

Supporting information

Synthesis of 6-alkynylated purine-containing DNA via on-column Sonogashira coupling and investigation of their base pairing properties

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1. HPLC analyses of the synthesized ODNs

The purified ODN3 and ODN4 incorporating N Pu and O Pu derivatives were analyzed by reverse-phase HPLC using a JASCO HPLC system (PU-2089 plus, UV-2075 plus, CO-2067 plus) equipped with a Nacalai Tesque COSMOSIL 5C₁₈-MS-II column (4.6 × 250 mm). The column oven was set to 50 °C and peak was detected at 254 nm. The following buffer system was used: buffer A: 0.1 M TEAA, pH 7.0 in H₂O, buffer B: acetonitrile. A flow rate of 1 ml/min with a gradient of 5 to 20% of buffer B in 25 min was applied.

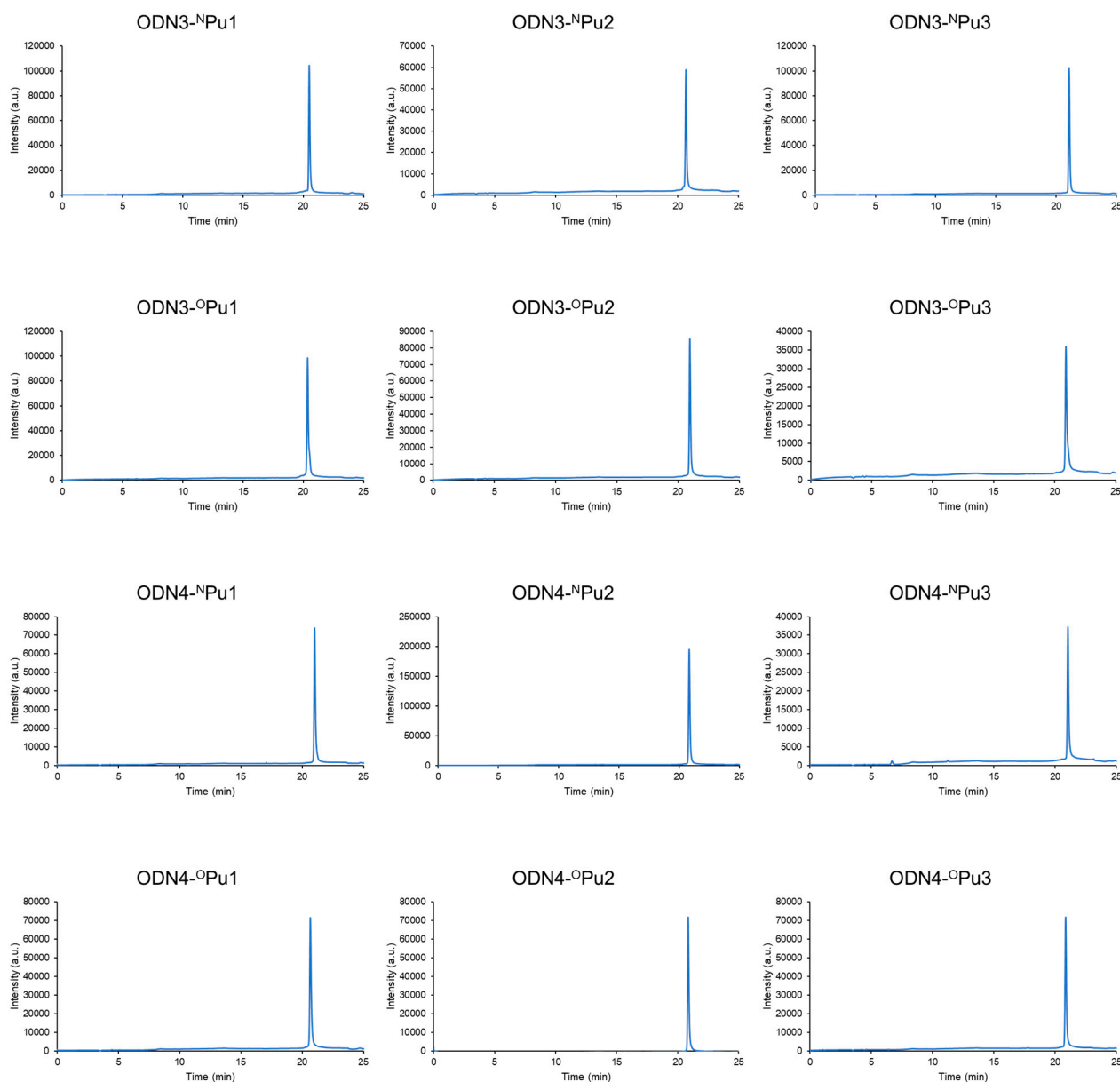


Figure S1. HPLC charts of the purified ODN3 and ODN4 incorporating the alkynylated purine derivatives.

2. UV melting curves and T_m values of the duplex DNAs

OND3: 5'-GCCTTAC**X**CTGAGAC-3'

ODN4: 3'-CGGAATG**Y**GACTCTG-5'

