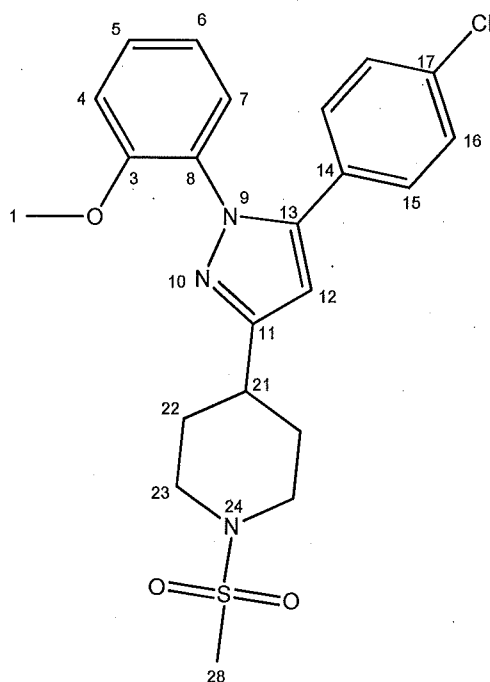


Verified Structure:



Key Points:

- 1.) The Proton and Nitrogen-15 chemical shift assignments were made using the chemical shift values and coupling patterns in the Proton spectrum (Figure 1) and HN HMBC spectrum (Figure 2).
- 2.) The proton chemical shifts, coupling patterns, and integration values observed in the proton spectrum are consistent with the structure shown above.
- 3.) In the HN HMBC spectrum, H21 has a three bond HN coupling to N10, which has a chemical shift of 305 ppm. This chemical shift is consistent with the chemical shift of a C=N nitrogen. This shows that N10 is the C=N nitrogen in the pyrazole ring and that the piperidine ring is at position 11. From this we can conclude that the methoxyphenyl group is bonded at N9 and is alpha to the parachlorephenyl group.
- 4.) The spectroscopy data are consistent with the structure shown.

Spectra: The spectra are shown in Figures 1 to 2.

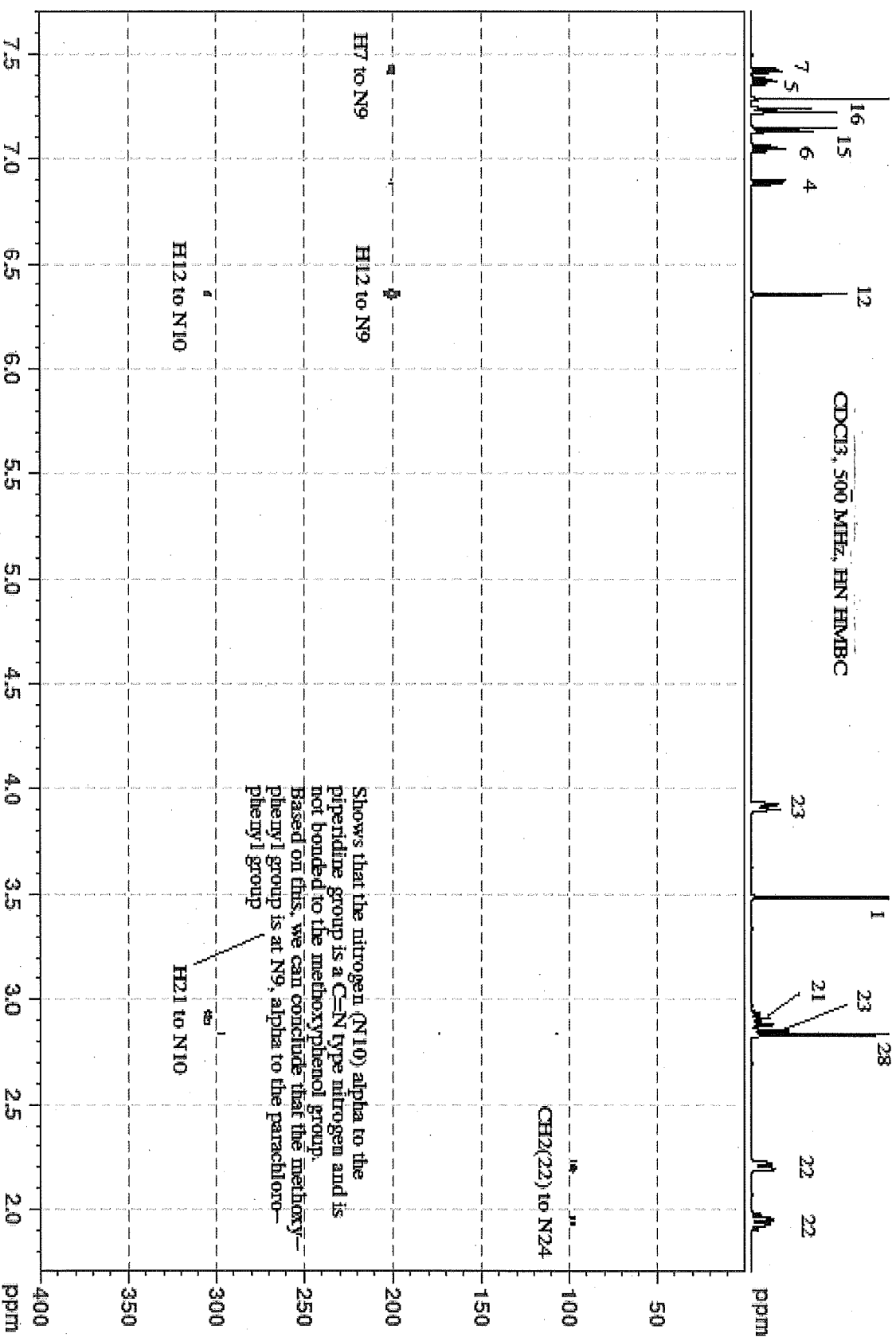
Figure 1 displays three ^1H NMR spectra of compound **1**. The top spectrum is recorded in CDCl_3 , the middle in $\text{DMSO}-d_6$, and the bottom in $\text{DMSO}-d_6$. The x-axis represents the chemical shift in ppm, ranging from 0 to 8.5. Integration values are provided for each peak.

