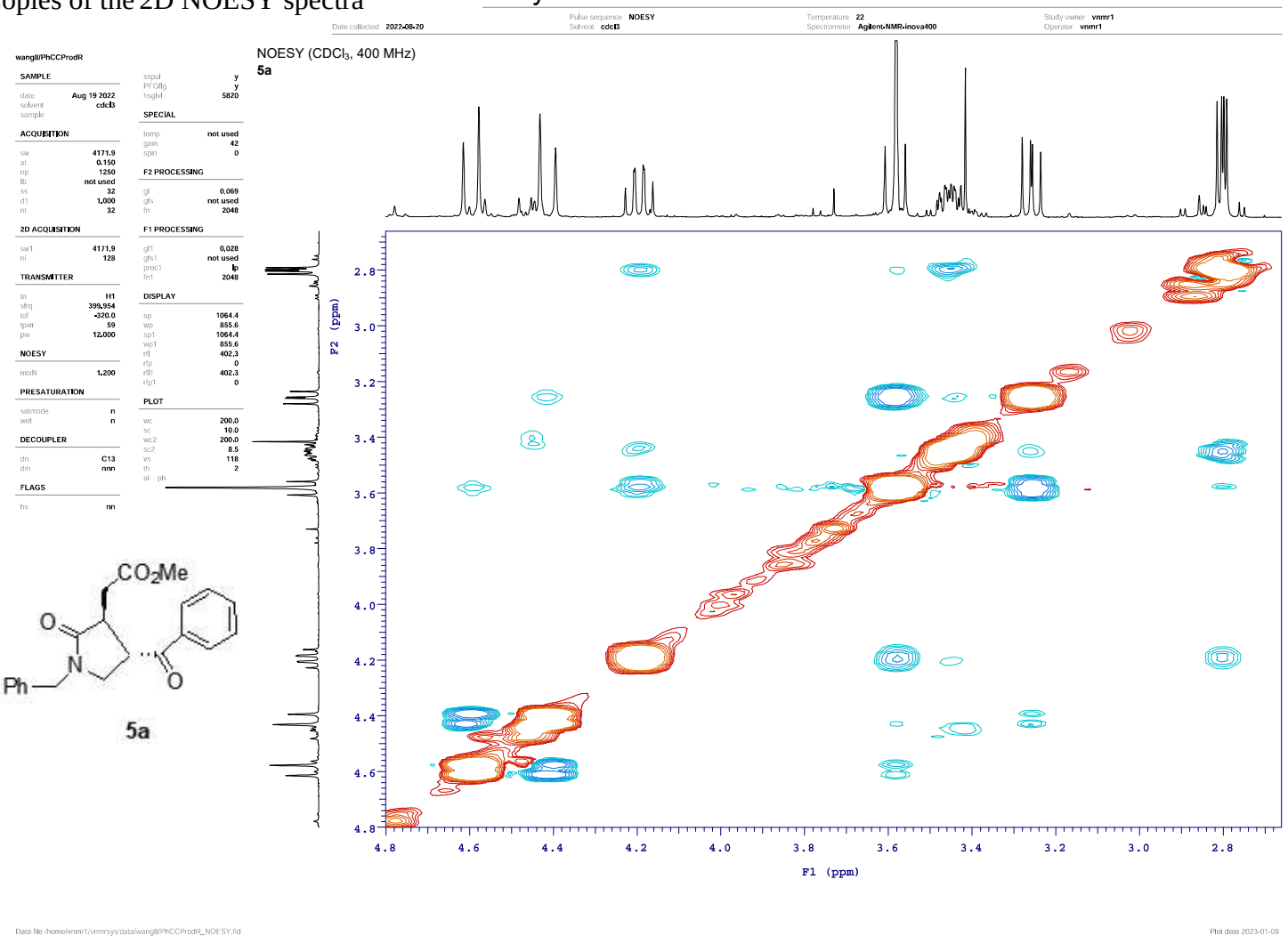
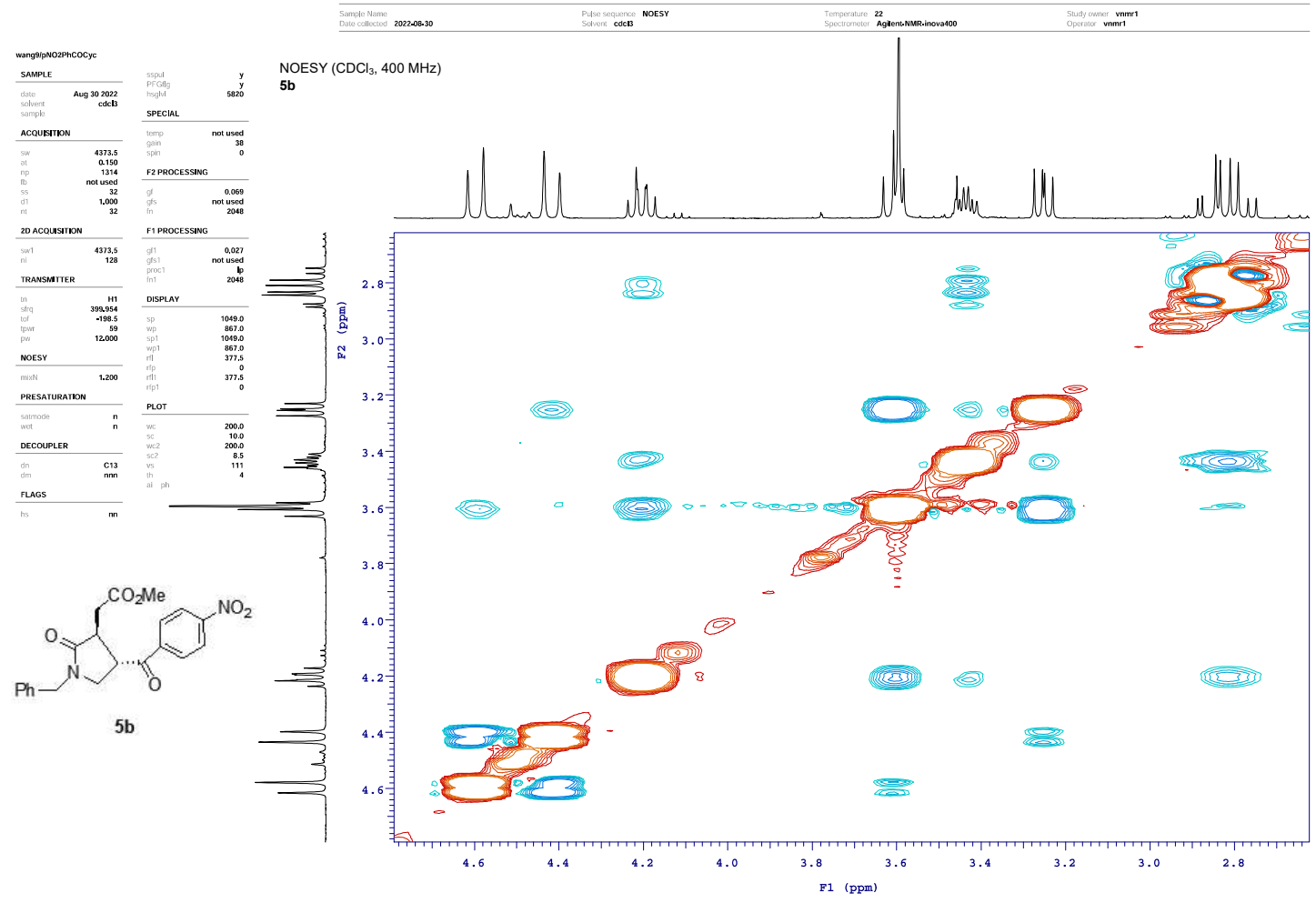
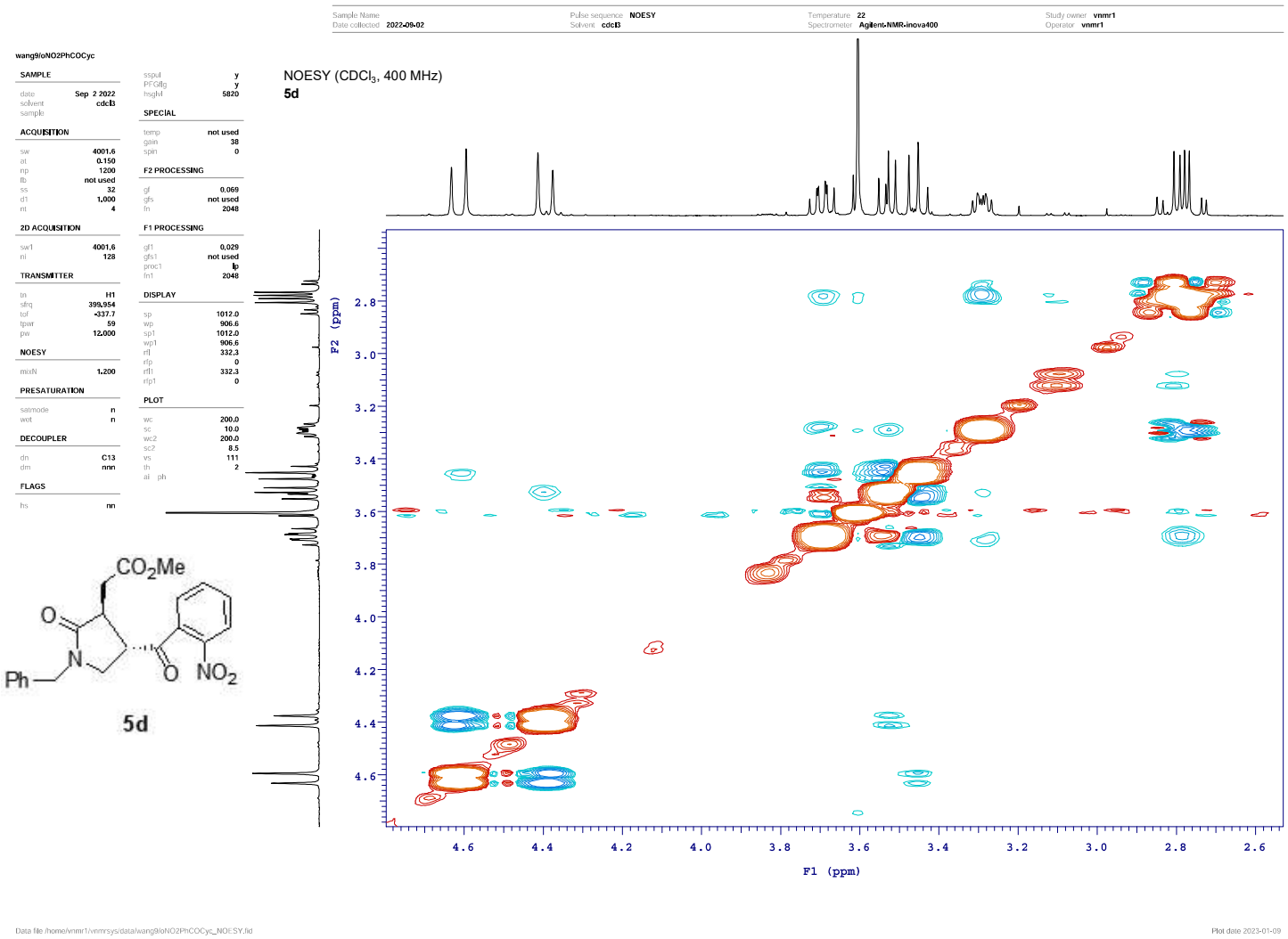
