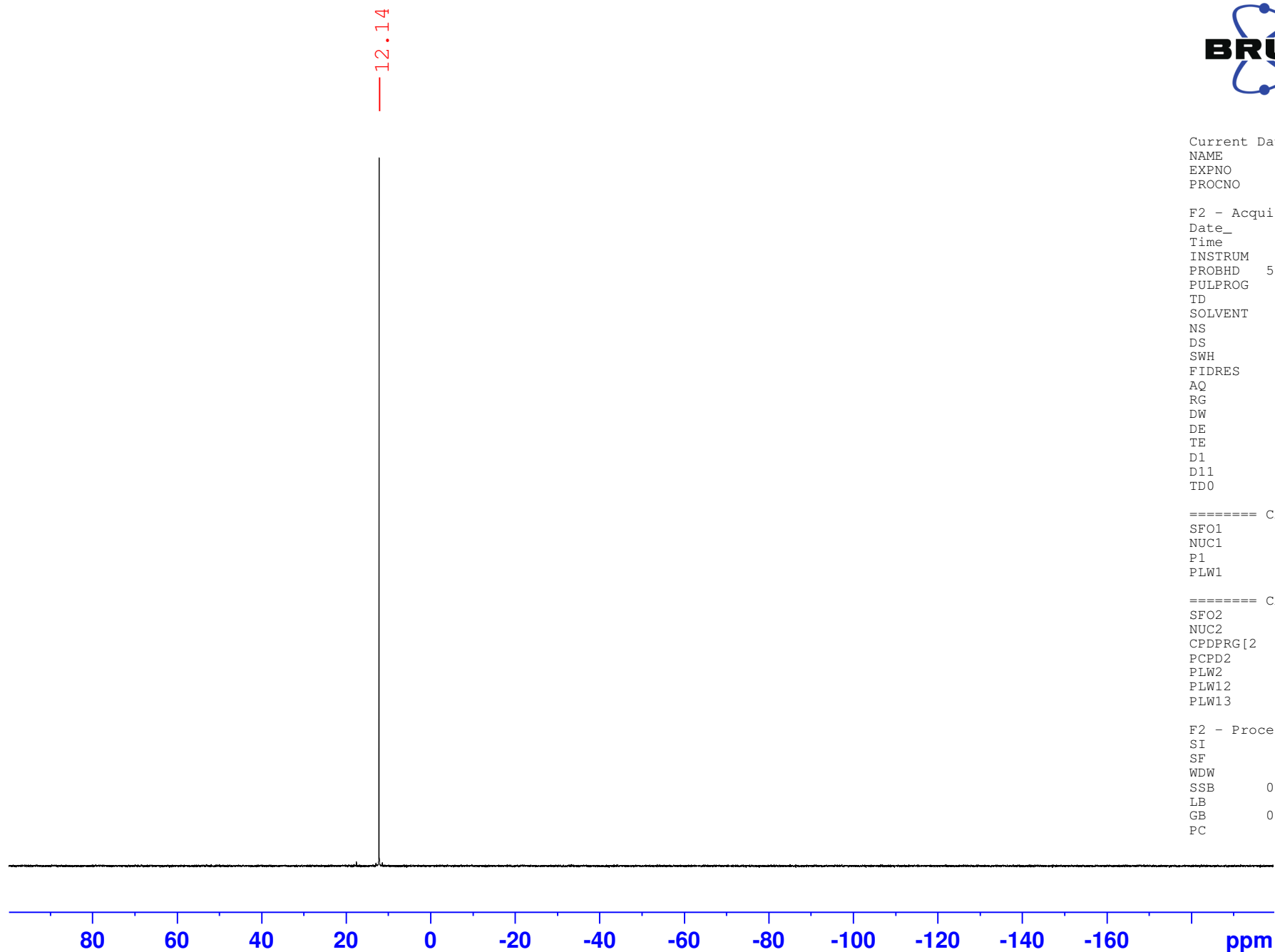




Current Data Parameters
NAME SF58
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210610
Time 13.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 49019.609 Hz
FIDRES 0.747980 Hz
AQ 0.6684672 sec
RG 1820
DW 10.200 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

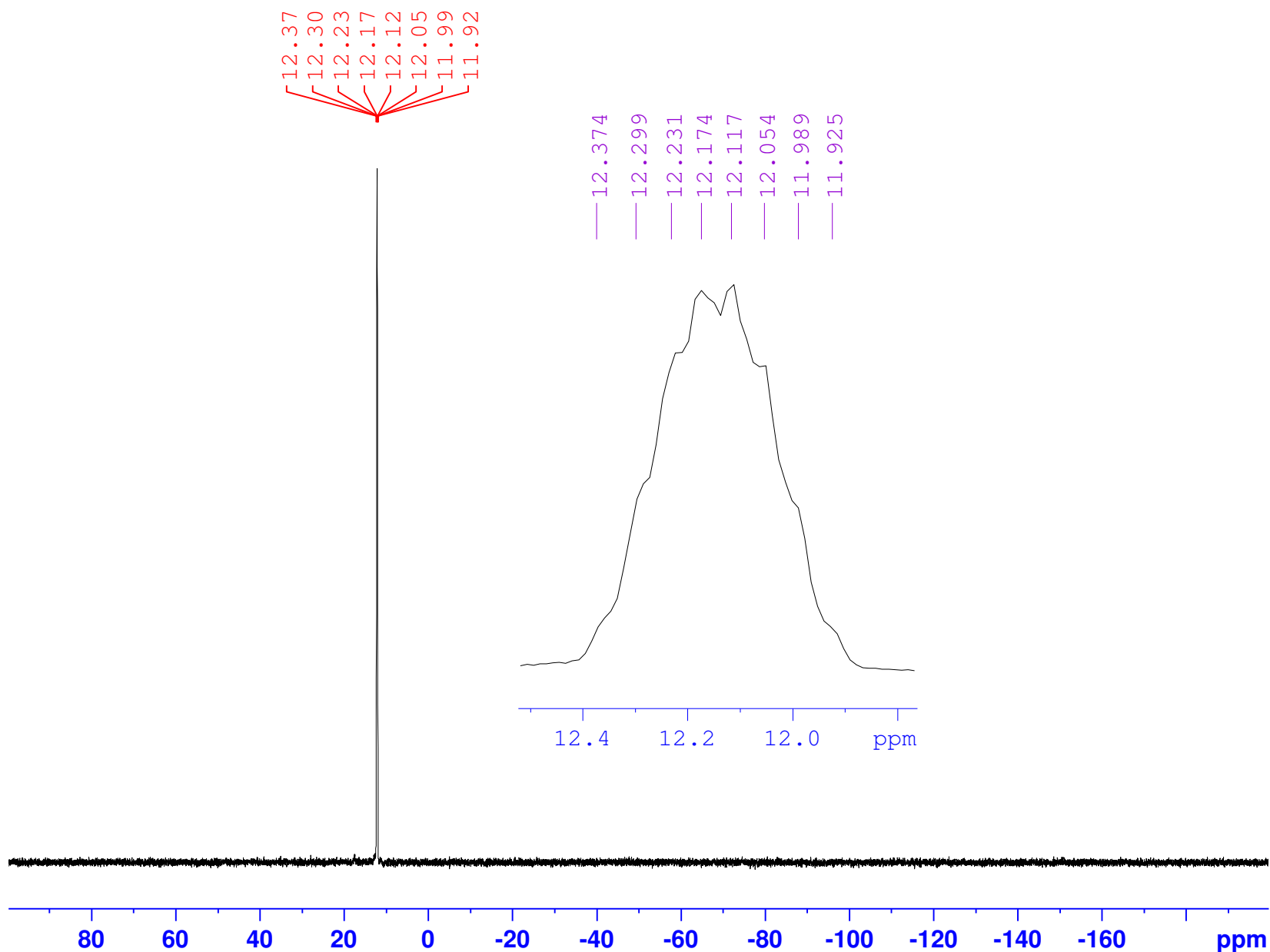
===== CHANNEL f1 =====
SFO1 121.4887762 MHz
NUC1 31P
P1 9.00 usec
PLW1 22.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.25861001 W
PLW13 0.13008000 W

F2 - Processing parameters
SI 32768
SF 121.4948510 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S1: Decoupled ^{31}P NMR spectrum of cycloadduct (3)