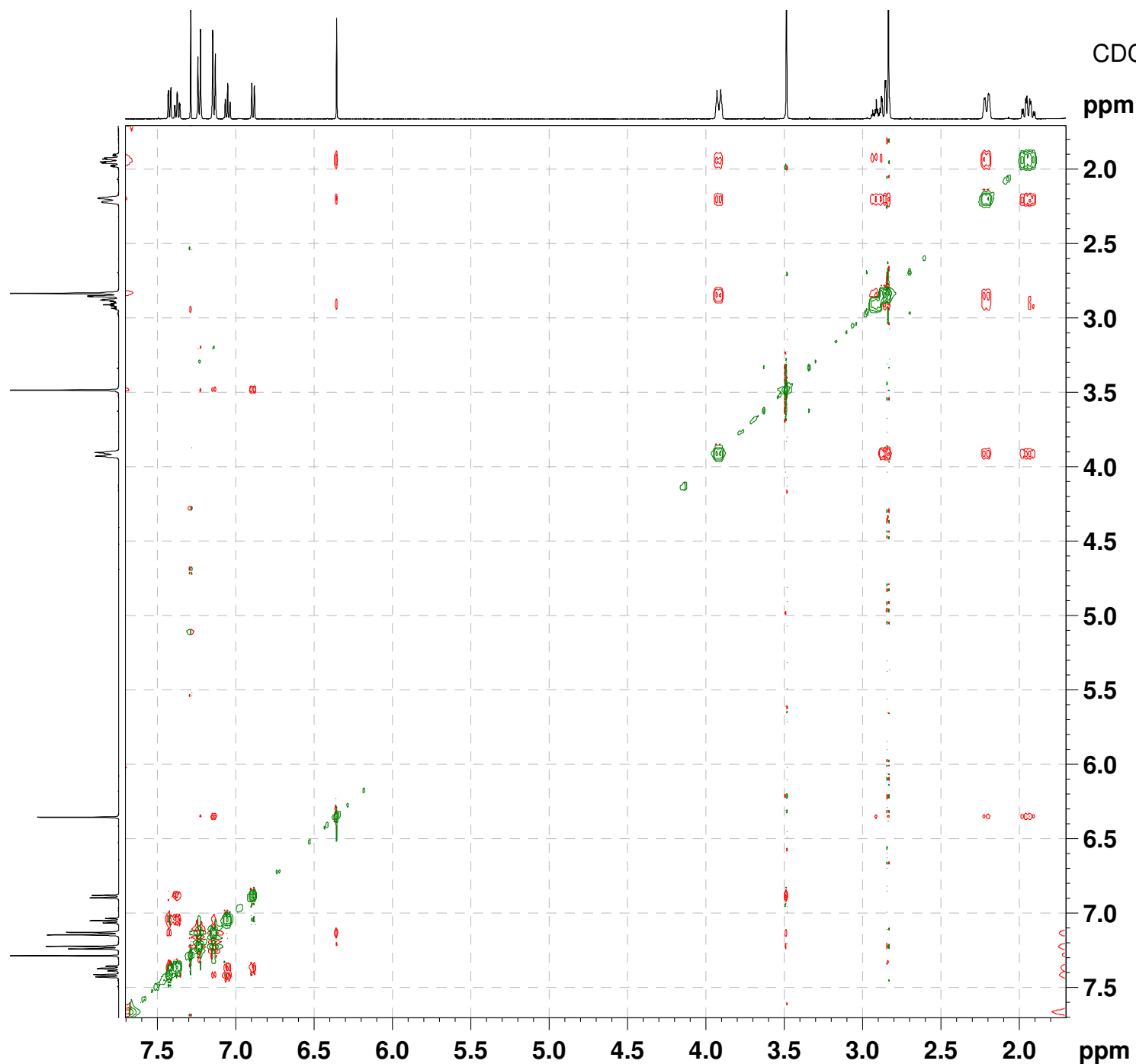
Peak Label	Chemical Shift (ppm)	Integration
12	~6.4	1.02
15	~7.1	2.06
16	~7.3	2.02
4	~6.9	1.03
6	~7.0	1.06
5	~7.2	2.02
7	~7.4	1.00
28	~2.8	6.23
23	~2.3	2.06
21	~2.9	3.14
22	~2.2	2.00
2	~2.0	2.00
1	~3.4	3.14
23	~3.9	2.06