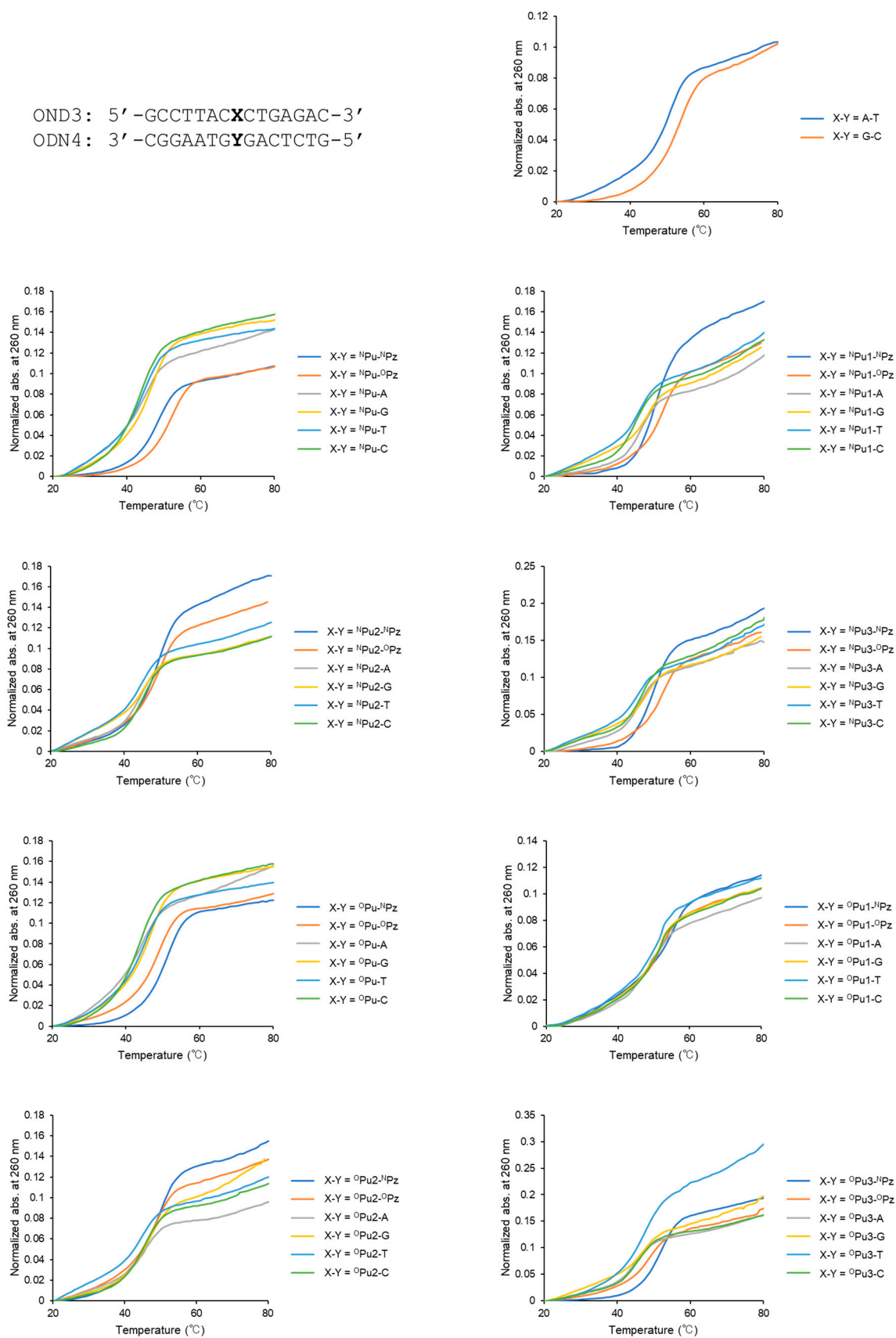


Figure S2. UV melting curves of the duplex DNAs incorporating different combinations of X-Y base pairs.

ODN4: 5'-GTCTCAG**X**GTAAGGC-3'
 ODN3: 3'-CAGAGTC**Y**CATTCCG-5'

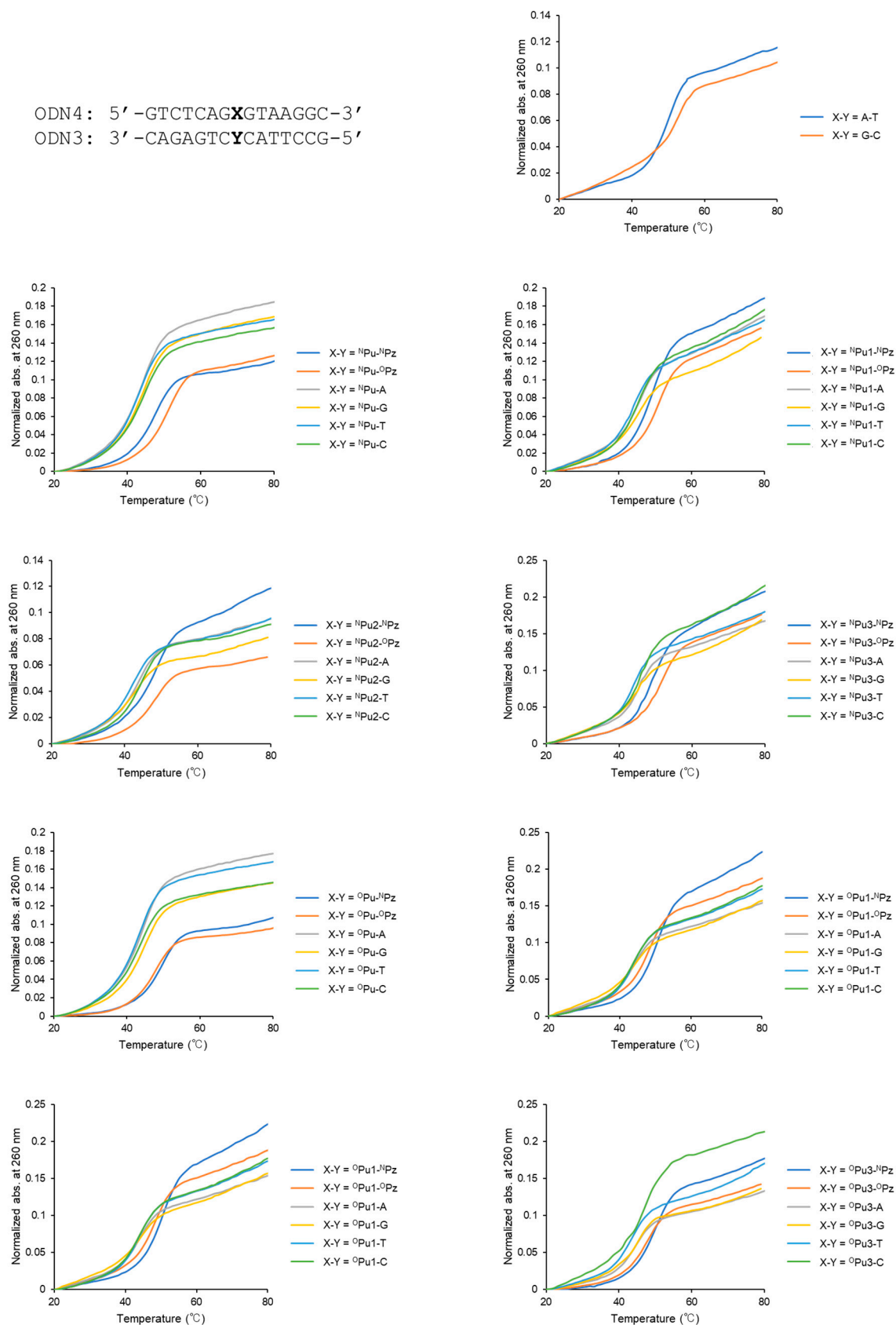


Figure S2 (continued). UV melting curves of the duplex DNAs incorporating different combinations of X-Y base pairs.

Table S1. T_m values of the duplex DNAs incorporating canonical as well as ^NPu and ^OPu derivatives at X-Y position in an inverted manner.