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)



Current Data Parameters
NAME SF58
EXPNO 7
PROCNO 1

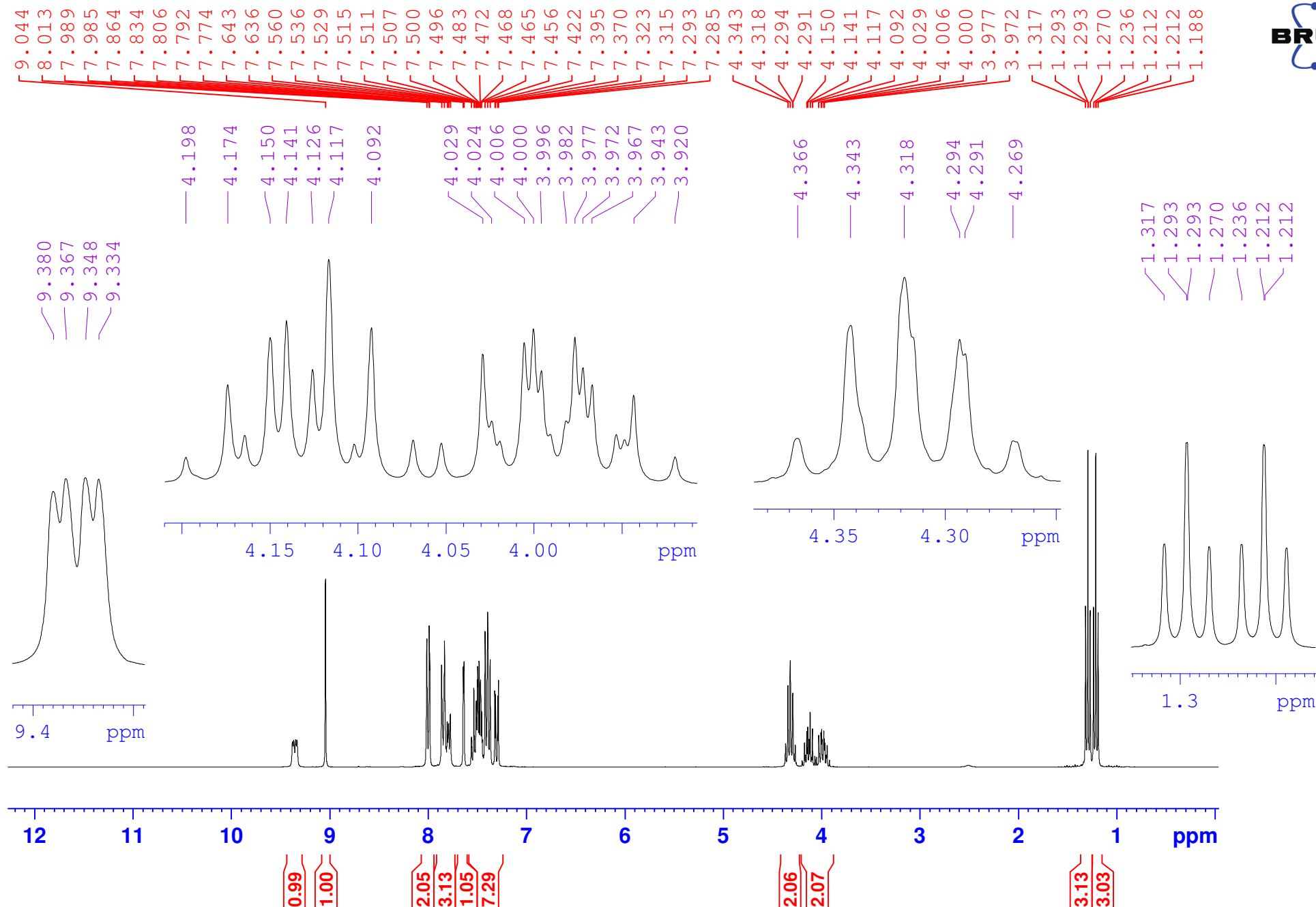
F2 - Acquisition Parameters
Date_ 20210610
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 64
DS 4
SWH 49019.609 Hz
FIDRES 0.747980 Hz
AQ 0.6684672 sec
RG 1820
DW 10.200 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 121.4887762 MHz
NUC1 31P
P1 9.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 32768
SF 121.4948510 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S2 : Coupled ^{31}P NMR spectrum of cycloadduct (3)

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)



Current Da
NAME
EXPNO
PROCNO

F2 - Acqui
Date_
Time
INSTRUM
PROBHD 5
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TD0

=====
SFO1
NUC1
P1
PLW1

F2 - Proce
SI
SF
WDW
SSB 0
LB
GB 0
PC

Figure S3: ¹H-NMR spectrum of cycloadduct (3)



Current Data Parameters
 NAME SF58
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210524
 Time 15.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 263
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175317 sec
 RG 1150
 DW 27.733 usec
 DE 6.50 usec
 TE 298.4 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 75.4752953 MHz
 NUC1 13C
 P1 8.20 usec
 P2 16.40 usec
 PLW1 41.00000000 W
 ===== CHANNEL f2 =====
 SFO2 300.1312005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 19.00000000 W
 PLW12 0.25861001 W

F2 - Processing parameters
 SI 32768
 SF 75.4677485 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