NAME	1
EXPNO	1
PROCNO	1
Date_	20120323
Time	15:46
INSTRUM	spec
PROBHD	5 mm PABBI 1H/
PULPROG	zg30
TD	65536
SOLVENT	CDCB
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157652 Hz
AQ	3.1770407 sec
RG	512
DW	48.400 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
TDO	1

CHANNEL f1	
NUC1	1H
P1	8.30 usec
PL1	6.00 dB
SFO1	500.130885 MHz
SF	37248
SF	500.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

Figure 2: HN HMBC Spectrum

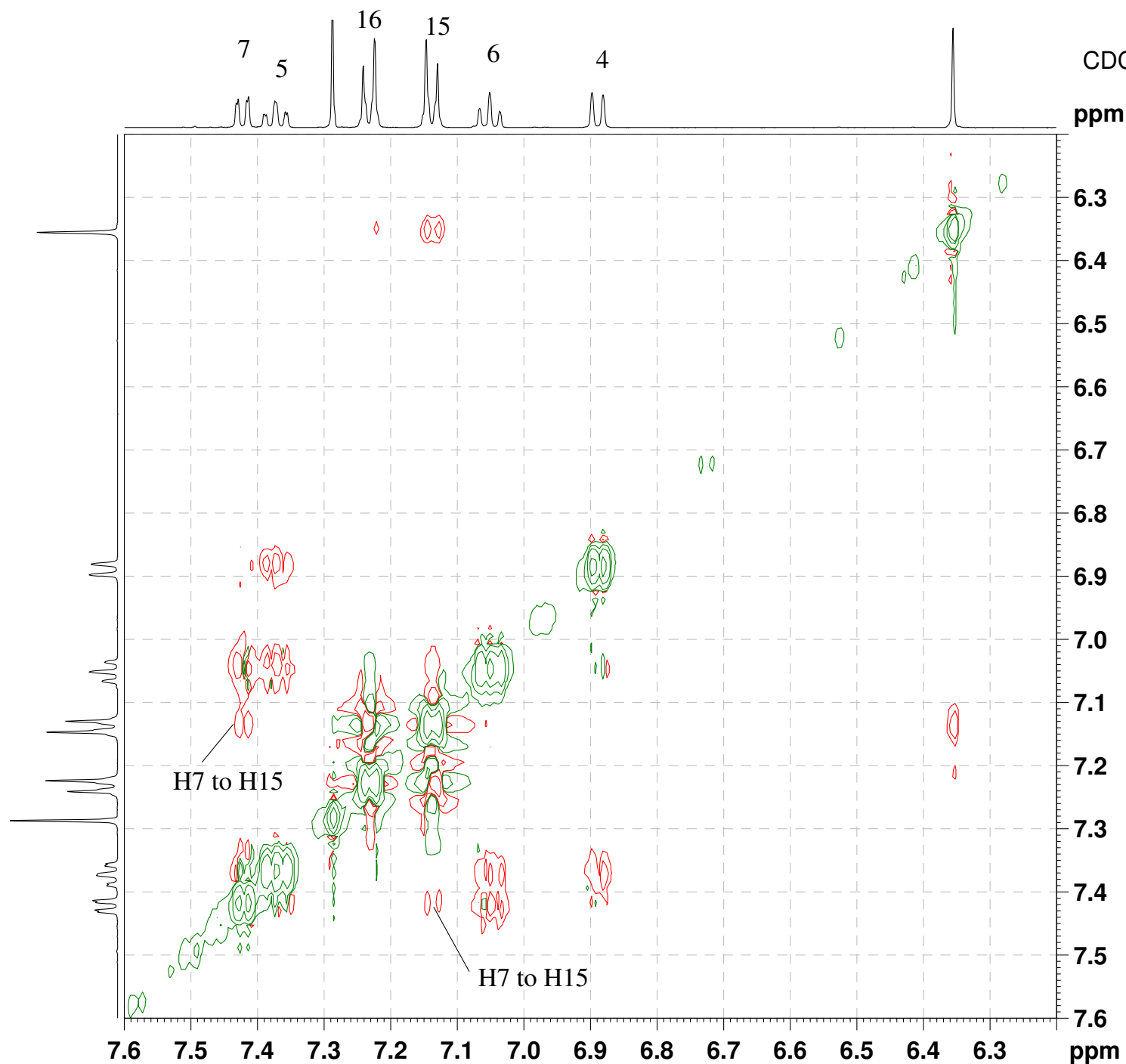




CDCl₃, 500 MHz, NOESY
d8 = 0.9 sec

ppm	NAME	Compound 2
	EXPNO	10
	PROCNO	1
	Date_	20120324
	Time	2.12
	INSTRUM	spect
	PROBHD	5 mm PABBI 1H/
	PULPROG	noesyph
	TD	2048
	SOLVENT	CDCl ₃
	NS	56
	DS	4
	SWH	3004.808 Hz
	FIDRES	1.467191 Hz
	AQ	0.3410036 sec
	RG	128
	DW	166.400 usec
	DE	12.00 usec
	TE	298.2 K
	d0	0.00015583 sec
	D1	2.00000000 sec
	D8	0.89999998 sec
	IN0	0.00033280 sec
	ST1CNT	0
	===== CHANNEL f1 =====	
	NUC1	¹ H
	P1	8.30 usec
	PL1	6.00 dB