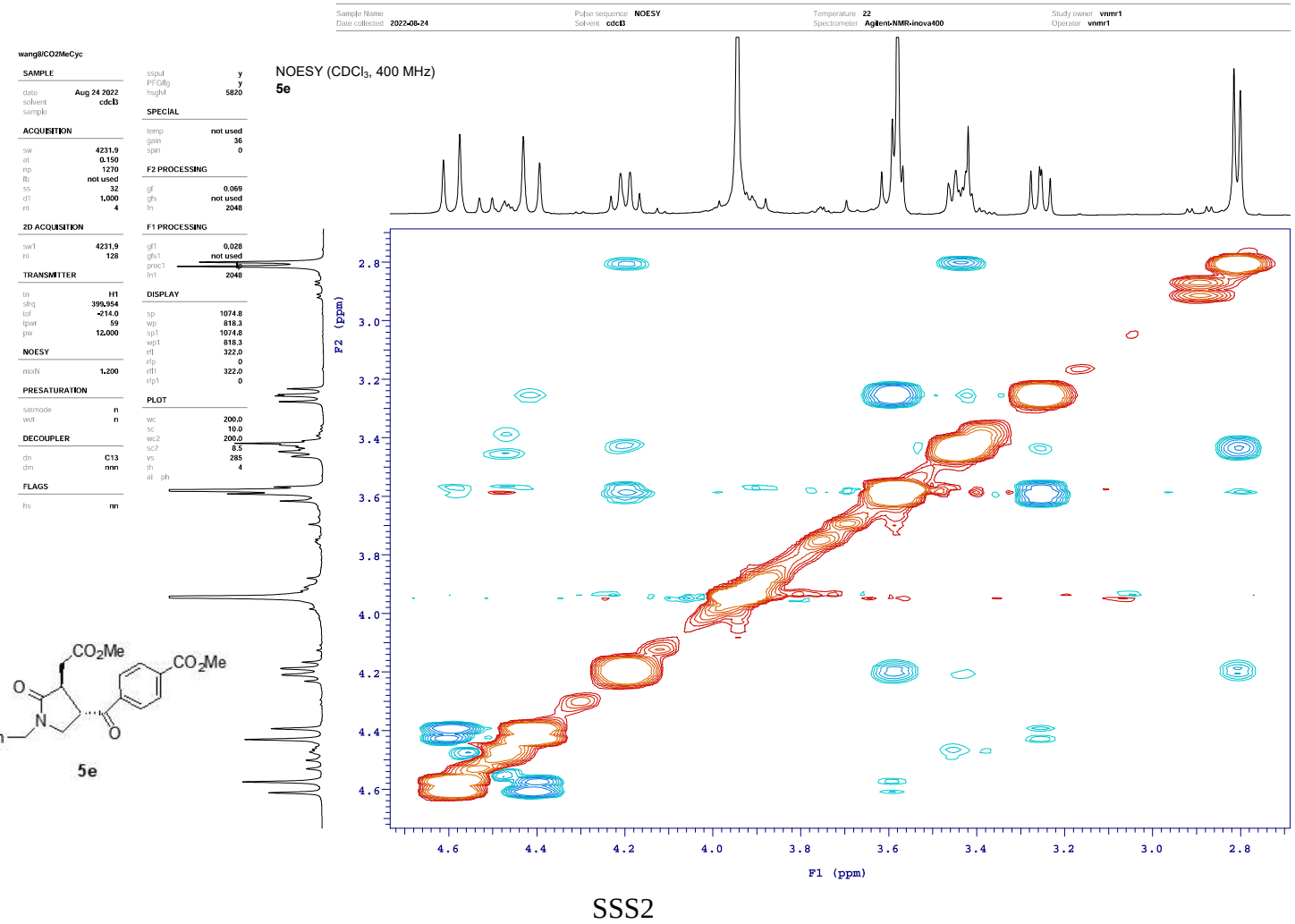
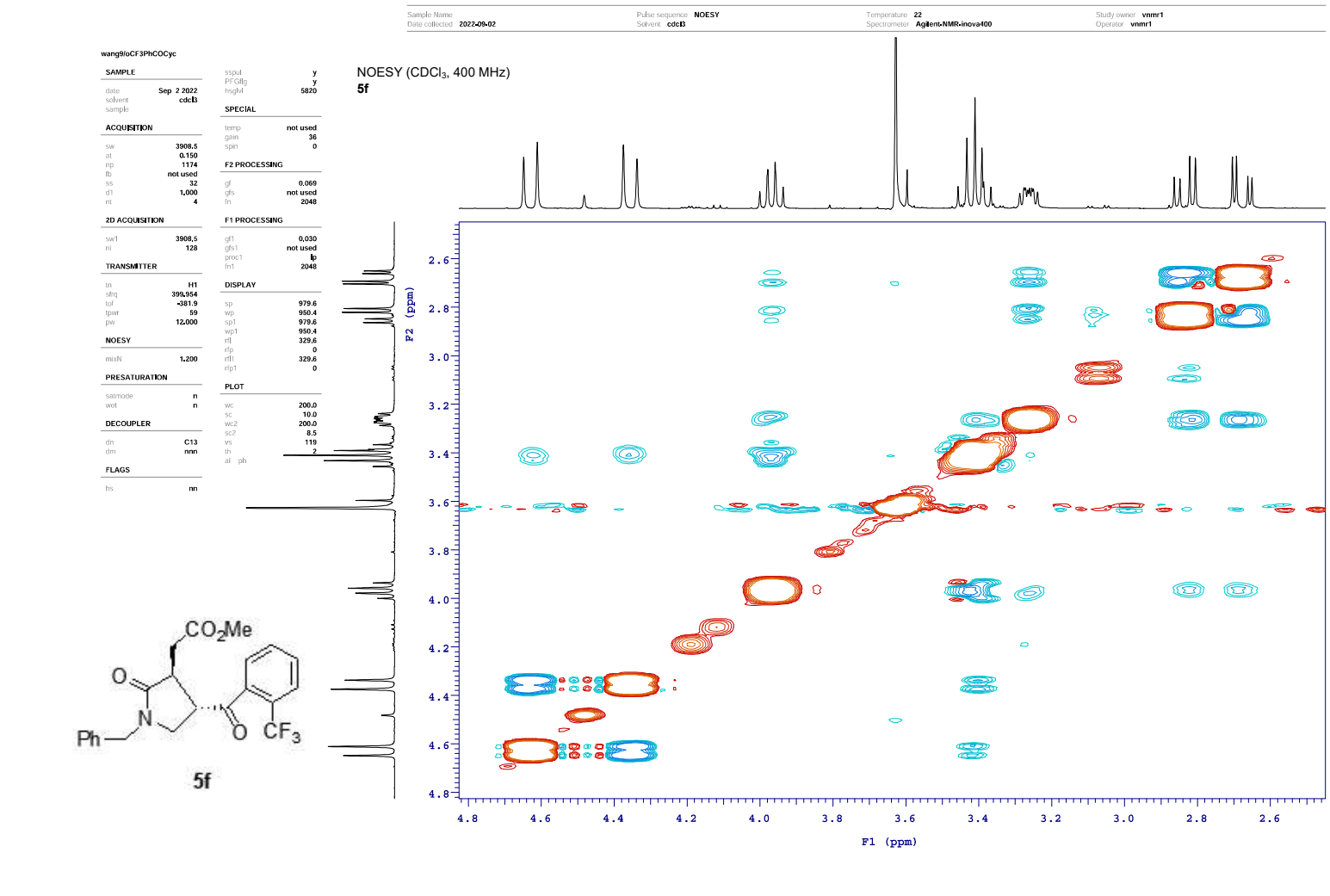
II. Copies of the 2D NOESY spectra