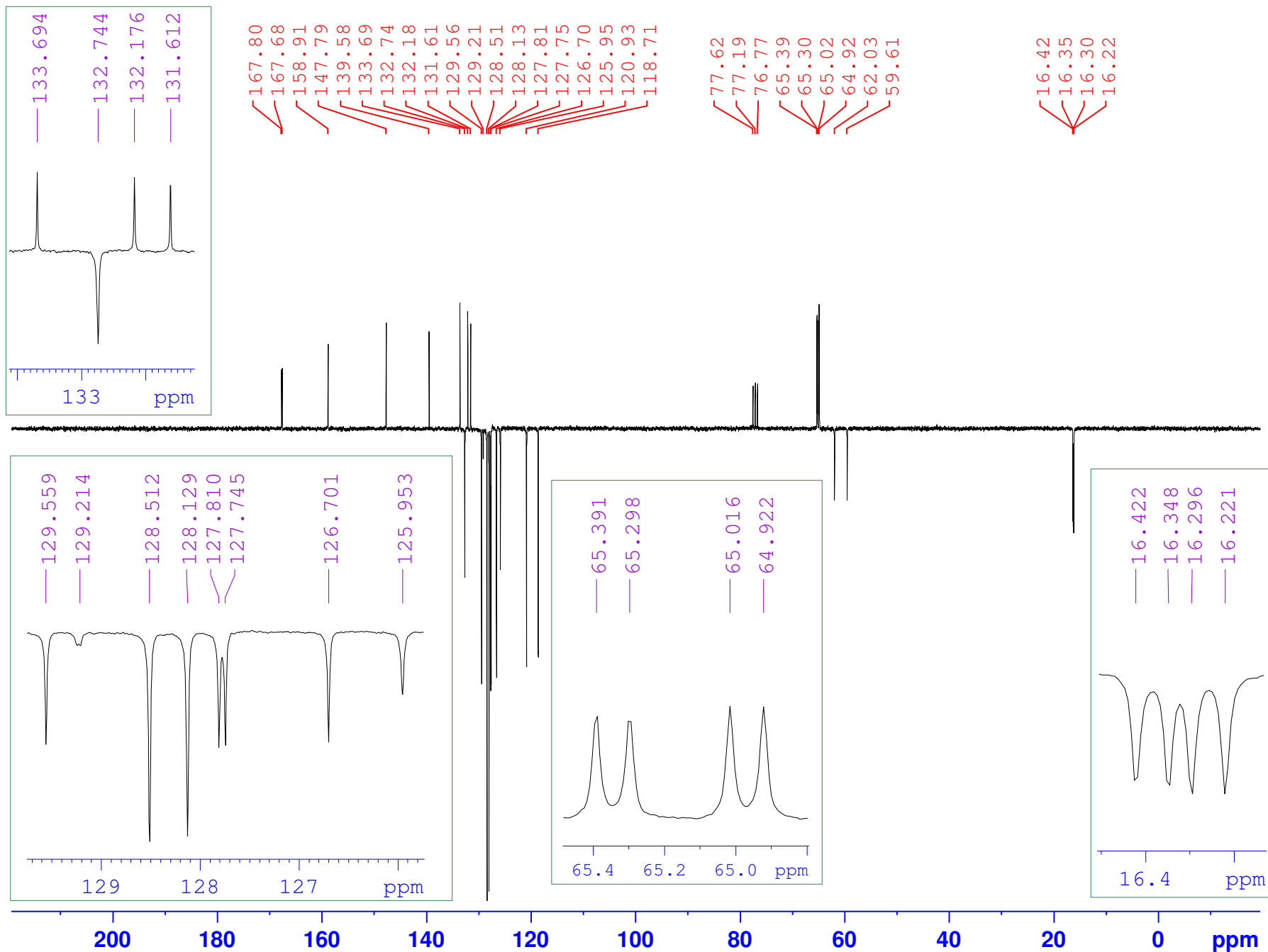
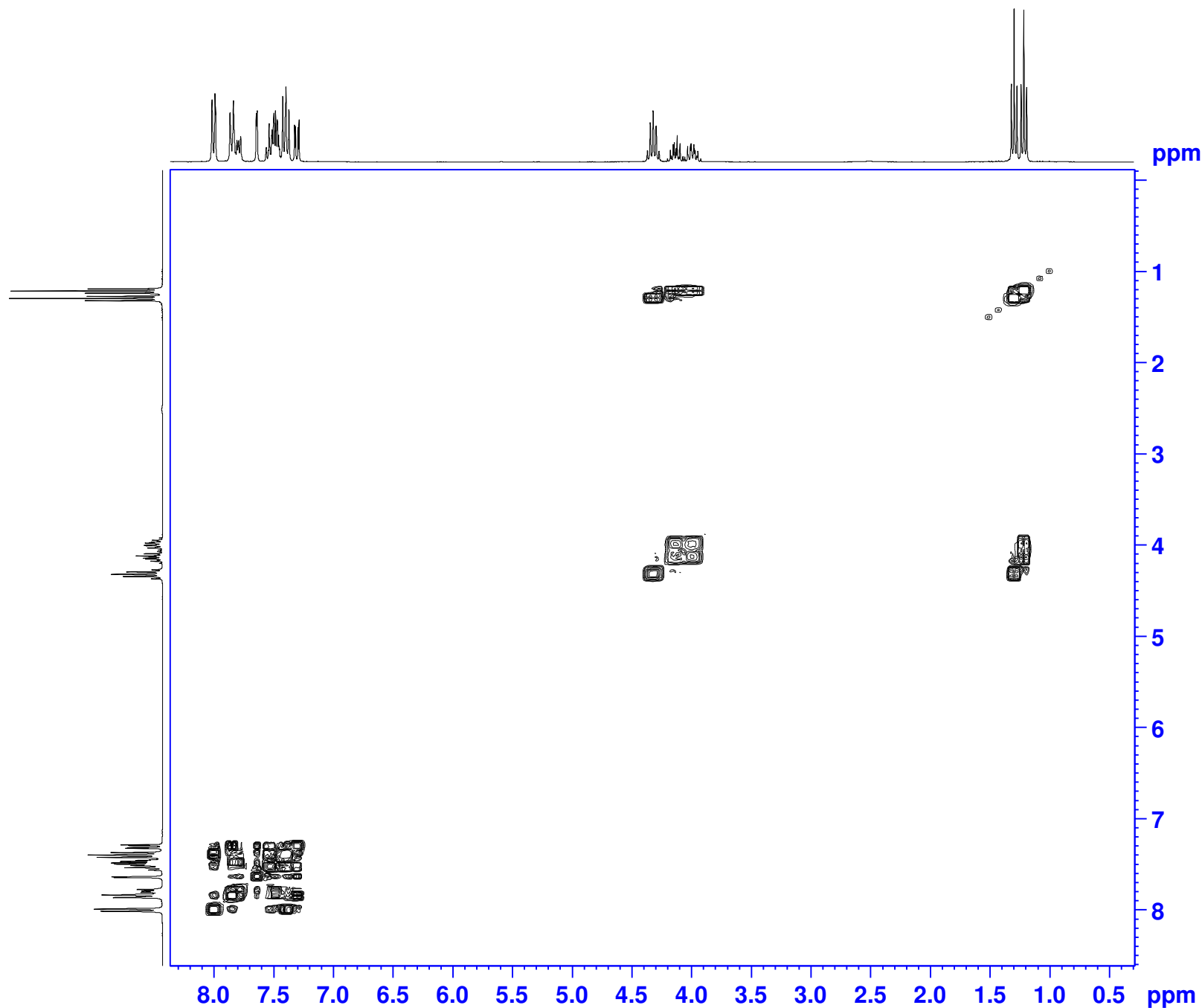


Figure S4: ¹³C-NMR spectrum of cycloadduct (3)

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)



Current Data Parameters
NAME SF58
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210524
Time 15.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDC13
NS 4
DS 8
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2555904 sec
RG 64
DW 124.800 usec
DE 6.50 usec
TE 297.9 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024960 sec

===== CHANNEL f1 =====
SFO1 300.1318044 MHz
NUC1 1H
P0 10.90 usec
P1 10.90 usec
P17 2500.00 usec
PLW1 19.00000000 W
PLW10 2.50589991 W

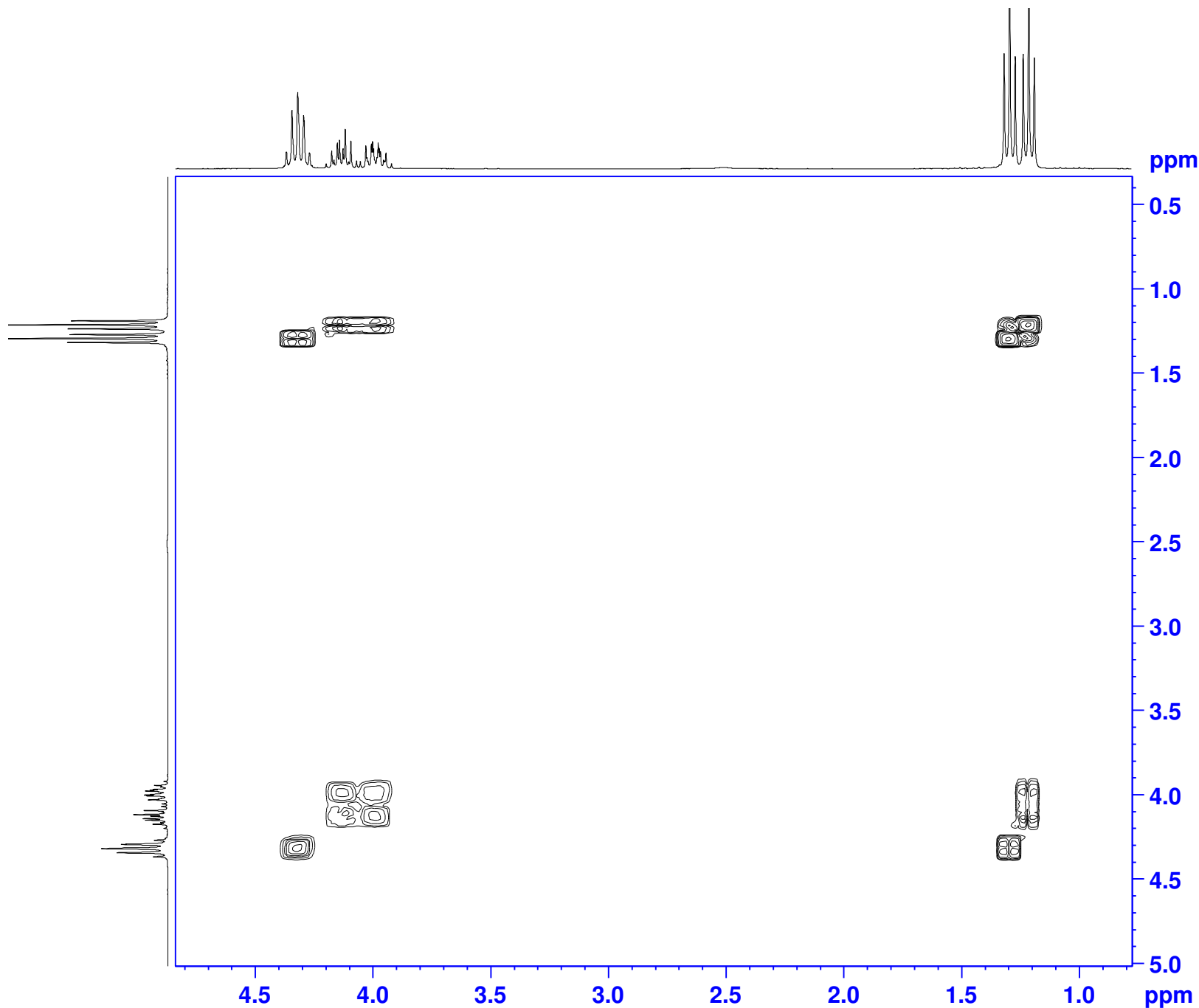
===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 109
SFO1 300.1318 MHz
FIDRES 36.756058 Hz
SW 13.349 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Figure S5: ^1H - ^1H COSY NMR spectrum of cycloadduct (3)