ODN4 : 5' -GTCTCAG X GTAAGGC-3' ODN3 : 3' -CAGAGTC Y CATTCCG-5'			
Base pair	T_m (°C)	Base pair	T_m (°C)
A - T	49.9 ± 0.1	G - C	52.4 ± 0.1
$^N\text{Pu} - ^O\text{Pz}$	51.2 ± 0.1	$^N\text{Pu} - ^N\text{Pz}$	47.5 ± 0.1
$^N\text{Pu1} - ^O\text{Pz}$	51.0 ± 0.2	$^N\text{Pu1} - ^N\text{Pz}$	49.2 ± 0.2
$^N\text{Pu2} - ^O\text{Pz}$	48.4 ± 0.1	$^N\text{Pu2} - ^N\text{Pz}$	48.6 ± 0.1
$^N\text{Pu3} - ^O\text{Pz}$	52.3 ± 0.2	$^N\text{Pu3} - ^N\text{Pz}$	49.7 ± 0.3
$^O\text{Pu} - ^N\text{Pz}$	49.6 ± 0.1	$^O\text{Pu} - ^O\text{Pz}$	47.7 ± 0.1
$^O\text{Pu1} - ^N\text{Pz}$	50.7 ± 0.3	$^O\text{Pu1} - ^O\text{Pz}$	47.9 ± 0.7
$^O\text{Pu2} - ^N\text{Pz}$	47.7 ± 0.3	$^O\text{Pu2} - ^O\text{Pz}$	47.9 ± 0.7
$^O\text{Pu3} - ^N\text{Pz}$	49.9 ± 0.1	$^O\text{Pu3} - ^O\text{Pz}$	47.9 ± 0.1

^aConditions: 2 μM duplex DNA, 10 mM sodium phosphate, 50 mM NaCl, pH 7.0.

Table S2. T_m values of the duplex DNAs incorporating the canonical nucleobases against ^NPu and ^OPu derivatives.

ODN3 : 5' - GCCTTAC X CTGAGAC - 3'			
ODN4 : 3' - CGGAATG Y GACTCTG - 5'			
Base pair (X-Y)	T_m (°C)	Base pair (X-Y)	T_m (°C)
^NPu - A	44.6 ± 0.1	^OPu - A	44.4 ± 0.1
^NPu - G	46.6 ± 0.1	^OPu - G	46.9 ± 0.1
^NPu - T	44.6 ± 0.1	^OPu - T	45.0 ± 0.1
^NPu - C	43.5 ± 0.1	^OPu - C	43.6 ± 0.1
$^N\text{Pu1}$ - A	46.5 ± 0.1	$^O\text{Pu1}$ - A	46.9 ± 0.2
$^N\text{Pu1}$ - G	48.2 ± 0.1	$^O\text{Pu1}$ - G	47.3 ± 0.3
$^N\text{Pu1}$ - T	45.8 ± 0.1	$^O\text{Pu1}$ - T	47.9 ± 0.5
$^N\text{Pu1}$ - C	45.0 ± 0.1	$^O\text{Pu1}$ - C	47.8 ± 0.2
$^N\text{Pu2}$ - A	44.5 ± 0.1	$^O\text{Pu2}$ - A	45.6 ± 0.1
$^N\text{Pu2}$ - G	45.5 ± 0.1	$^O\text{Pu2}$ - G	46.8 ± 0.2
$^N\text{Pu2}$ - T	44.7 ± 0.2	$^O\text{Pu2}$ - T	44.7 ± 0.1
$^N\text{Pu2}$ - C	45.1 ± 0.1	$^O\text{Pu2}$ - C	45.3 ± 0.1
$^N\text{Pu3}$ - A	46.5 ± 0.1	$^O\text{Pu3}$ - A	45.1 ± 0.1
$^N\text{Pu3}$ - G	47.7 ± 0.1	$^O\text{Pu3}$ - G	47.0 ± 0.1
$^N\text{Pu3}$ - T	46.0 ± 0.1	$^O\text{Pu3}$ - T	45.6 ± 0.1
$^N\text{Pu3}$ - C	47.0 ± 0.4	$^O\text{Pu3}$ - C	45.8 ± 0.2

^aConditions: 2 μM duplex DNA, 10 mM sodium phosphate, 50 mM NaCl, pH 7.0.

Table S3. T_m values of the duplex DNAs incorporating the canonical nucleobases against ^NPu and ^OPu derivatives at X-Y position in an inverted manner.

ODN4 : 5' -GTCTCAG X GTAAGGC-3' ODN3 : 3' -CAGAGTC Y CATTCCG-5'			
Base pair (X-Y)	T_m (°C)	Base pair (X-Y)	T_m (°C)
^NPu - A	43.9 ± 0.1	^OPu - A	44.4 ± 0.1
^NPu - G	44.2 ± 0.1	^OPu - G	44.8 ± 0.1
^NPu - T	43.2 ± 0.2	^OPu - T	43.5 ± 0.1
^NPu - C	44.5 ± 0.1	^OPu - C	43.5 ± 0.1
$^N\text{Pu1}$ - A	45.6 ± 0.1	$^O\text{Pu1}$ - A	44.3 ± 0.3
$^N\text{Pu1}$ - G	45.4 ± 0.1	$^O\text{Pu1}$ - G	44.4 ± 0.3
$^N\text{Pu1}$ - T	44.0 ± 0.1	$^O\text{Pu1}$ - T	44.1 ± 0.3
$^N\text{Pu1}$ - C	45.3 ± 0.1	$^O\text{Pu1}$ - C	44.1 ± 0.3
$^N\text{Pu2}$ - A	43.5 ± 0.4	$^O\text{Pu2}$ - A	47.0 ± 0.2
$^N\text{Pu2}$ - G	42.7 ± 0.1	$^O\text{Pu2}$ - G	44.4 ± 0.3
$^N\text{Pu2}$ - T	42.1 ± 0.1	$^O\text{Pu2}$ - T	44.0 ± 0.2
$^N\text{Pu2}$ - C	44.3 ± 0.1	$^O\text{Pu2}$ - C	45.1 ± 0.2
$^N\text{Pu3}$ - A	46.0 ± 0.5	$^O\text{Pu3}$ - A	44.5 ± 0.2
$^N\text{Pu3}$ - G	45.8 ± 0.2	$^O\text{Pu3}$ - G	44.9 ± 0.5
$^N\text{Pu3}$ - T	44.6 ± 0.2	$^O\text{Pu3}$ - T	43.4 ± 0.3
$^N\text{Pu3}$ - C	47.2 ± 0.1	$^O\text{Pu3}$ - C	45.2 ± 0.2

^aConditions: 2 μM duplex DNA, 10 mM sodium phosphate, 50 mM NaCl, pH 7.0.

