

## Supporting Information

### Structure-activity studies of phosphopeptidomimetic prodrugs targeting the Src homology

### 2 (SH2) domain of signal transducer and activator of transcription 3 (Stat3)

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**Table S1**  $^1\text{H}$  NMR (500MHz,  $\text{CDCl}_3$ )  $\delta$  for *trans* **27**:

	bMe-Cinn	POM	Nle	4,4-Me <sub>2</sub> Pro	4-Aminopentamide
NH			6.92 (d, $J = 8.0$ Hz)		6.35 (d, $J = 9.0$ Hz)
$\alpha$ -H	6.12 (s, 1H)		4.78 (m, 1H)	4.30 (t, 1H, $J = 8.5$ Hz)	3.99 (m, 1H)
$\beta$ -H			1.73 (m, 1H) 1.51 (m, 1H)	1.89 (d, $J = 8.5$ Hz)	1.88 (m, 1H), 1.54 (m, 1H), 1.10 (d, $J = 6.5$ Hz, 3H)
$\gamma$ -H	2.51 (s, 3H)		1.3 (m)		2.32 (m) 2.19 (m)
$\delta$ -H			0.83 (br tr)	3.35 (d, $J = 10.0$ Hz, 1H) 3.70 (d, $J = 10.0$ Hz, 1H)	
Aromatic	7.56 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 8.0$ Hz, 2H)				
NH <sub>2</sub>					6.92 (brs, 1H), 5.87 (brs, 1H)
Methyl				1.16 (s, 3H), 1.04 (s, 3H)	
Methylene		5.71 (m, 2H), 5.63 (m, 2H)			
<i>tert</i> -Butyl		1.20 (s)			

**Table S2.**  $^1\text{H}$ NMR (500MHz,  $\text{CDCl}_3$ )  $\delta$  Table for *cis* **27**:

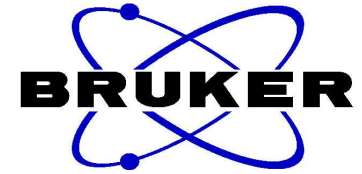
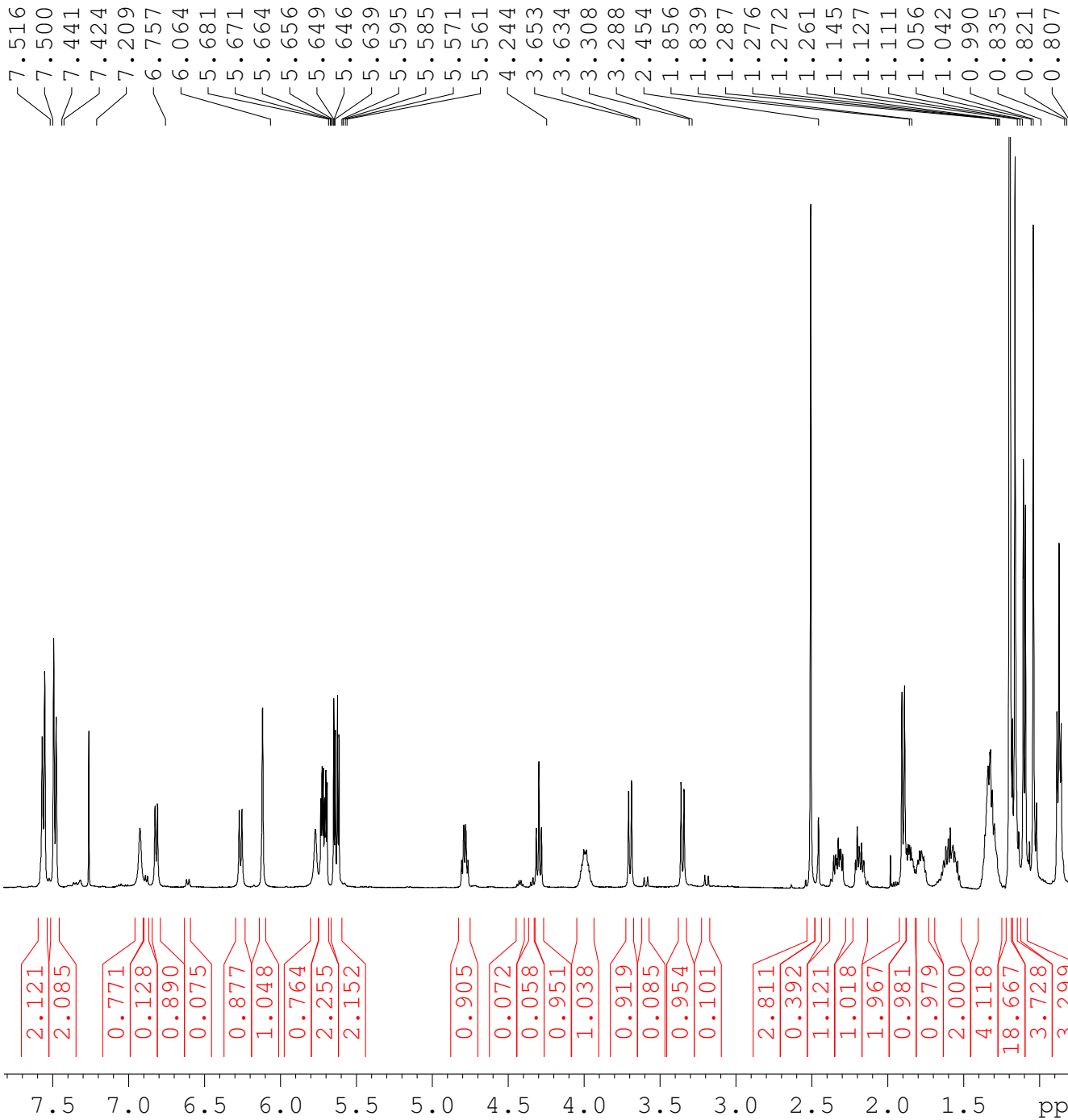
	bMe-Cinn	POM	Nle	4,4-Me <sub>2</sub> Pro	4-Aminopentamide
NH			6.88		6.61
$\alpha$ -H			4.42	4.335	4.01
$\beta$ -H					
$\gamma$ -H					
$\delta$ -H			3.14, 3.59		
Aromatic					
NH <sub>2</sub>					
Methyl	2.45				
Methylene					
<i>tert</i> -Butyl					