Current Data Parameters
NAME SF58
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210524
Time 15.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppgf
TD 2048
SOLVENT CDC13
NS 4
DS 8
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2555904 sec
RG 64
DW 124.800 usec
DE 6.50 usec
TE 297.9 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024960 sec

===== CHANNEL f1 =====
SFO1 300.1318044 MHz
NUC1 1H
P0 10.90 usec
P1 10.90 usec
P17 2500.00 usec
PLW1 19.00000000 W
PLW10 2.50589991 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 109
SFO1 300.1318 MHz
FIDRES 36.756058 Hz
SW 13.349 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Figure S6 : Expanded region of ^1H - ^1H COSY NMR spectrum (0.5 – 5.0 ppm and 0.5 – 5.0 ppm) of cycloadduct (3)

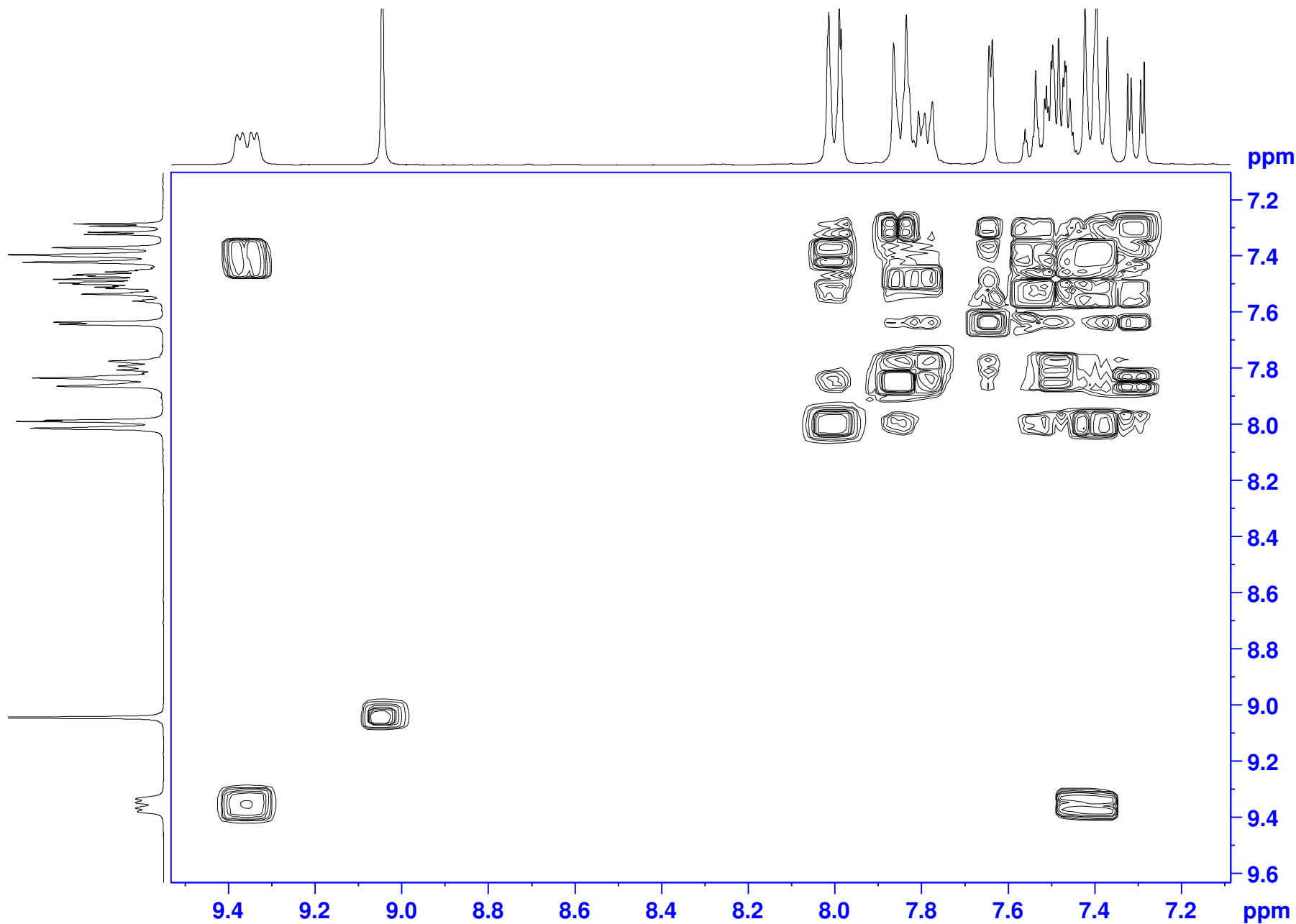


Figure S7 : Expanded region of ^1H - ^1H COSY NMR spectrum (7.2 – 9.5 ppm and 7.2 – 9.5 ppm) of cycloadduct (3)

Current Data Parameters
NAME SF58
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210524
Time 15.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2555904 sec
RG 64
DW 124.800 usec
DE 6.50 usec
TE 297.9 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024960 sec

===== CHANNEL f1 =====
SFO1 300.1318044 MHz
NUC1 1H
P0 10.90 usec
P1 10.90 usec
P17 2500.00 usec
PLW1 19.00000000 W
PLW10 2.50589991 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 109
SFO1 300.1318 MHz
FIDRES 36.756058 Hz
SW 13.349 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)