3. Speculated recognition modes of the alkynylated purine derivatives

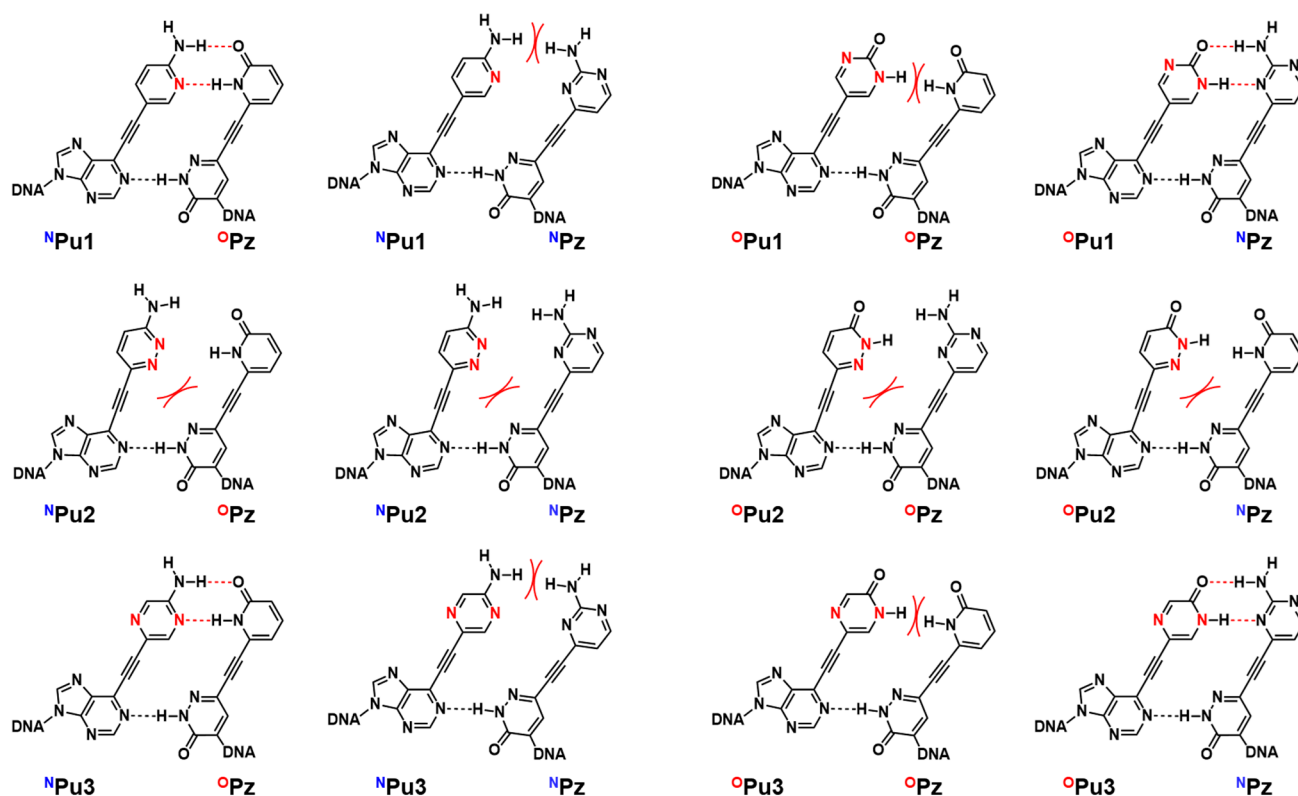
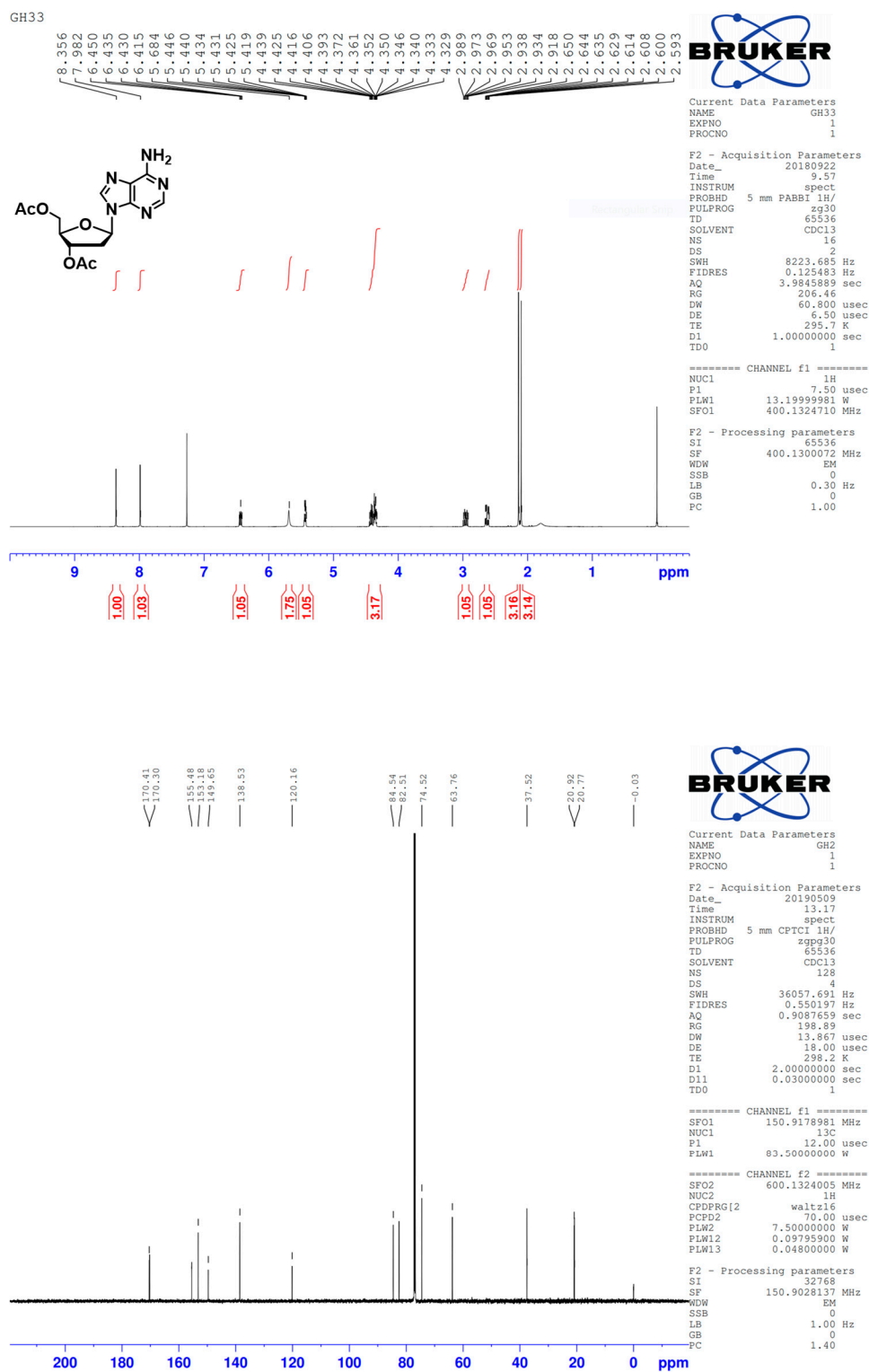