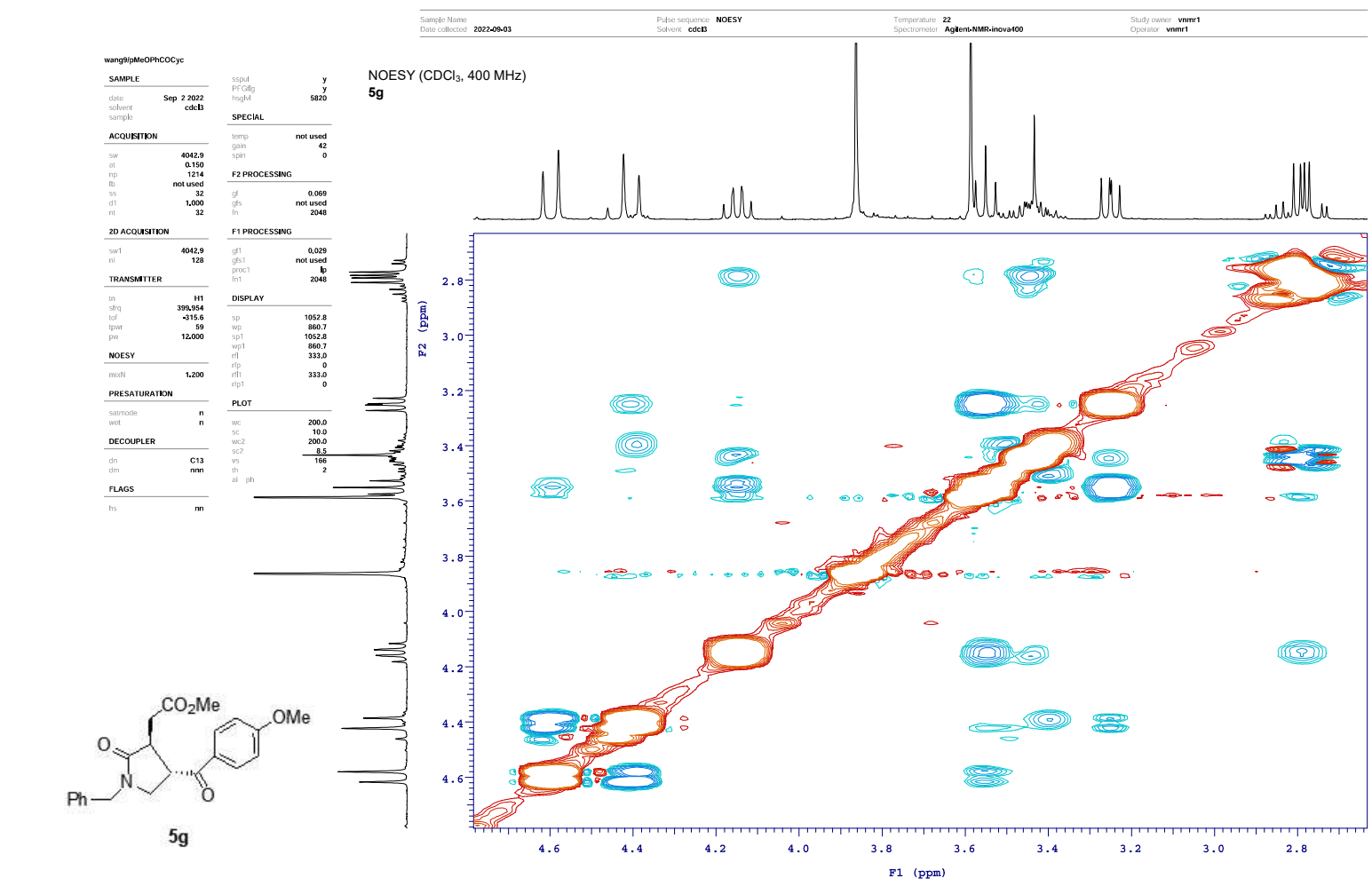

Sample Name
Date collected 2022-06-02
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
wang9/oNO2PhCOCyc
SAMPLE
date Sep 2 2022
solvent cdcl3
sample
ACQUISITION
sw 4001.6
at 0.150
np 1200
fb not used
ss 32
d1 1.000
nt 4
2D ACQUISITION
sw1 4001.6
ni 128
TRANSMITTER
tn H1
sfrq 399.954
tof -337.7
tpwr 59
pw 12.000
NOESY
mixN 1.200
PRESATURATION
satmode n
wet n
DECOUPLER
dn C13
dm nnn
FLAGS
hs nn
sspul y
PFGflg y
hsglvl 5820
SPECIAL
temp not used
gain 38
spin 0
F2 PROCESSING
gf 0.069
gfs not used
fn 2048
F1 PROCESSING
gf1 0.029
gfs1 not used
proc1 lp
fn1 2048
DISPLAY
sp 1012.0
wp 906.6
sp1 1012.0
wp1 906.6
rfl 332.3
rfp 0
rfl1 332.3
rfp1 0
PLOT
wc 200.0
sc 10.0
wc2 200.0
sc2 8.5
vs 111
th 2
al ph
NOESY (CDCl3, 400 MHz)
5d
CO2Me
O
N
Ph
O
NO2
5d
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/wang9/oNO2PhCOCyc_NOESY.fid
Plot date 2023-01-09