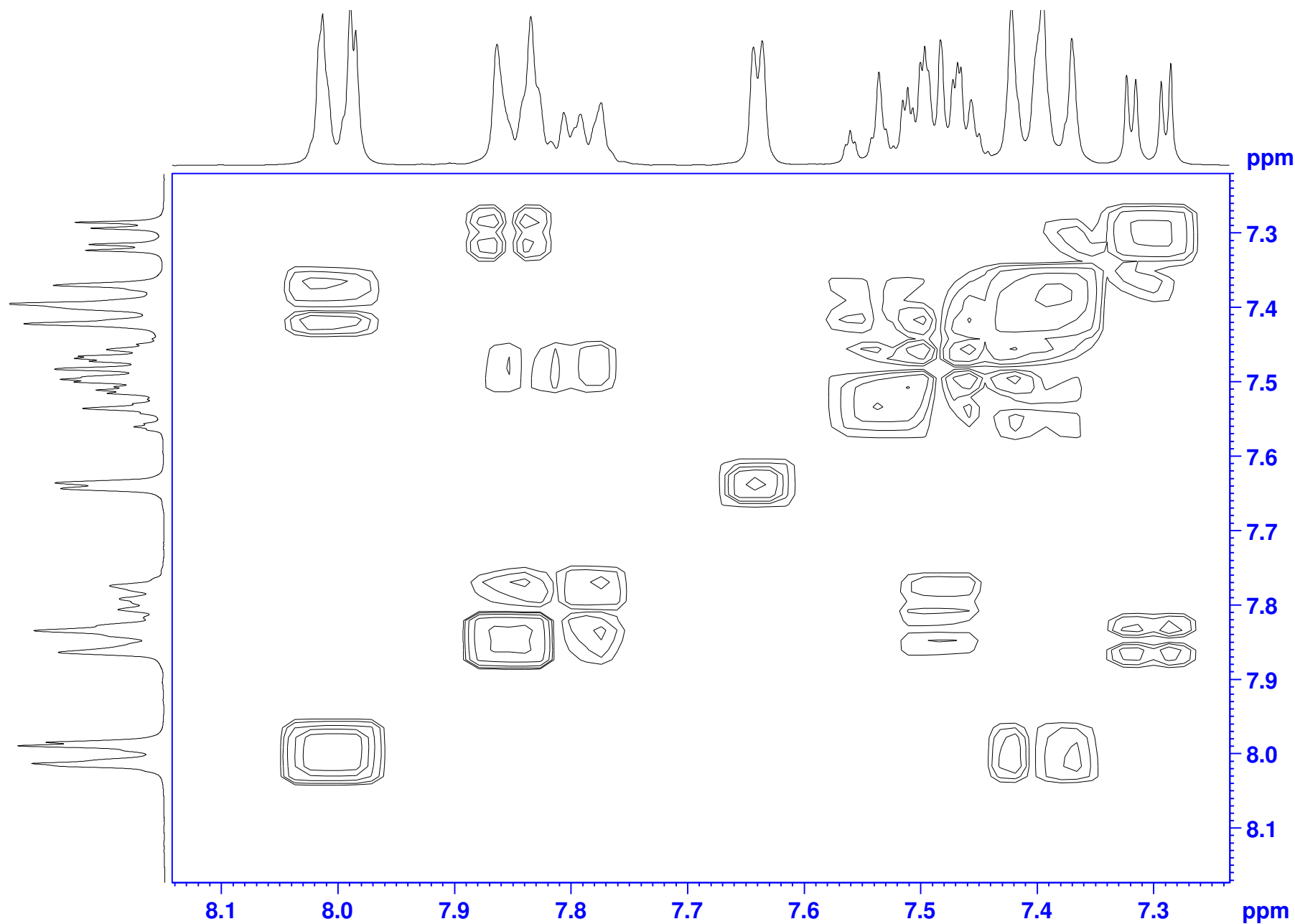


Figure S8 : Expanded region of ^1H - ^1H COSY NMR spectrum (7.25 – 8.1 ppm and 7.25 – 8.1 ppm) of cycloadduct (3)

Current Data Parameters
NAME SF58
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210524
Time 15.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 4006.410 Hz
FIDRES 1.956255 Hz
AQ 0.2555904 sec
RG 64
DW 124.800 usec
DE 6.50 usec
TE 297.9 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024960 sec

===== CHANNEL f1 =====
SFO1 300.1318044 MHz
NUC1 1H
P0 10.90 usec
P1 10.90 usec
P17 2500.00 usec
PLW1 19.00000000 W
PLW10 2.50589991 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 109
SFO1 300.1318 MHz
FIDRES 36.756058 Hz
SW 13.349 ppm
FhMODE QF

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)

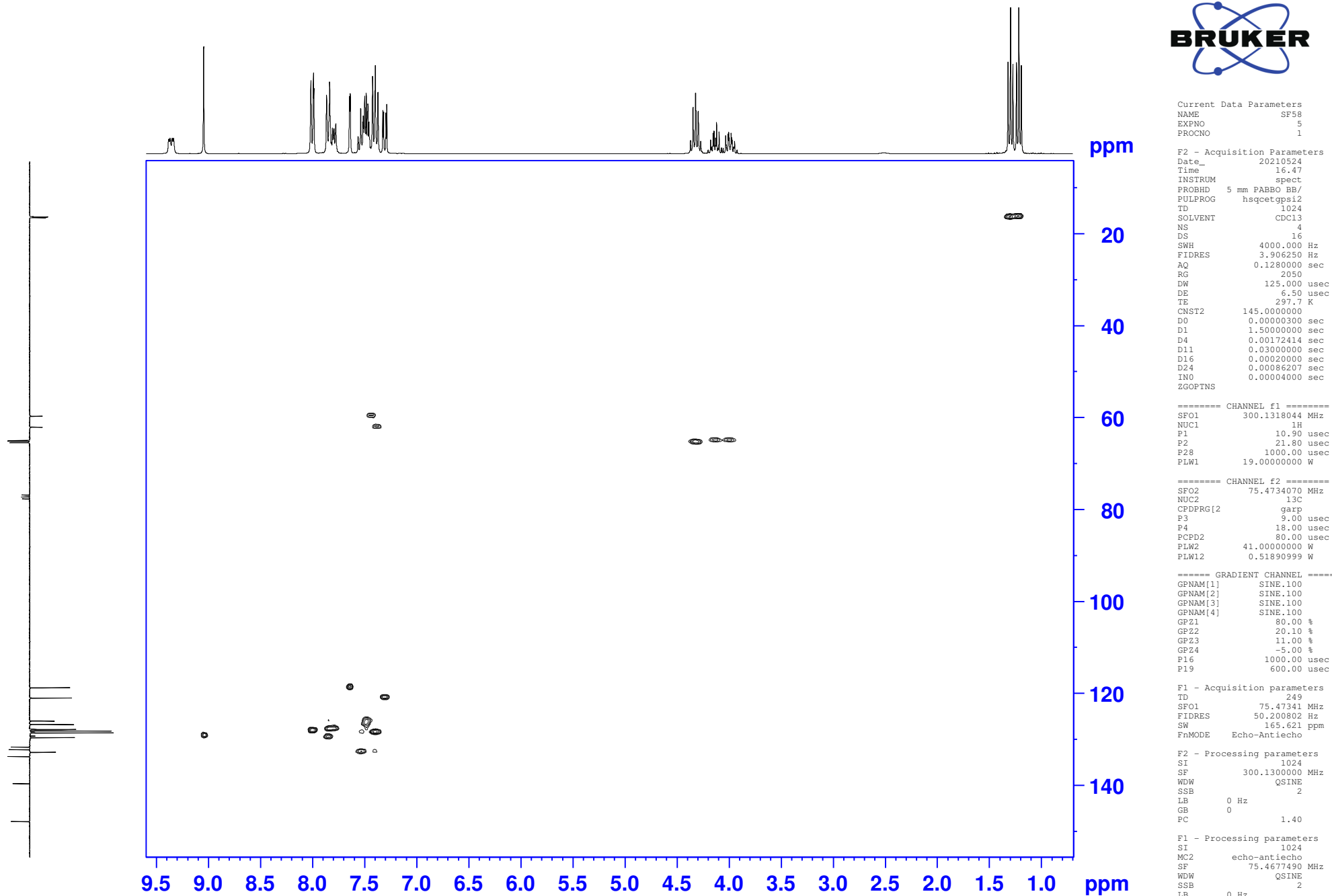


Figure S9 : ^1H - ^{13}C HSQC NMR spectrum of cycloadduct (3)