Major isomer:

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  13.9, 17.5, 21.3, 22.5, 25.5, 26.0, 26.3, 26.7, 27.2, 32.0, 32.4, 33.3, 38.7, 38.8, 42.4, 44.7, 50.6, 50.7, 60.3, 60.8, 82.4, 82.5, 121.1, 126.4, 126.5, 145.5, 149.8, 166.1, 171.4, 172.2, 176.3, 176.5.

Minor isomer:

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  22.6, 25.8, 26.9, 27.4, 36.7, 45.0, 116.1, 117.9, 131.5

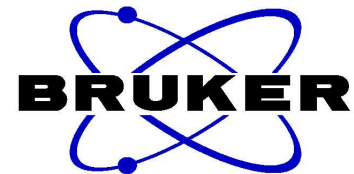


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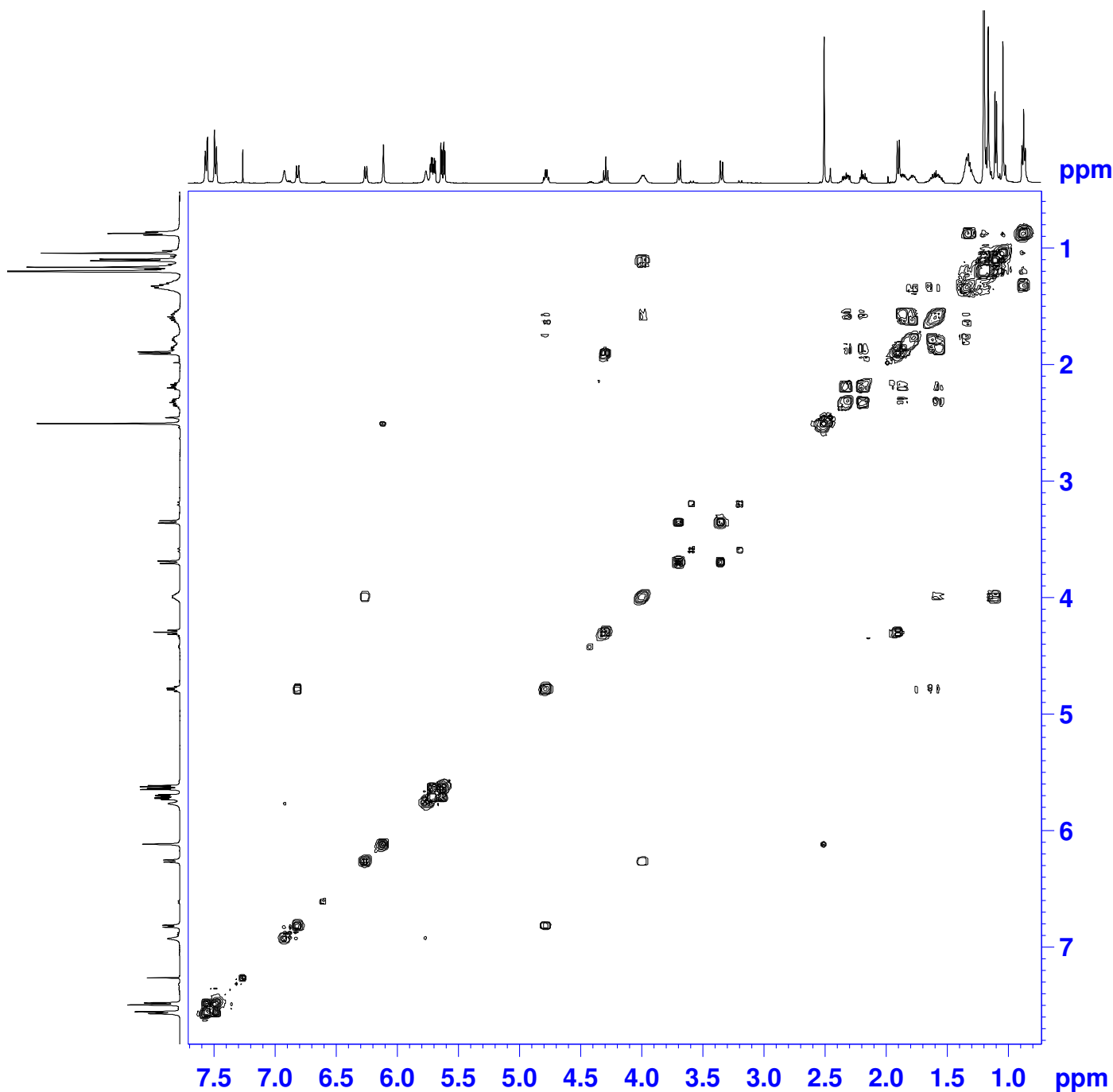
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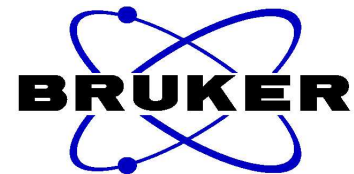


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RG 64  
DW 75.000 usec  
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d13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00015000 sec