Sample Name
Date collected 2022-08-24
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
wang8/CO2MeCyc
SAMPLE
date Aug 24 2022
solvent cdcl3
sample
ACQUISITION
sw 4231.9
at 0.150
np 1270
fb not used
ss 32
d1 1.000
nt 4
2D ACQUISITION
sw1 4231.9
ni 128
TRANSMITTER
tn H1
sfrq 399.954
tof -214.0
tpwr 59
pw 12.000
NOESY
mixN 1.200
PRESATURATION
satmode n
wet n
DECOUPLER
dn C13
dm nnn
FLAGS
hs nn
sspul y
PFGflg y
hsglvl 5820
SPECIAL
temp not used
gain 36
spin 0
F2 PROCESSING
gf 0.069
gfs not used
fn 2048
F1 PROCESSING
gf1 0.028
gfs1 not used
proc1 lp
fn1 2048
DISPLAY
sp 1074.8
wp 818.3
sp1 1074.8
wp1 818.3
rfl 322.0
rfp 0
rfl1 322.0
rfp1 0
PLOT
wc 200.0
sc 10.0
wc2 200.0
sc2 8.5
vs 285
th 4
al ph
NOESY (CDCl3, 400 MHz)
5e
CO2Me
CO2Me
O
N
Ph
O
5e
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/wang8/CO2MeCyc_NOESY.fid
Plot date 2023-01-08


Sample Name
Date collected 2022-09-02
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
wang9/oCF3PhCOCyc
NOESY (CDCl3, 400 MHz)
5f
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/wang9/oCF3PhCOCyc_NOESY.fid
Plot date 2023-01-09

CO2Me
O
N
Ph
O
CF3

5f


Sample Name
Date collected 2022-09-03
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1
wang9/pMeOPhCOCyc
NOESY (CDCl3, 400 MHz)
5g
F2 (ppm)
F1 (ppm)
Data file /home/vnmr1/vnmrsys/data/wang9/pMeOPhCOCyc_NOESY.fid
Plot date 2023-01-09

CO2Me
OMe
O
N
Ph
O

5g

Sample Name | Pulse sequence NOESY | Temperature 22 | Study owner vnmr1
Date collected 2022-09-24 | Solvent cdcl3 | Spectrometer Agilent-NMR-inova400 | Operator vnmr1

wang9/MePhCyc

SAMPLE
date Sep 23 2022
solvent cdcl3
sample

ACQUISITION
sw 3870.0
at 0.150
np 1162
fb not used
ss 32
d1 1.000
nt 32

2D ACQUISITION
sw1 3870.0
ni 128

TRANSMITTER
tn H1
sfrq 399.954
tof -344.3
tpwr 59
pw 12.000

NOESY
mixN 1.200

PRESATURATION
satmode n
wet n

DECOUPLER
dn C13
dm nnn

FLAGS
hs nn

sspul y
PFGflg y
hsghd 5820

SPECIAL
temp not used
gain 42
spin 0

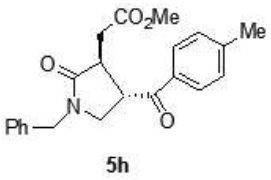
F2 PROCESSING
gf 0.069
gfs not used
fn 2048

F1 PROCESSING
gf1 0.030
gfs1 not used
proc1 lp
fn1 2048

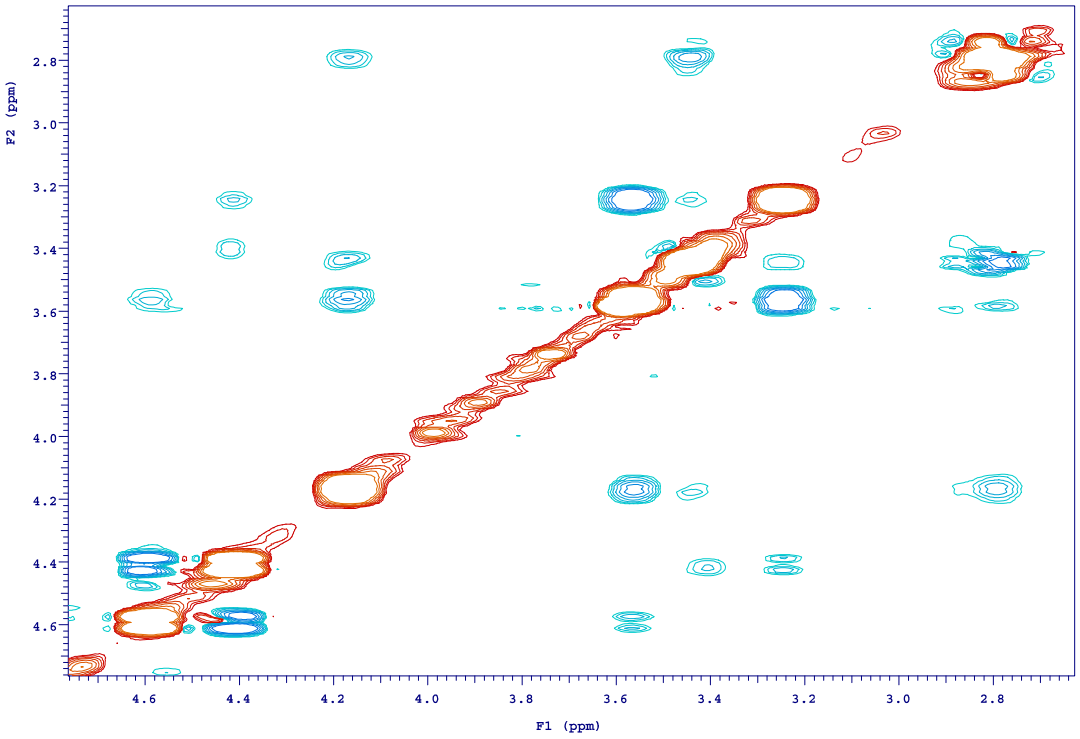
DISPLAY
sp 1050.9
wp 854.1
sp1 1050.9
wp1 854.1
rfl 275.6
rfp 0
rfl1 275.6
rfp1 0

PLOT
wc 200.0
sc 10.0
wc2 200.0
sc2 8.5
vs 229
th 3
ai ph

NOESY ($CDCl_3$, 400 MHz)
5h (trans/cis = 13 : 1)



5h



Data file /home/vnmr1/vnmrsys/data/wang9/MePhCyc_NOESY.fid

Plot date 2023-01-09

Sample Name | Pulse sequence NOESY | Temperature 22 | Study owner vnmr1
Date collected 2022-09-28 | Solvent cdcl3 | Spectrometer Agilent-NMR-inova400 | Operator vnmr1

wang9/MePhCycmix

SAMPLE
date Sep 28 2022
solvent cdcl3
sample

ACQUISITION
sw 4042.9
at 0.150
np 1212
fb not used
ss 32
d1 1.000
nt 4

2D ACQUISITION
sw1 4042.9
ni 128

TRANSMITTER
tn H1
sfrq 399.954
tof -304.6
tpwr 59
pw 12.000

NOESY
mixN 1.200

PRESATURATION
satmode n
wet n

DECOUPLER
dn C13
dm nnn

FLAGS
hs nn

sspul y
PFGflg y
hsghd 5820

SPECIAL
temp not used
gain 20
spin 0

F2 PROCESSING
gf 0.069
gfs not used
fn 2048

F1 PROCESSING
gf1 0.029
gfs1 not used
proc1 lp
fn1 2048

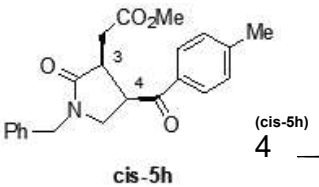
DISPLAY
sp 926.8
wp 963.3
sp1 926.8
wp1 963.3
rfl 320.8
rfp 0
rfl1 320.8
rfp1 0

PLOT
wc 200.0
sc 10.0
wc2 200.0
sc2 8.5
vs 221
th 3
ai ph

NOESY ($CDCl_3$, 400 MHz)
5h (trans/cis = 1.2 : 1)