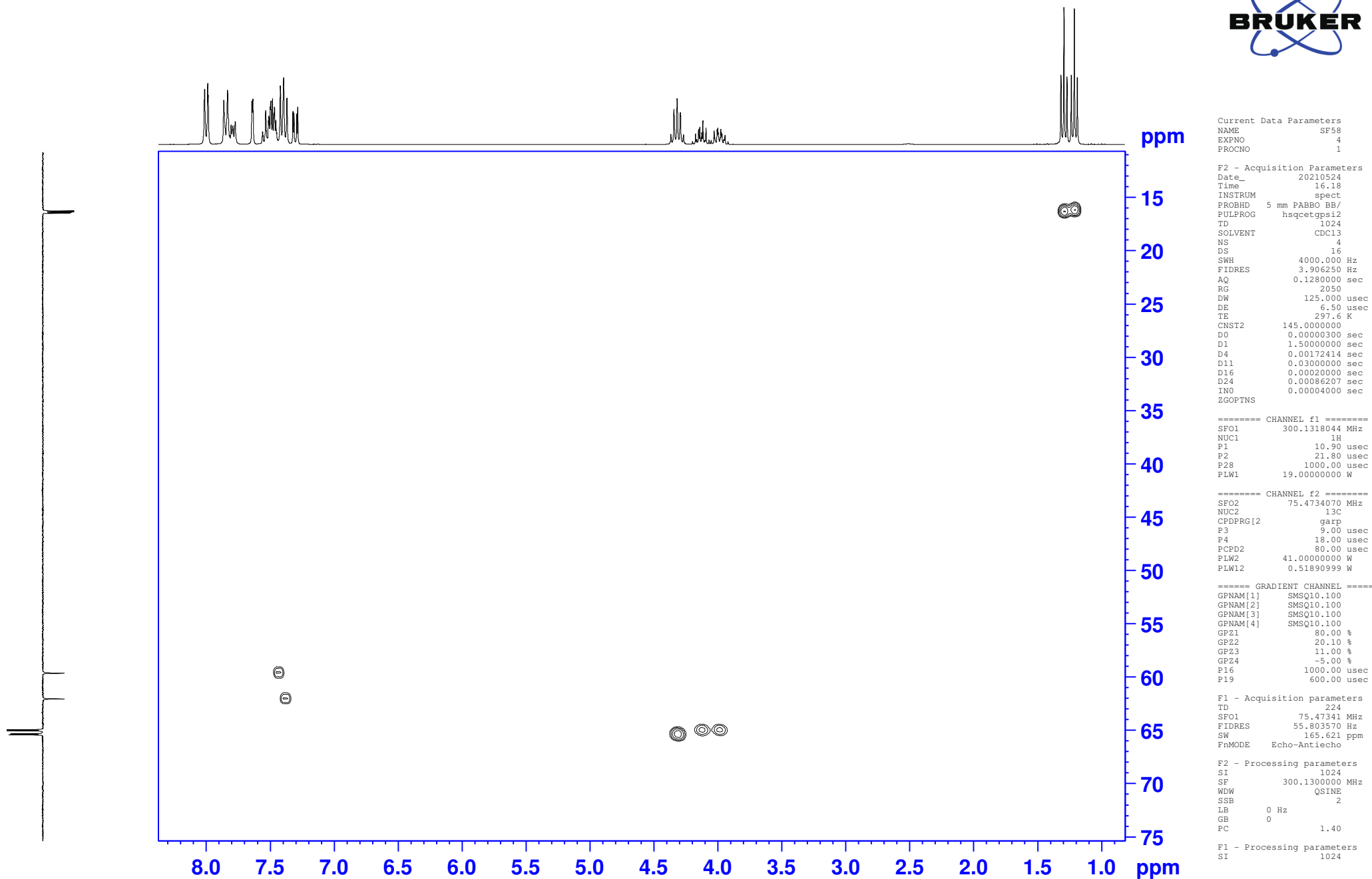


Figure S10 : Expanded region of ^1H - ^{13}C HSQC NMR spectrum (1.0 – 8.0 ppm and 15 – 75 ppm) of cycloadduct (3)

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)

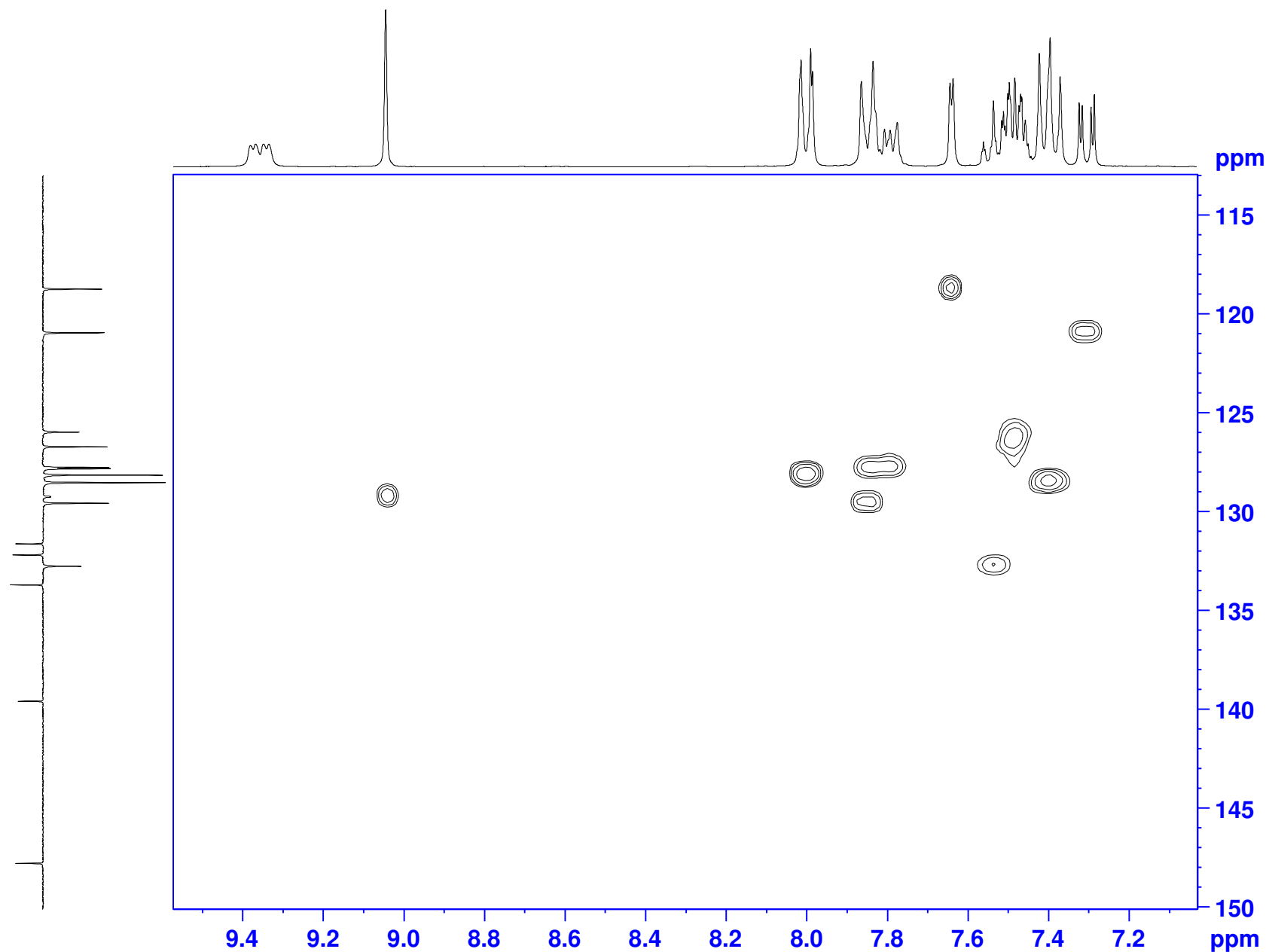


Figure S11 : Expanded region of ^1H - ^{13}C HSQC NMR spectrum (7.1 – 9.5 ppm and 113 – 150 ppm) of cycloadduct (3)

Current Data Parameters
NAME SF58
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210524
Time 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetps12
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4000.000 Hz
FIDRES 3.906250 Hz
AQ 0.1280000 sec
RG 2050
DW 125.000 usec
DE 6.50 usec
TE 297.6 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00004000 sec
ZGPTNS

===== CHANNEL f1 =====
SFO1 300.1318044 MHz
NUC1 ^1H
P1 10.90 usec
P2 21.80 usec
P28 1000.00 usec
PLW1 19.00000000 W