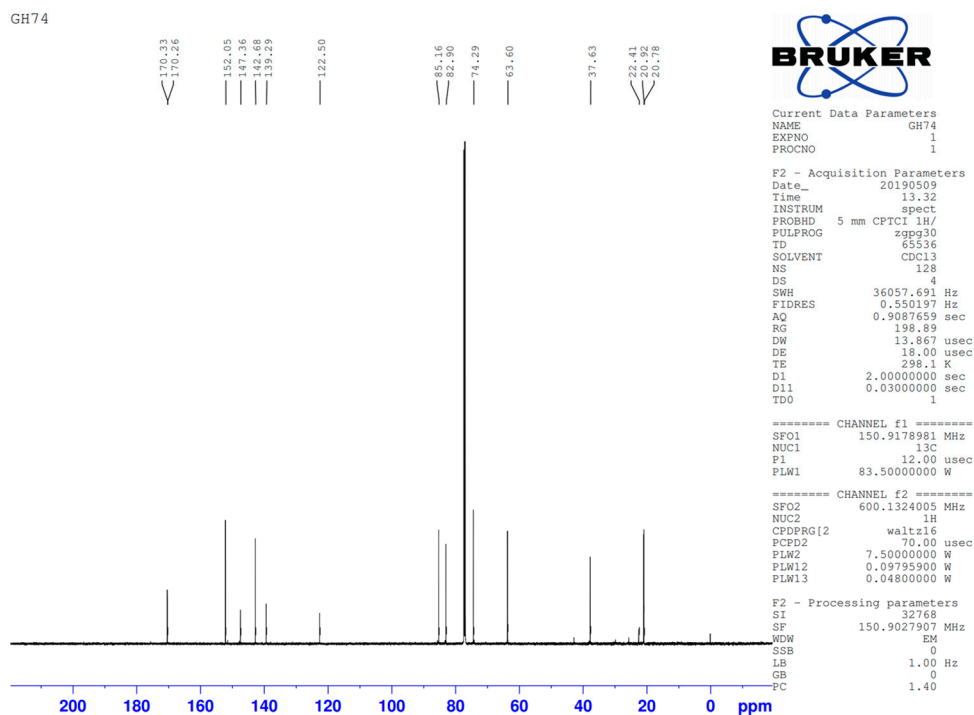
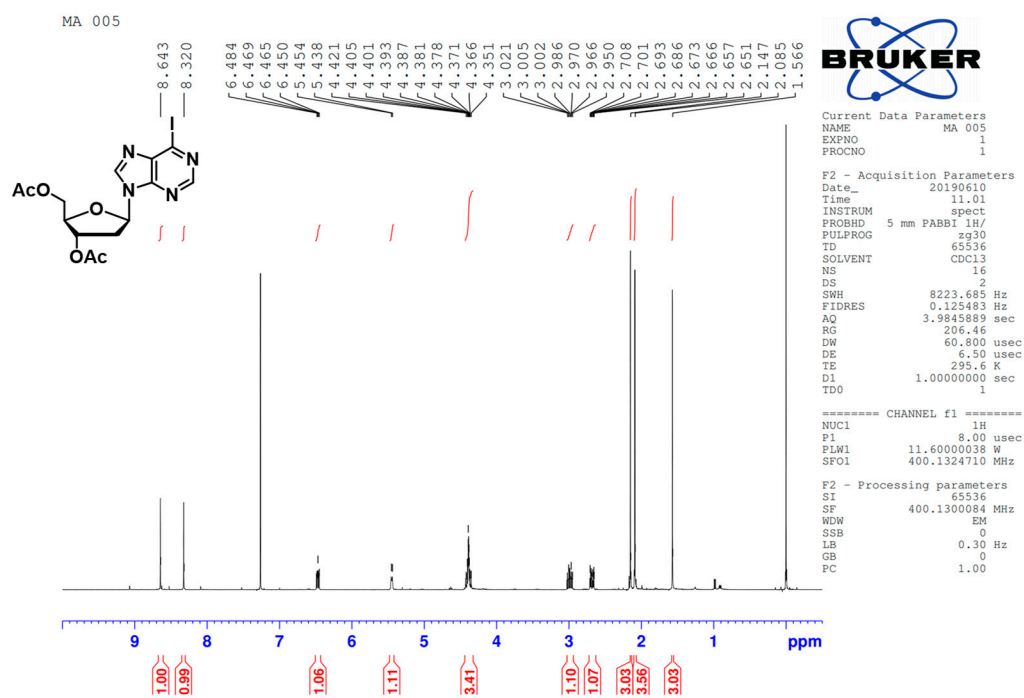
Figure S3. Speculated recognition modes of the alkynylated purine derivatives pairing with the alkynylated pyridazines.