(cis-5h) 4

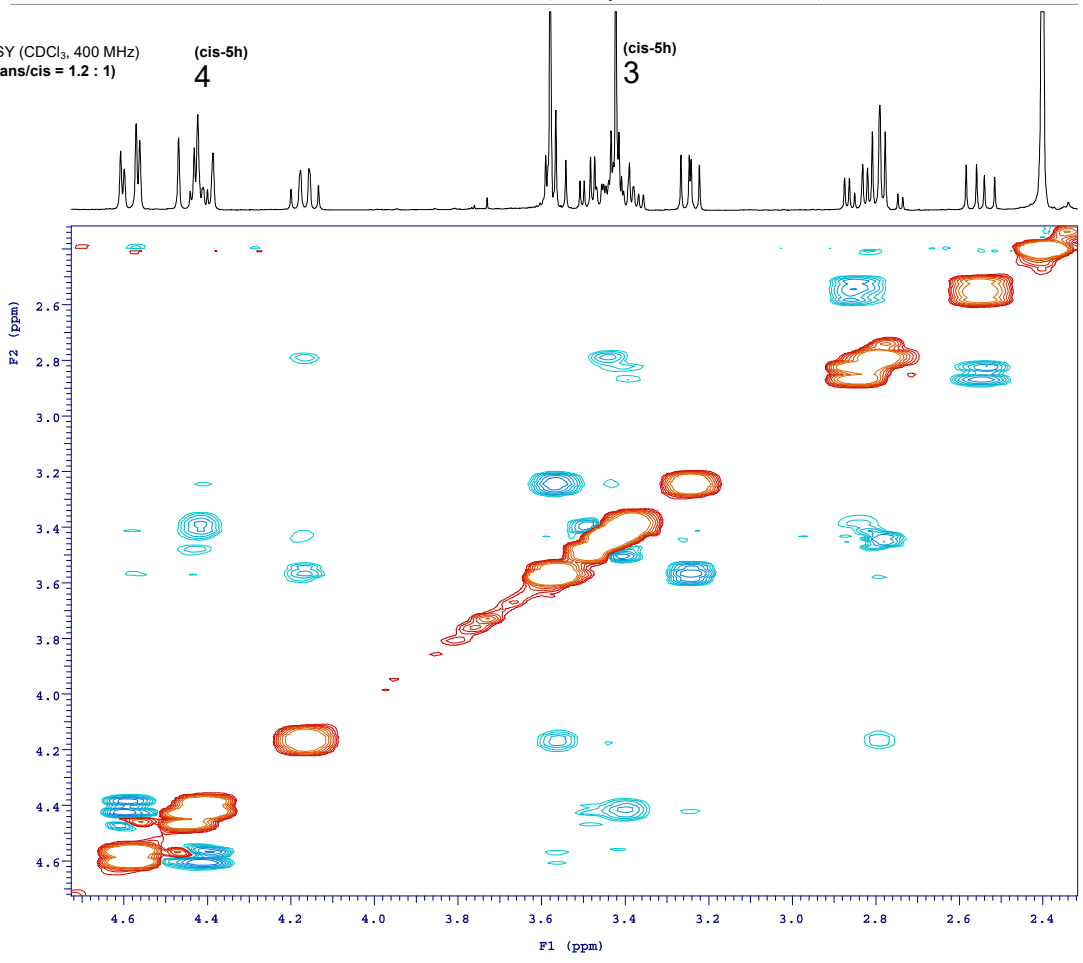
(cis-5h) 3



cis-5h

(cis-5h) 3

(cis-5h) 4



Data file /home/vnmr1/vnmrsys/data/wang9/MePhCycmix_NOESY.fid

Plot date 2023-01-09

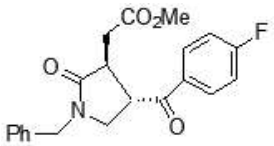
Sample Name | Pulse sequence NOESY | Temperature 22 | Study owner vnmr1
Date collected 2022-09-07 | Solvent cdcl3 | Spectrometer Agilent-NMR-inova400 | Operator vnmr1

wang9/FPhCOCyc

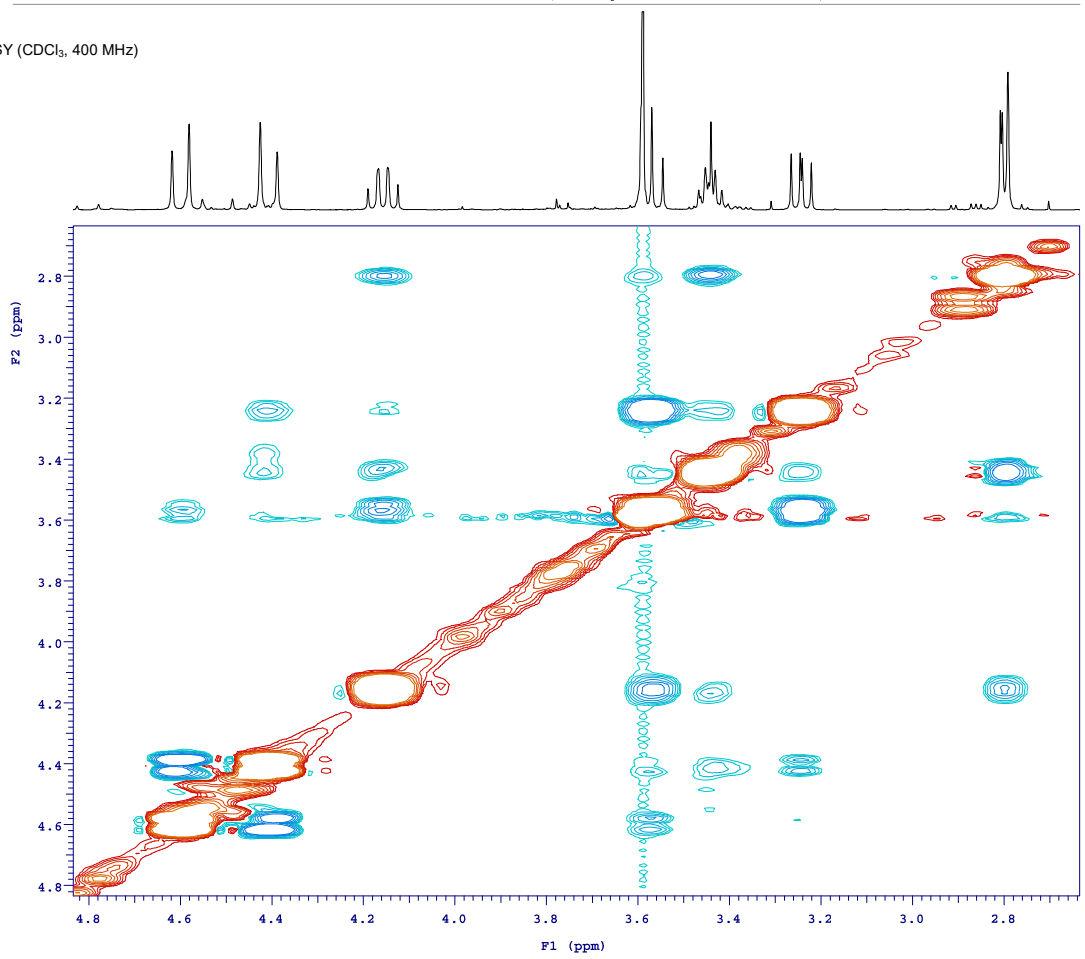
NOESY ($CDCl_3$, 400 MHz)

5i

SAMPLE			
date	Sep 7 2022	sspul	y
solvent	cdcl3	PFGflg	y
sample		hsglvl	5820
ACQUISITION		**SPECIAL**	
sw	4056.8	temp	not used
at	0.150	gain	38
np	1216	spin	0
fb	not used	**F2 PROCESSING**	
ss	32	gf	0.069
d1	1.000	gfs	not used
nt	32	fn	2048
2D ACQUISITION		**F1 PROCESSING**	
sw1	4056.8	gf1	0.029
ni	128	gfs1	not used
TRANSMITTER		proc1	lp
tn	H1	fn1	2048
sfrq	399.954	**DISPLAY**	
tof	-258.2	sp	1053.9
tpwr	59	wp	879.5
pw	12.000	sp1	1053.9
NOESY		wp1	879.5
mixN	1.200	rfl	281.2
PRESATURATION		rfp	0
satmode	n	rfl1	281.2
wet	n	rfp1	0
DECOUPLER		**PLOT**	
dn	C13	wc	200.0
dm	nnn	sc	10.0
FLAGS		wc2	200.0
hs	nn	sc2	8.5
		vs	167
		th	2
		ai ph	