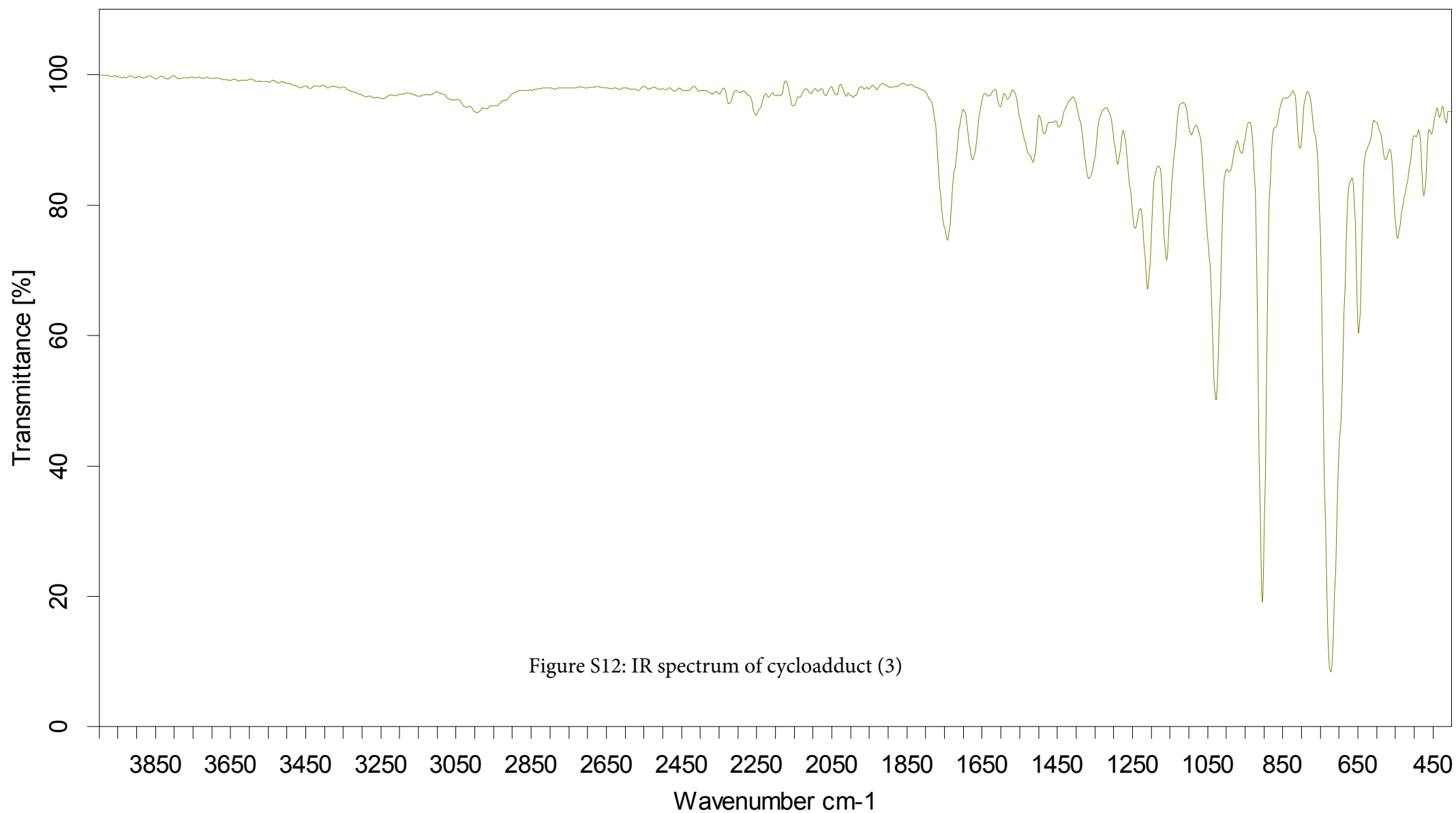
===== CHANNEL f2 =====
SFO2 75.4734070 MHz
NUC2 ^{13}C
CPDPRG2 garp
P3 9.00 usec
P4 18.00 usec
PCPD2 80.00 usec
PLW2 41.00000000 W
PLW12 0.51890999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 224
SFO1 75.47341 MHz
FIDRES 55.803570 Hz
SW 165.621 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 75.4677485 MHz
WDW QSINE



Résolution : 4 cm⁻¹ (16 scans)

Echantillon : SF58

Technique : FTIR - VERTEX 70 - BRUKER

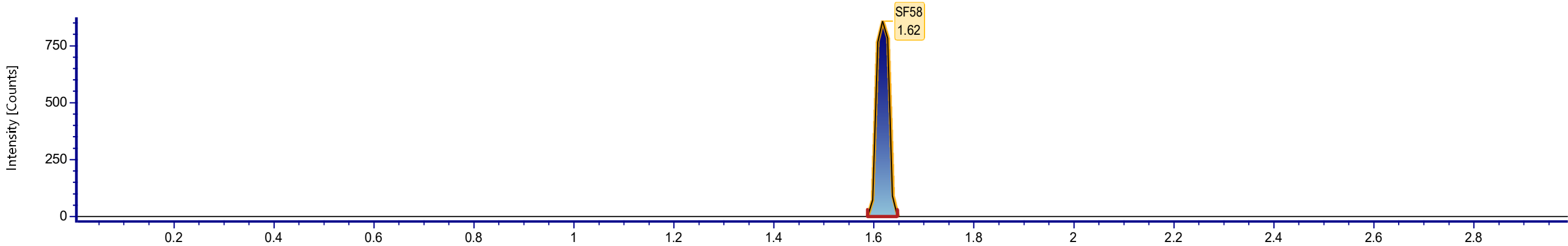
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Sample Information

Item name:	SF58 50 PPM	Sample type:	Reference
Item description:		Sample position:	2:A,6
Acquisition start time:	Jun 09, 2021 17:27:16 W. Europe Daylight Time	Injection volume:	2.00

	Component name	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Observed RT (min)	Observed CCS (Å)	Response	Adducts
1	SF58	508.15117	509.1595	2.1	1.62	283.26	742	+H
2	SF58	508.15117	531.1404	0.0	1.62	237.35	98621	+Na, +H

Channel name: SF58 [+H] : (10.00 mDa) 509.1595 : DT=7.78 to 8.39 ms



Channel name: SF58 [+Na] : (10.00 mDa) 531.1404 : DT=6.24 to 6.81 ms

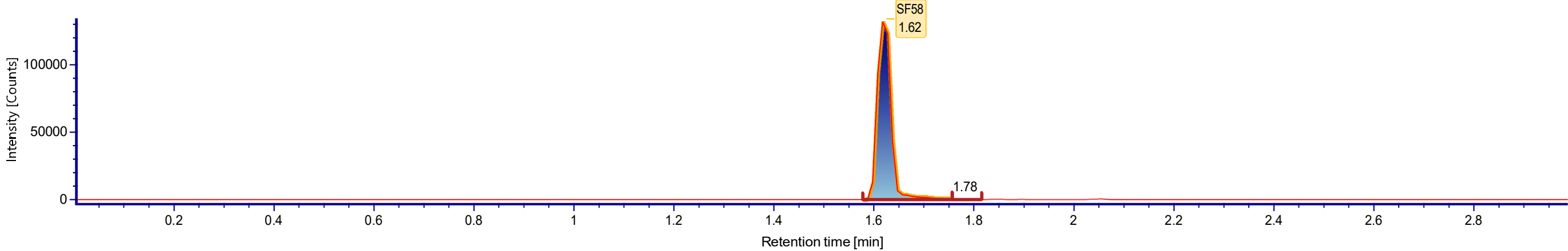


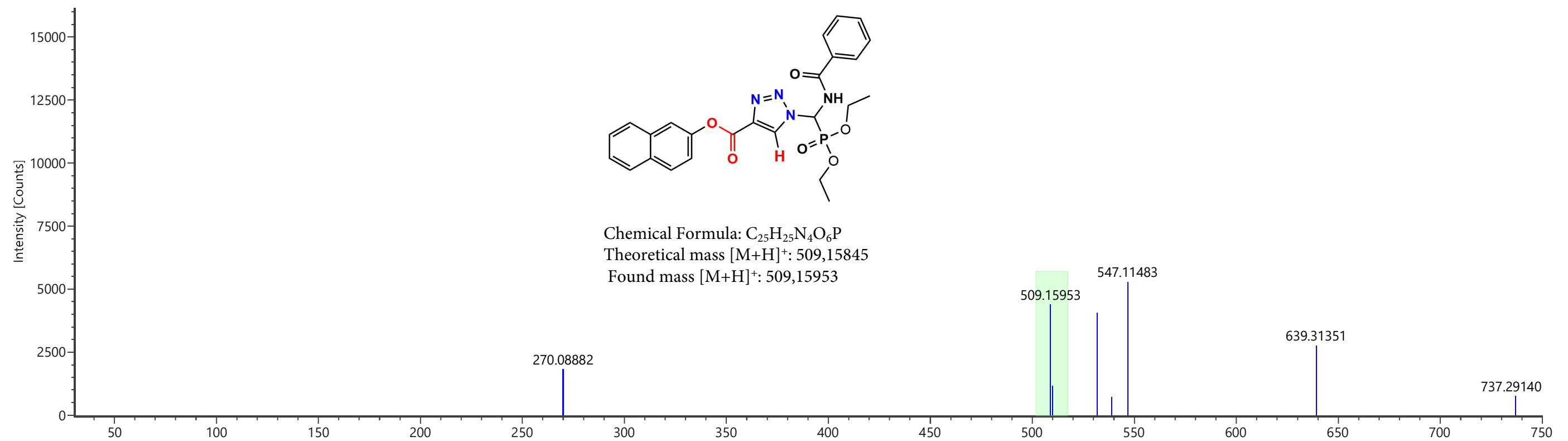
Figure S13 : LC-HRMS Chromatogram of cycloadduct (3)

