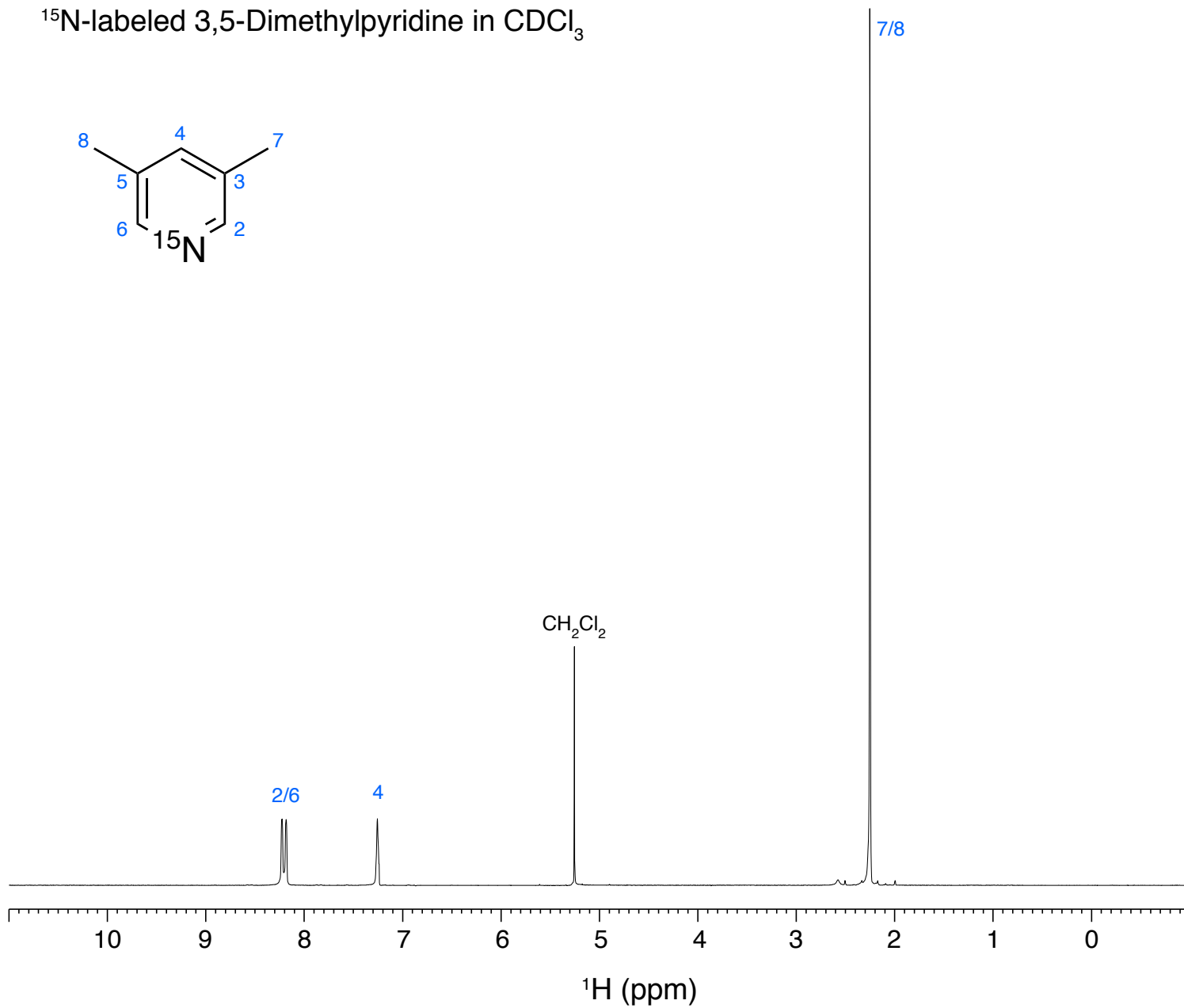


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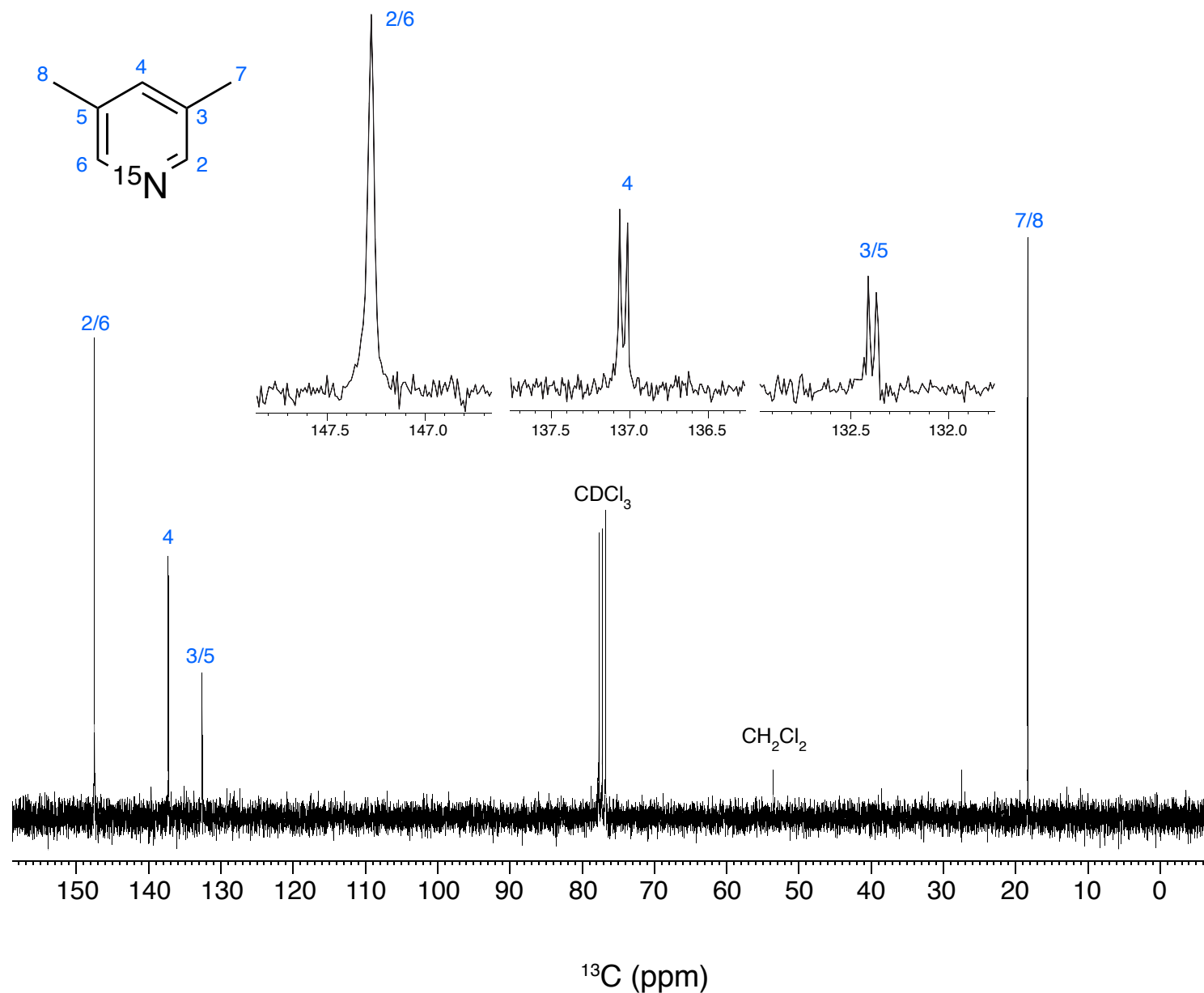


¹⁵N-labeled 3,5-Dimethylpyridine in CDCl₃

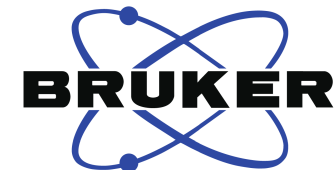


Current Data Parameters
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EXPNO 1
PROCNO 1

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SI 16384
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WDW no
SSB 0
LB 2.00 Hz
GB 0
PC 4.00



^{15}N -labeled 3,5-Dimethylpyridine in CDCl_3



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 50.6976064 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