5i



Data file /home/vnmr1/vnmrsys/data/wang9/FPhCOCyc_NOESY.fid

Plot date 2023-01-09

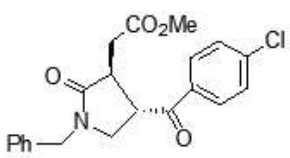
Sample Name | Pulse sequence NOESY | Temperature 22 | Study owner vnmr1
Date collected 2022-10-24 | Solvent cdcl3 | Spectrometer Agilent-NMR-inova400 | Operator vnmr1

torii/4ClPhCOCyc

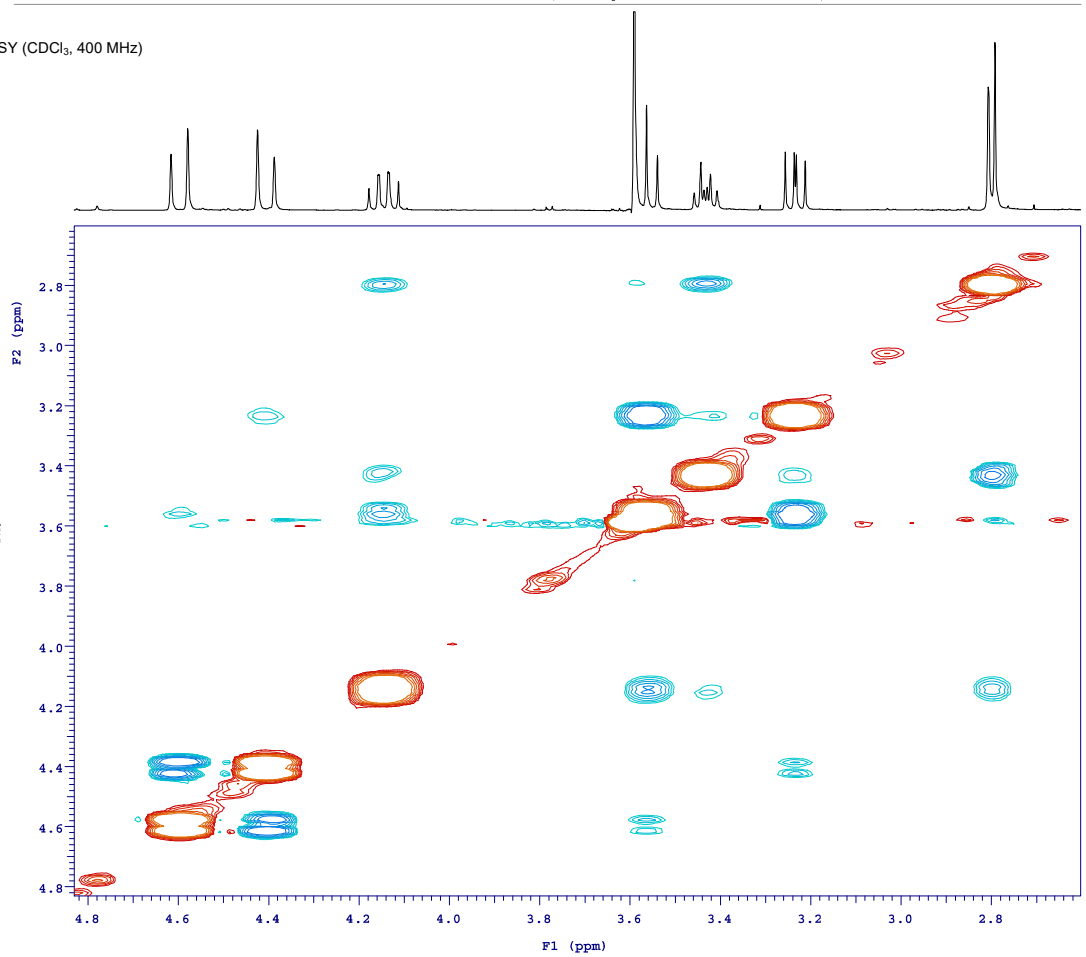
NOESY ($CDCl_3$, 400 MHz)

5j

SAMPLE			
date	Oct 24 2022	sspul	y
solvent	cdcl3	PFGflg	y
sample		hsglvl	5820
ACQUISITION		**SPECIAL**	
sw	4128.0	temp	not used
at	0.150	gain	42
np	1240	spin	0
fb	not used	**F2 PROCESSING**	
ss	32	gf	0.069
d1	1.000	gfs	not used
nt	4	fn	2048
2D ACQUISITION		**F1 PROCESSING**	
sw1	4128.0	gf1	0.029
ni	128	gfs1	not used
TRANSMITTER		proc1	lp
tn	H1	fn1	2048
sfrq	399.954	**DISPLAY**	
tof	-205.7	sp	1041.0
tpwr	59	wp	890.9
pw	12.000	sp1	1041.0
NOESY		wp1	890.9
mixN	1.200	rfl	265.1
PRESATURATION		rfp	0
satmode	n	rfl1	265.1
wet	n	rfp1	0
DECOUPLER		**PLOT**	
dn	C13	wc	200.0
dm	nnn	sc	10.0
FLAGS		wc2	200.0
hs	nn	sc2	8.6
		vs	104
		th	2
		ai ph	



5j



Data file /home/vnmr1/vnmrsys/data/torii/4ClPhCOCyc_NOESY.fid

Plot date 2023-01-07

Sample Name
Date collected 2022-12-09
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1

miyake12/2ClCOPh

SAMPLE
date Dec 9 2022
solvent cdcl3
sample

ACQUISITION
sw 3807.3
at 0.150
np 1140
fb not used
ss 32
d1 1.000
nt 32

2D ACQUISITION
sw1 3807.3
ni 128

TRANSMITTER
tn H1
sfrq 399.953
tof -458.9
tpwr 59
pw 12.000

NOESY
mixN 1.200

PRESATURATION
satmode n
wet n

DECOUPLER
dn C13
dm nnn

FLAGS
hs nn

sspul y
PFGflg y
hsglvl 5820

SPECIAL
temp not used
gain 36
spin 0

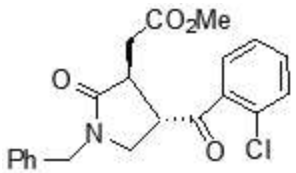
F2 PROCESSING
gf 0.069
gfs not used
fn 2048