4. ^1H , ^{13}C and ^{31}P NMR spectra of the synthesized compounds

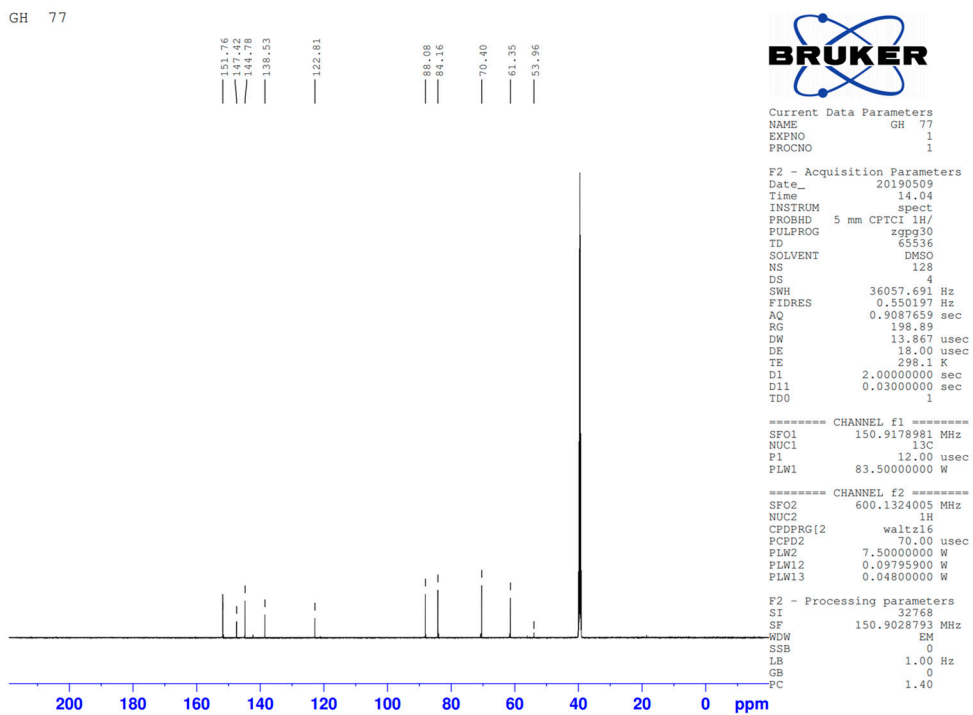
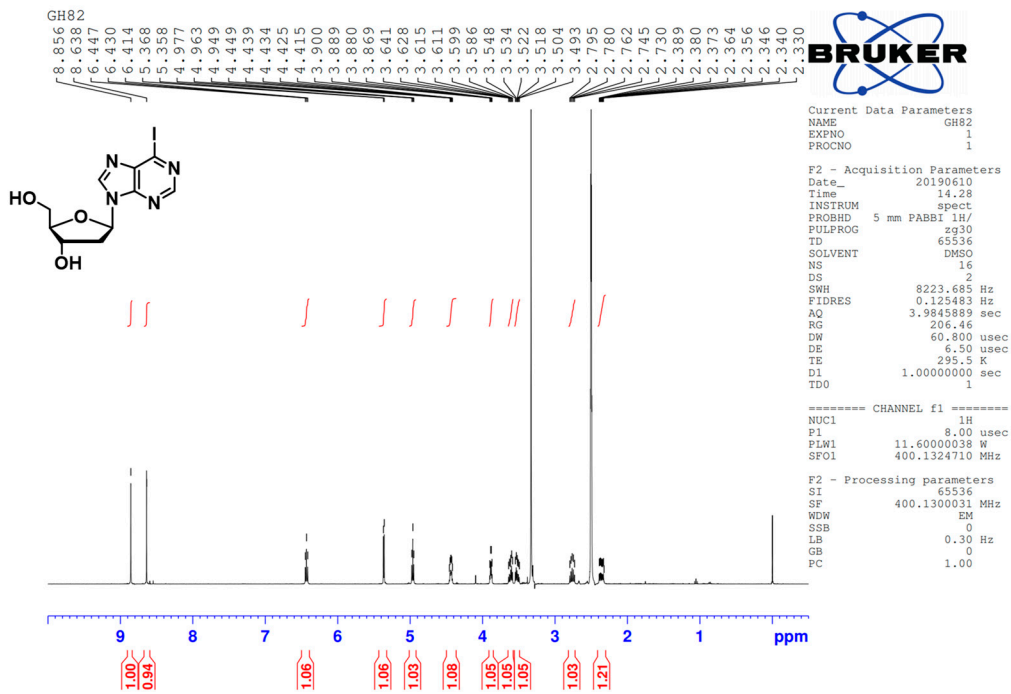
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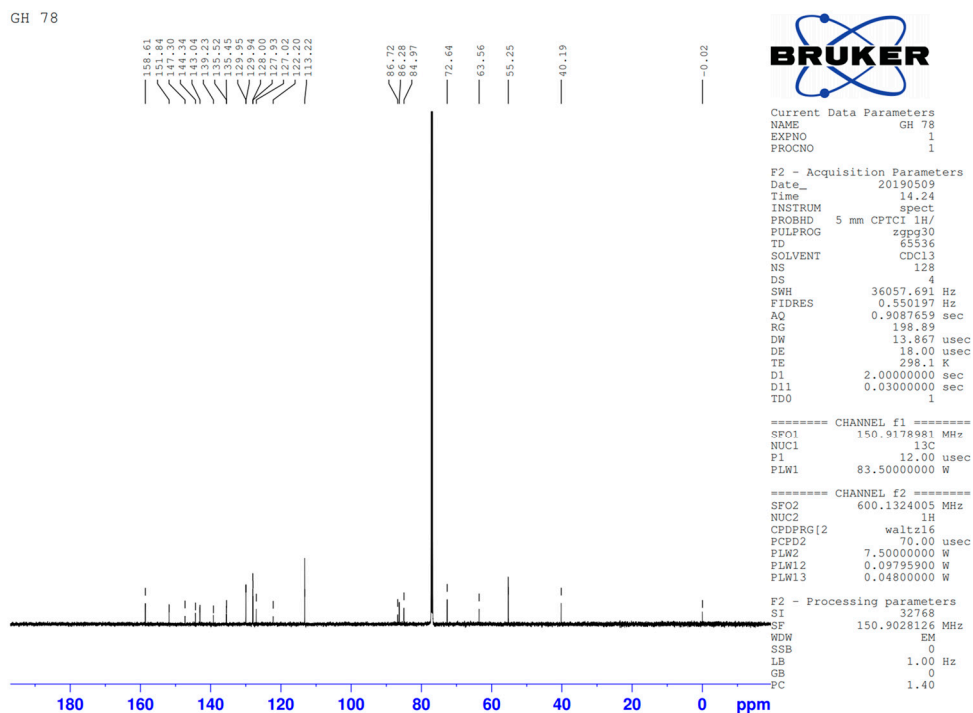
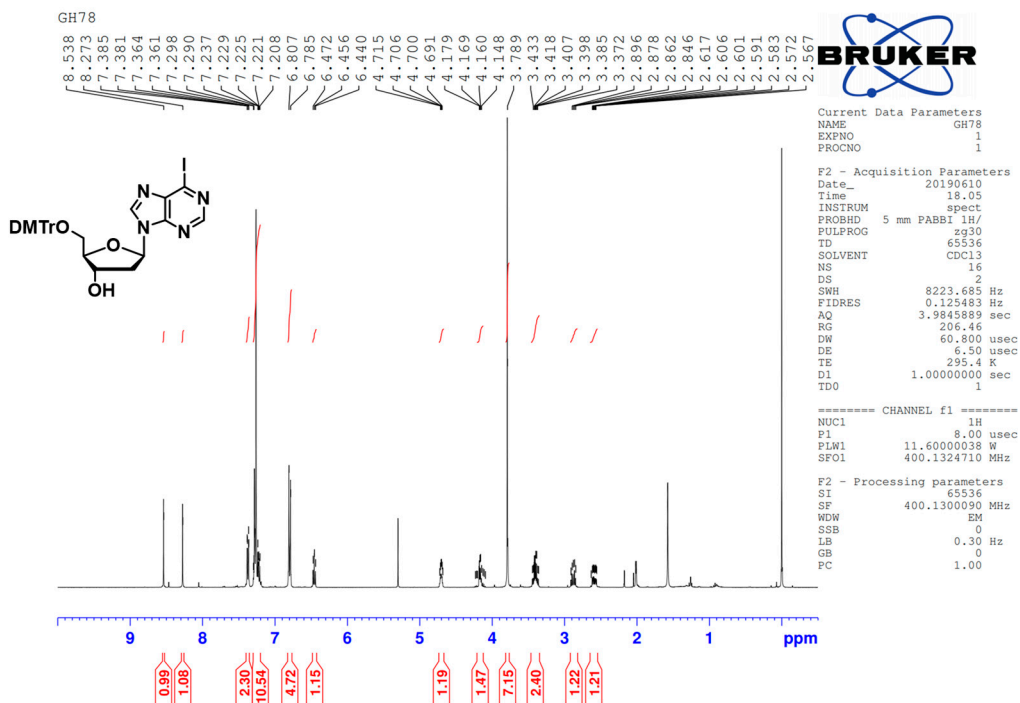
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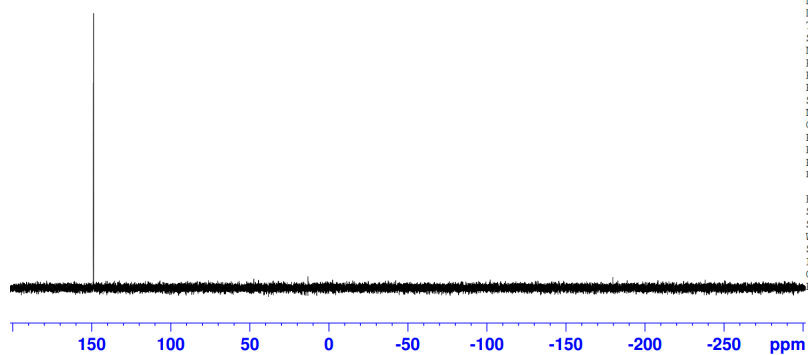
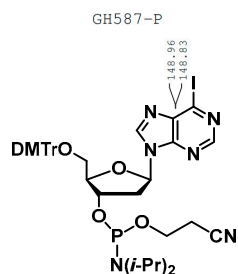
Compound 4