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (**3**)

Item name: SF58 50 PPM

Item description:

Channel name: Low energy : Time 1.6196 +/- 0.0181 minutes : Drift Times: 8.09 +/- 0.31 ms



Item name: SF58 50 PPM

Item description:

Channel name: High energy : Time 1.6196 +/- 0.0181 minutes : Drift Times: 8.05 +/- 0.31 ms

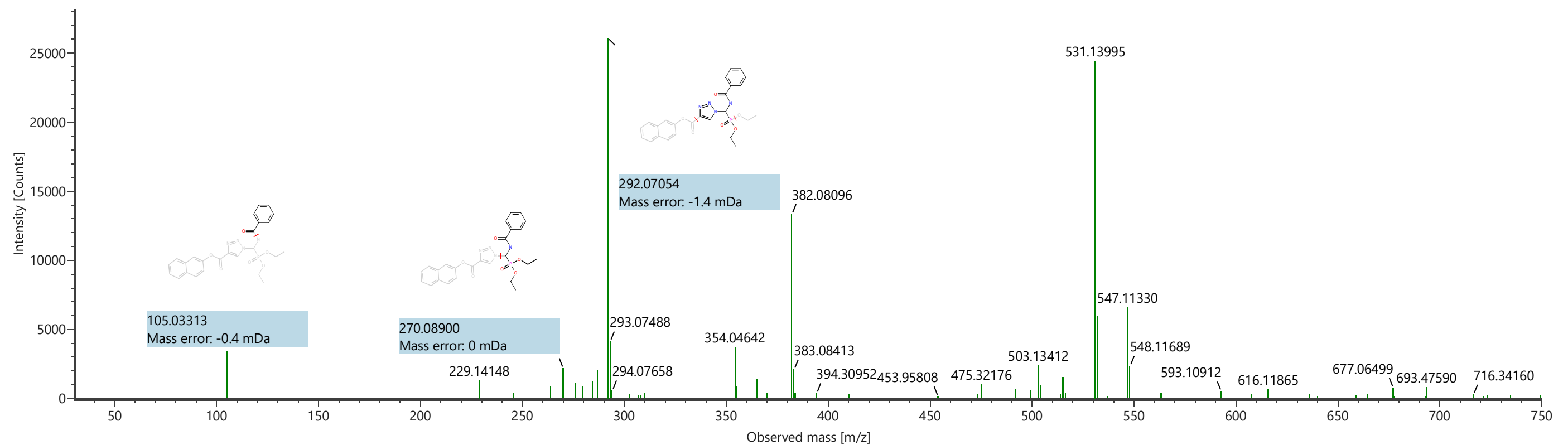
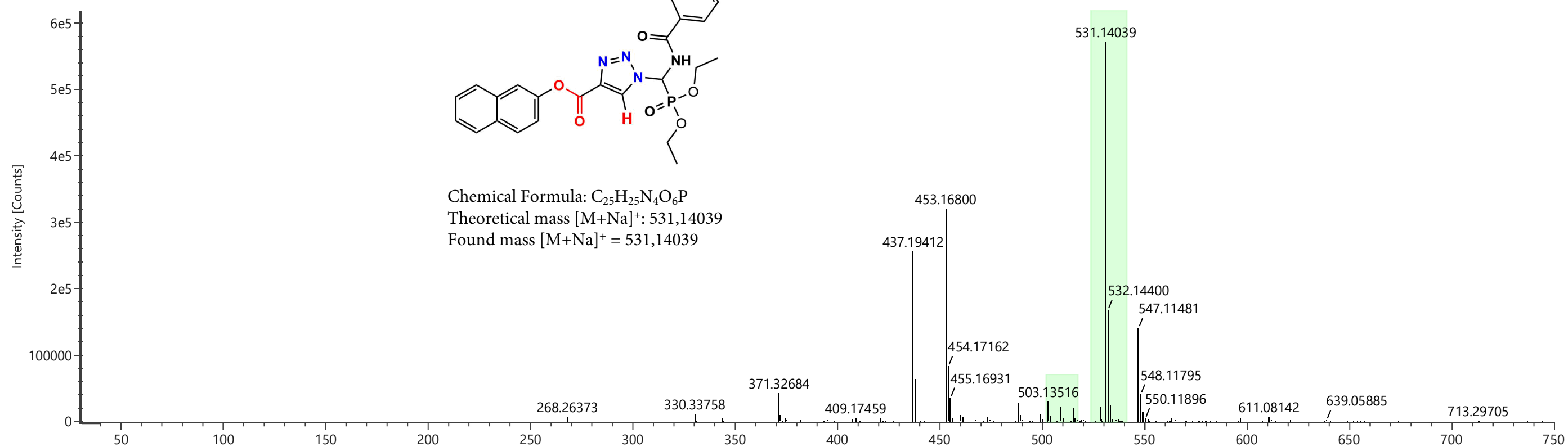


Figure S14 : HRMS spectrum of cyloadduct (**3**) showing a $[M + H]^+$ ion at m/z 508,15953

Supplementary Materials of naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate (3)

Item name: SF58 50 PPM
Item description:

Channel name: Low energy : Time 1.6216 +/- 0.0181 minutes : Drift Times: 6.52 +/- 0.29, 5.56 +/- 0.27 ms



Item name: SF58 50 PPM
Item description:

Channel name: High energy : Time 1.6216 +/- 0.0181 minutes : Drift Times: 6.47 +/- 0.29, 5.51 +/- 0.27 ms

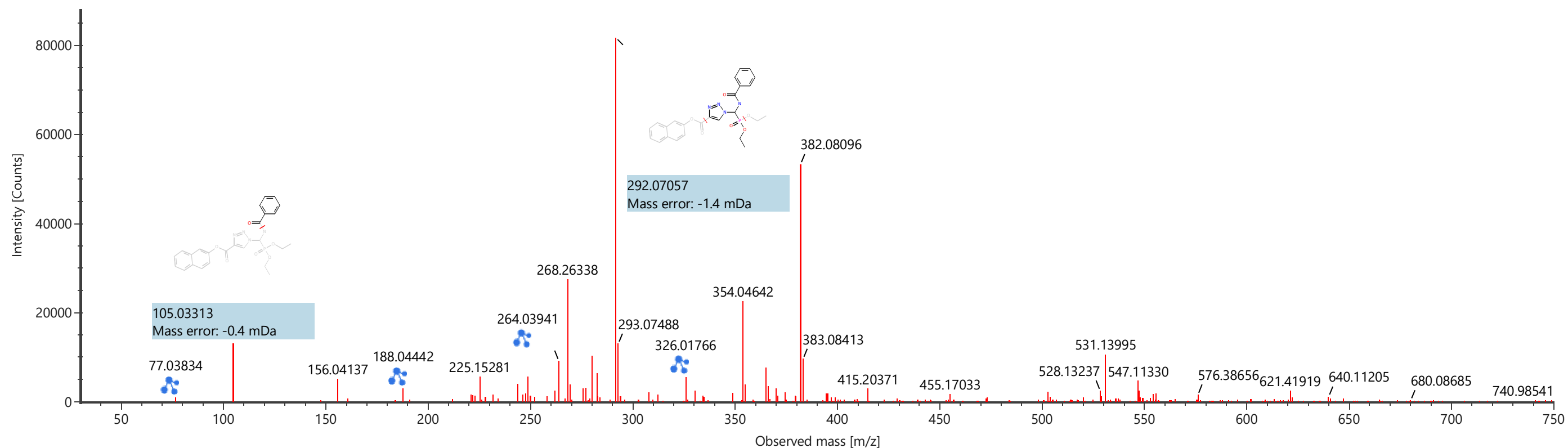


Figure S15 : HRMS spectrum of cyloadduct (3) showing a $[M + Na]^+$ ion at m/z 531,14039.