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SF 500.0550106 MHz  
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SSB 0  
LB 0.00 Hz  
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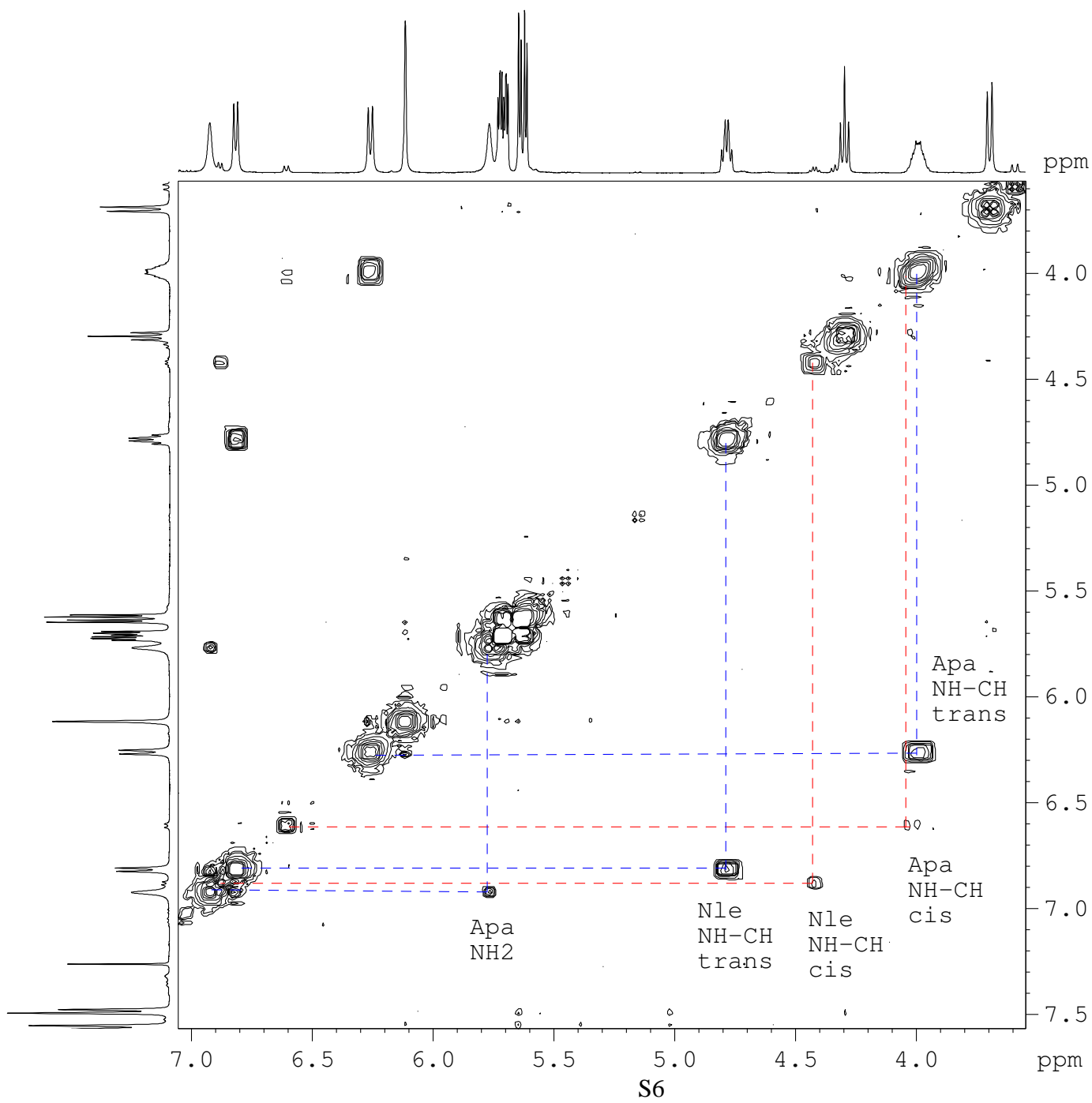


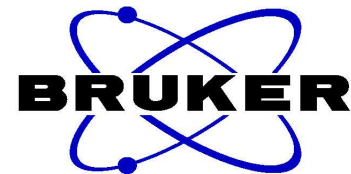


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PULPROG cosygpgqf  
TD 2048  
SOLVENT DMSO  
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DS 8  
SWH 6666.667 Hz  
FIDRES 3.255208 Hz  
AQ 0.1537250 sec  
RG 64  
DW 75.000 usec  
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D1 1.48689198 sec  
d13 0.00000400 sec  
D16 0.00020000 sec  
IN0 0.00015000 sec