Compound 5



Compound 6



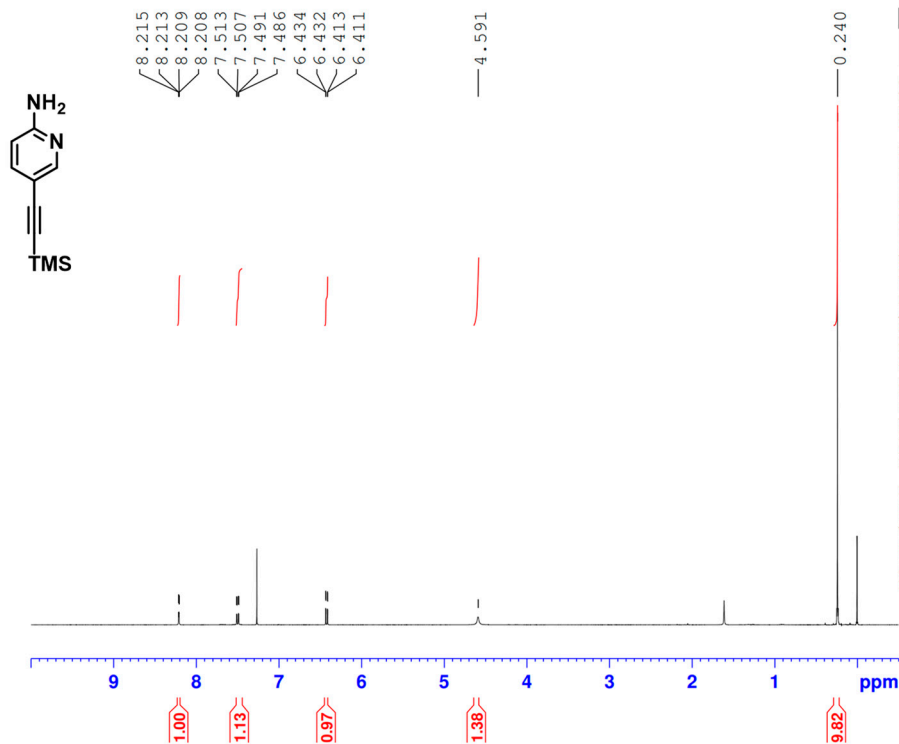
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Compound 8