	SFO1	500.1323506 MHz
	ND0	1
	TD	256
	SFO1	500.1324 MHz
	FIDRES	11.737530 Hz
	SW	6.008 ppm
	FnMODE	States-TPPI
	SI	1024
	SF	500.1300000 MHz
	WDW	QSINE
	SSB	2
	LB	0.00 Hz
	GB	0
	PC	1.00
	SI	512
	MC2	States-TPPI
	SF	500.1300000 MHz
	WDW	QSINE
	SSB	2
	LB	0.00 Hz

GB 0



CDCl₃, 500 MHz, NOESY
d8 = 0.9 sec

NAME	Compound 2
EXPNO	10
PROCNO	1
Date_	20120324
Time	2.12
INSTRUM	spect
PROBHD	5 mm PABBI 1H/
PULPROG	noesyph
TD	2048
SOLVENT	CDCl ₃
NS	56
DS	4
SWH	3004.808 Hz
FIDRES	1.467191 Hz
AQ	0.3410036 sec
RG	128
DW	166.400 usec
DE	12.00 usec
TE	298.2 K
d0	0.00015583 sec
D1	2.00000000 sec
D8	0.89999998 sec
IN0	0.00033280 sec
ST1CNT	0

===== CHANNEL f1 =====

NUC1	1H
P1	8.30 usec
PL1	6.00 dB
SFO1	500.1323506 MHz
ND0	1
TD	256
SFO1	500.1324 MHz
FIDRES	11.737530 Hz
SW	6.008 ppm
FnMODE	States-TPPI
SI	1024
SF	500.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	512
MC2	States-TPPI
SF	500.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz

GB 0