===== CHANNEL f1 =====  
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P1 8.65 usec  
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GPNAM1 SINE.100  
GPNAM2 SINE.100  
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GPZ2 10.00 %  
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FIDRES 52.083332 Hz  
SW 13.332 ppm  
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SF 500.0550106 MHz  
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SSB 0  
LB 0.00 Hz  
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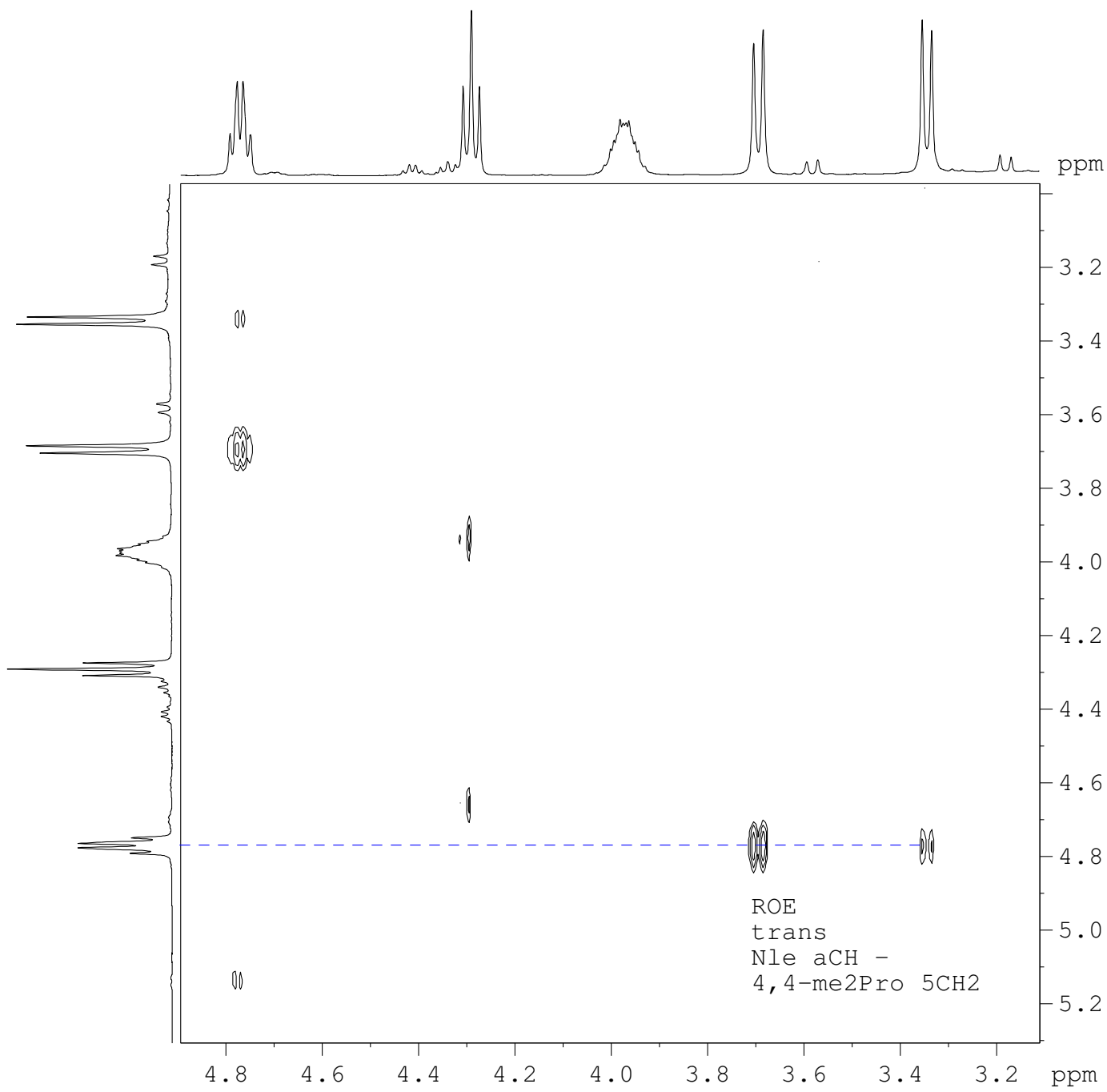




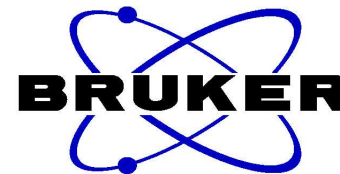
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LB 0.00 Hz  
GB 0  
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SI 1024  
MC2 echo-antiecho  
SF 500.0550109 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0



ROE  
trans  
Nle aCH -  
4,4-me2Pro 5CH2



176.52  
176.30  
172.21  
171.39  
166.06

149.74  
145.51

131.47  
126.51  
126.39  
121.08  
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77.04  
76.78  
60.77  
60.26  
50.66  
44.71  
42.41  
38.83  
38.72  
36.74  
33.31  
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32.04  
27.39  
27.21  
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26.73  
26.02  
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