F1 PROCESSING
gf1 0.031
gfs1 not used
proc1 lp
fn1 2048

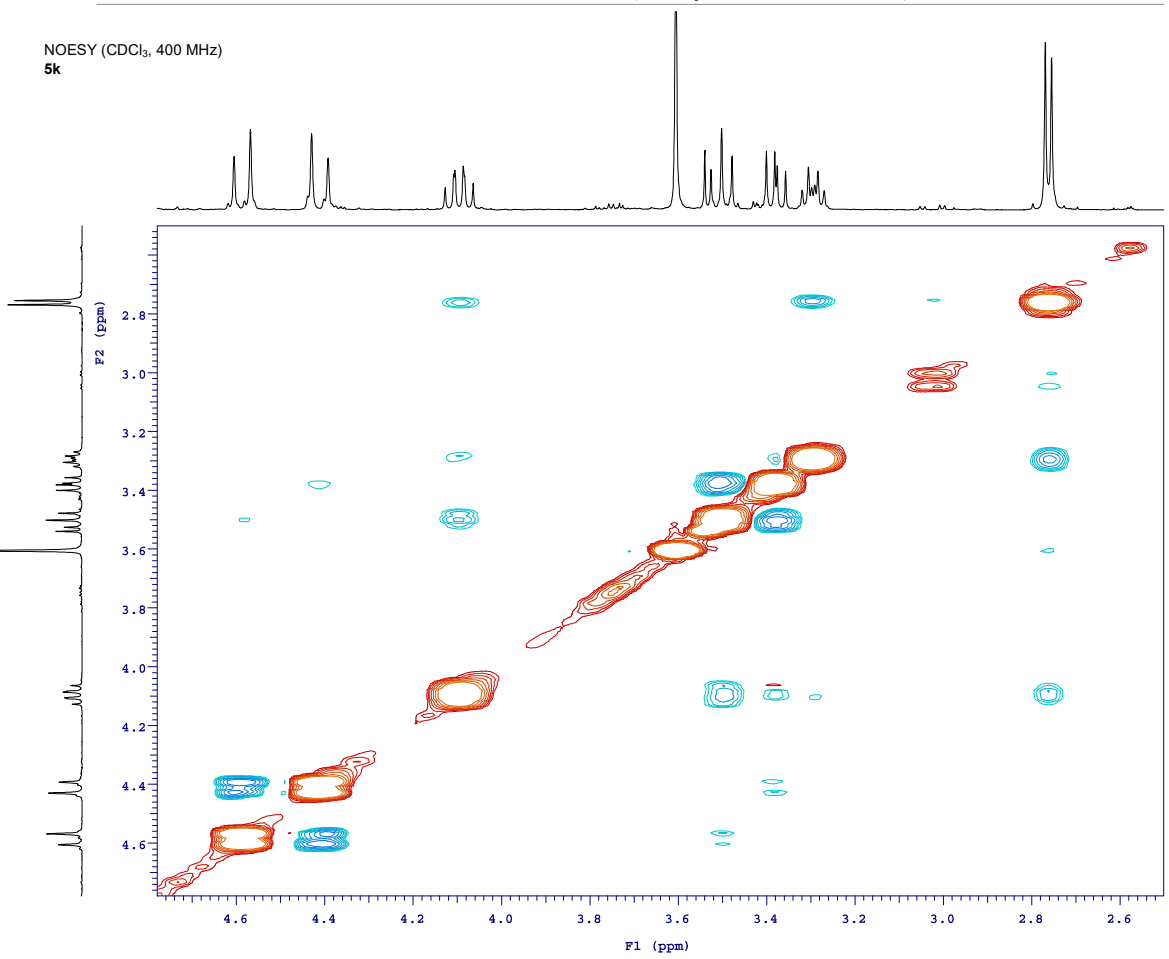
DISPLAY
sp 1000.5
wp 910.9
sp1 1000.5
wp1 910.9
rfl 356.6
rfp 0
rfl1 356.6
rfp1 0

PLOT
wc 200.0
sc 10.0
wc2 200.0
sc2 8.5
vs 173
th 2
ai ph

NOESY ($CDCl_3$, 400 MHz)
5k



5k

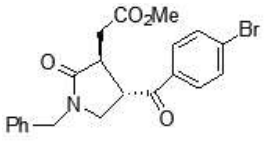


Data file /home/vnmr1/vnmrsys/data/miyake12/2ClCOPh_NOESY.fid

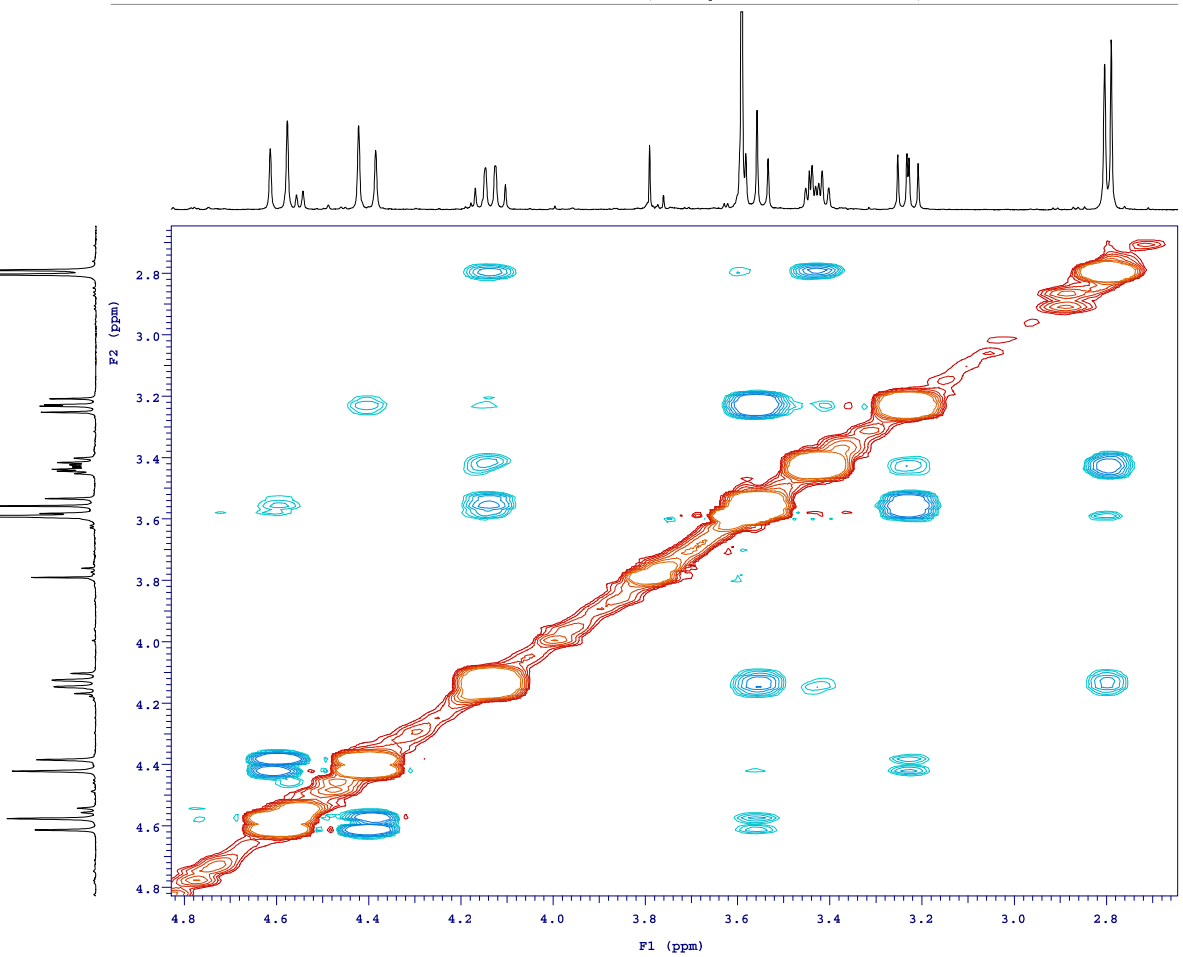
Plot date 2023-01-07

Sample Name
Date collected 2022-10-17
Pulse sequence NOESY
Solvent cdcl3
Temperature 22
Spectrometer Agilent-NMR-inova400
Study owner vnmr1
Operator vnmr1

NOESY ($CDCl_3$, 400 MHz)
5l



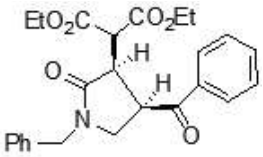
5l



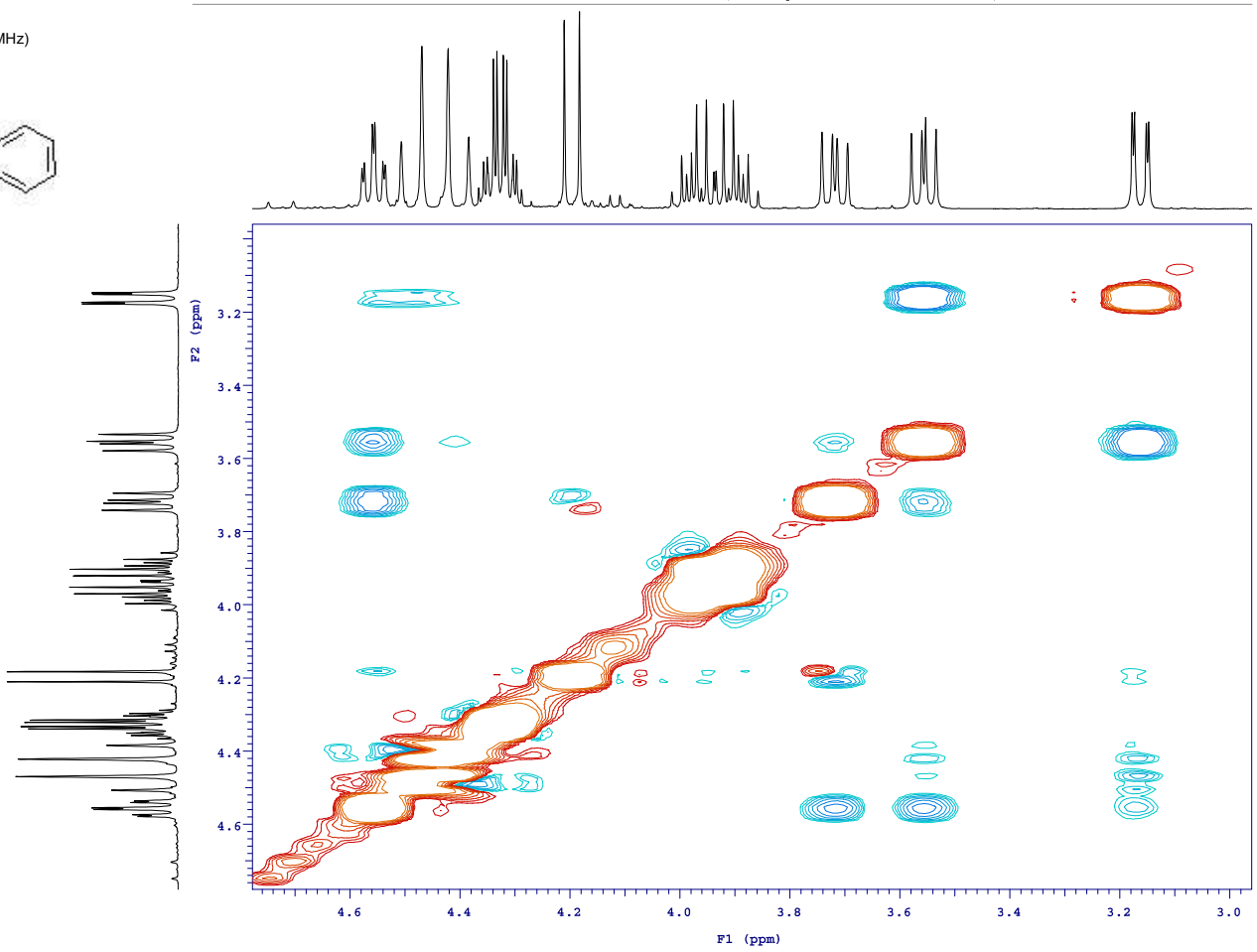
Data file /home/vnmr1/vnmrsys/data/wang10/BrPhCOCyc_NOESY.fid

Plot date 2023-01-13

NOESY ($CDCl_3$, 400 MHz)
7a



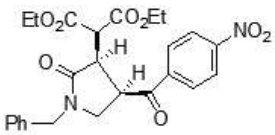
7a



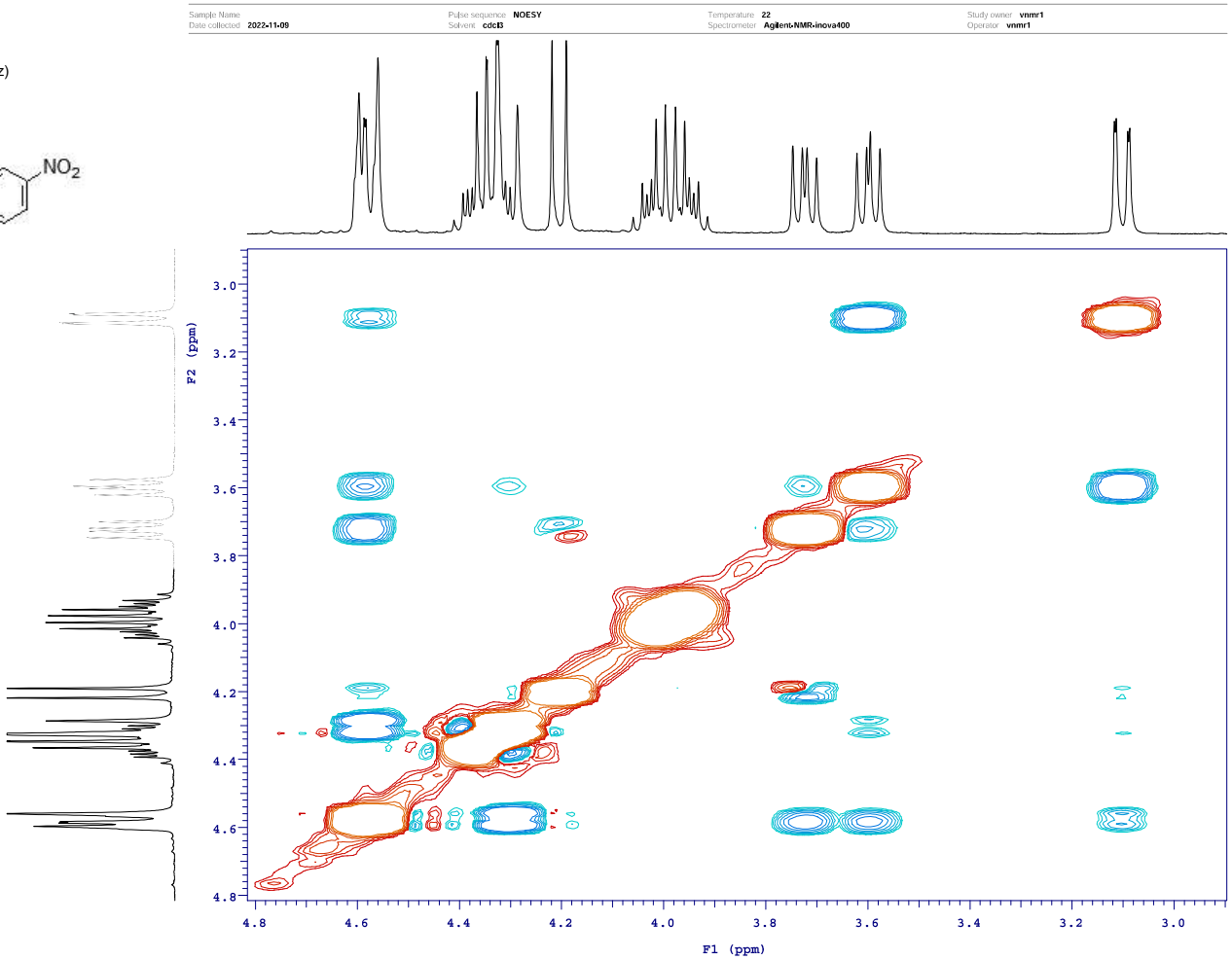
Data file /home/vnmr1/vnmrsys/data/wang10/dil:PhCycR_NOESY.fid

Plot date 2023-01-11

NOESY ($CDCl_3$, 400 MHz)
7b



7b

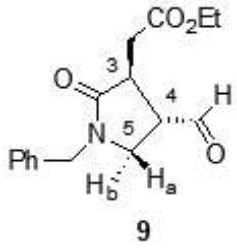


Data file /home/vnmr1/vnmrsys/data/wang10/dil:pNO2PhCyc_NOESY.fid

Plot date 2023-01-11

wang10/Et2CCHCyc

NOESY ($CDCl_3$, 400 MHz)
9_1



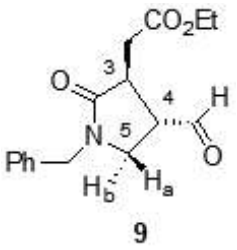
9

Data file /home/vnmr1/vnmrsys/data/wang10/Et2CCHCyc_NOESY.fid

Plot date 2023-01-20

NOESY ($CDCl_3$, 400 MHz)
9_2

wang10/Et2CCHCyc



9

Data file /home/vnmr1/vnmrsys/data/wang10/Et2CCHCyc_NOESY.fid

Plot date 2023-01-20