GH486

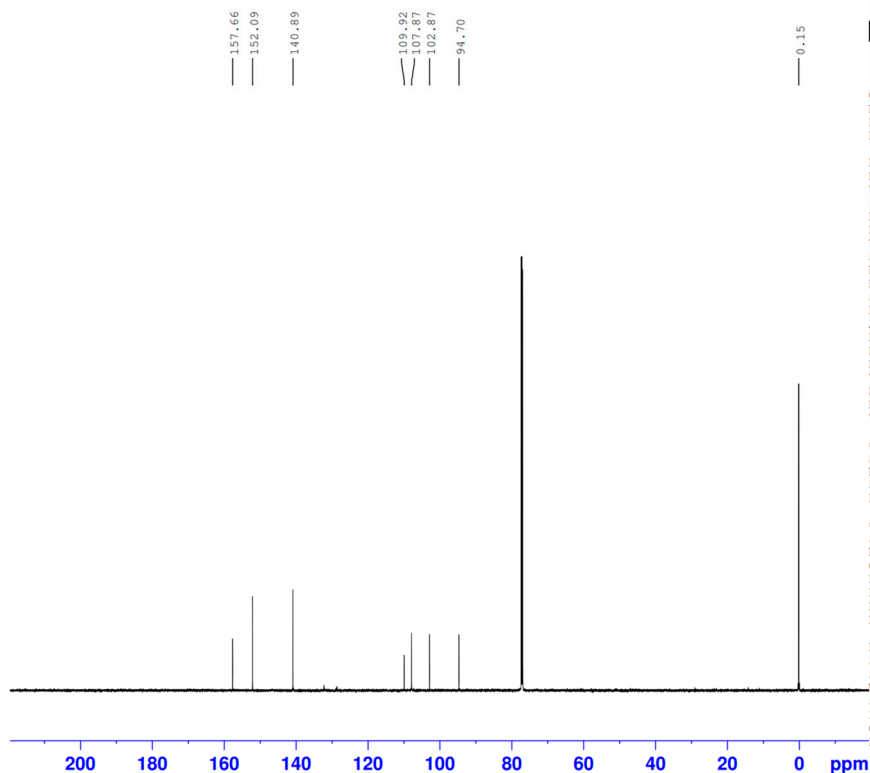


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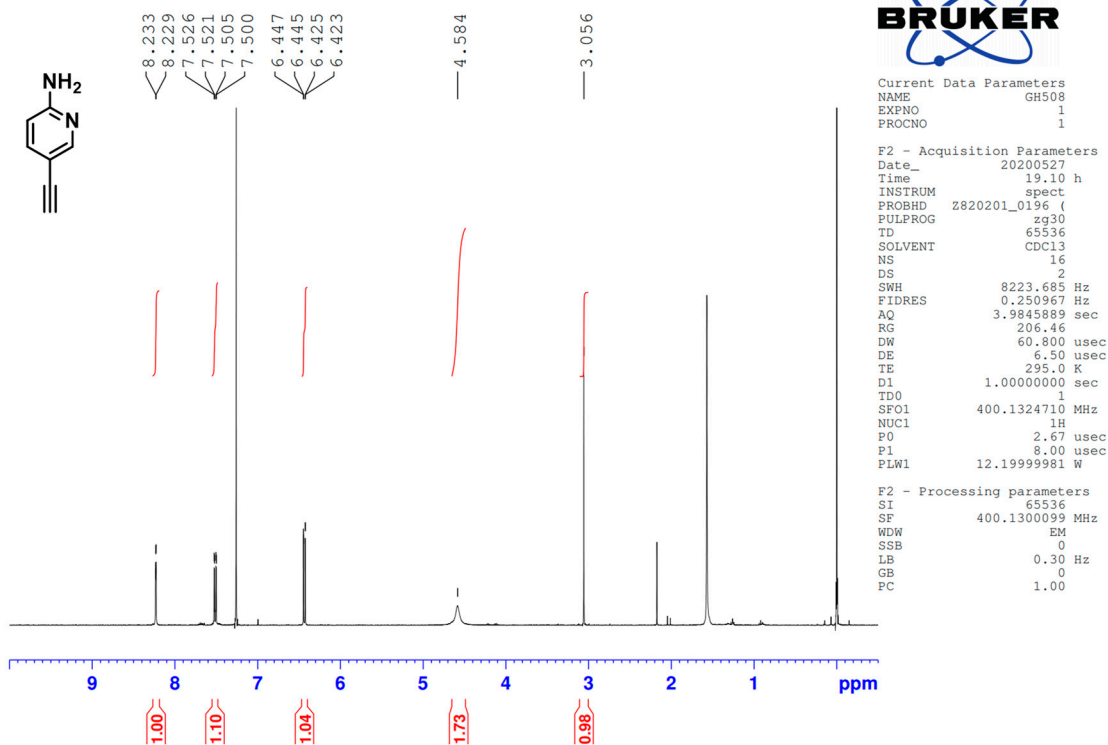
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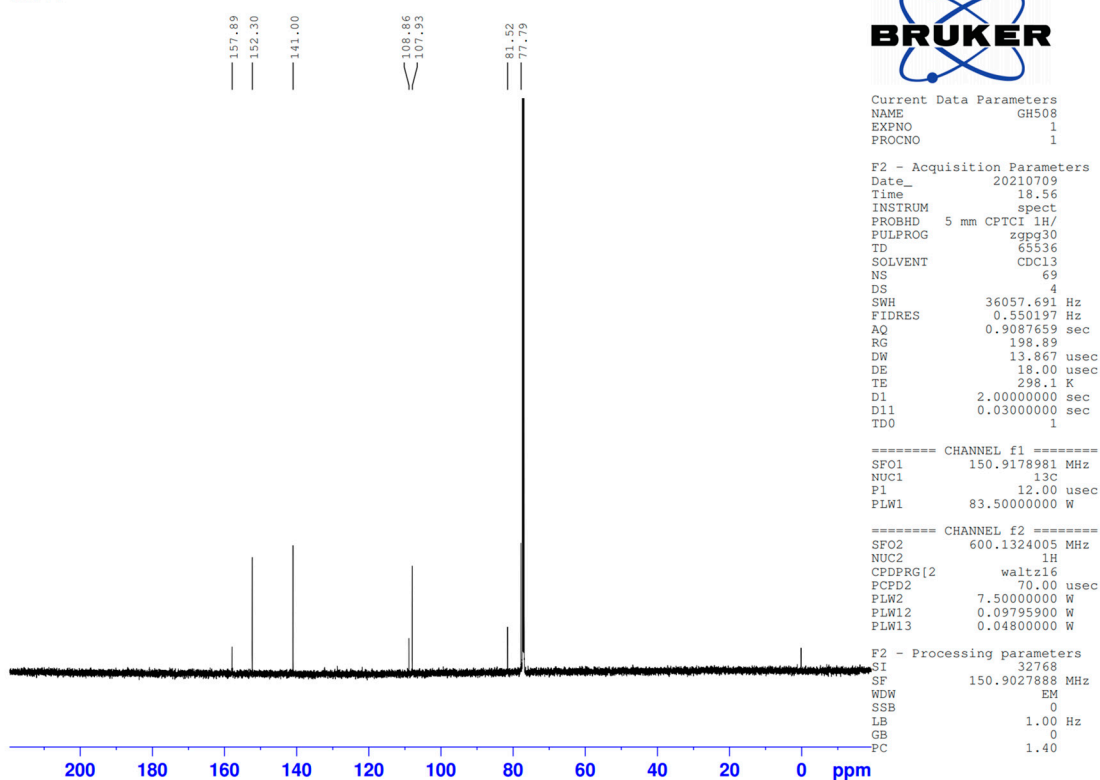
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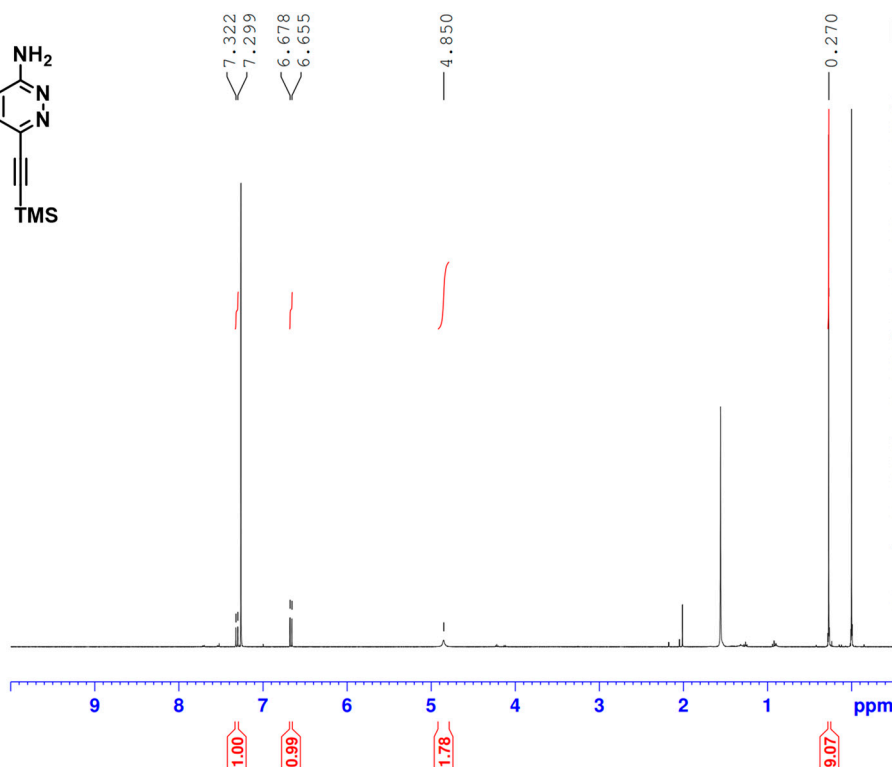
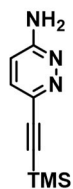


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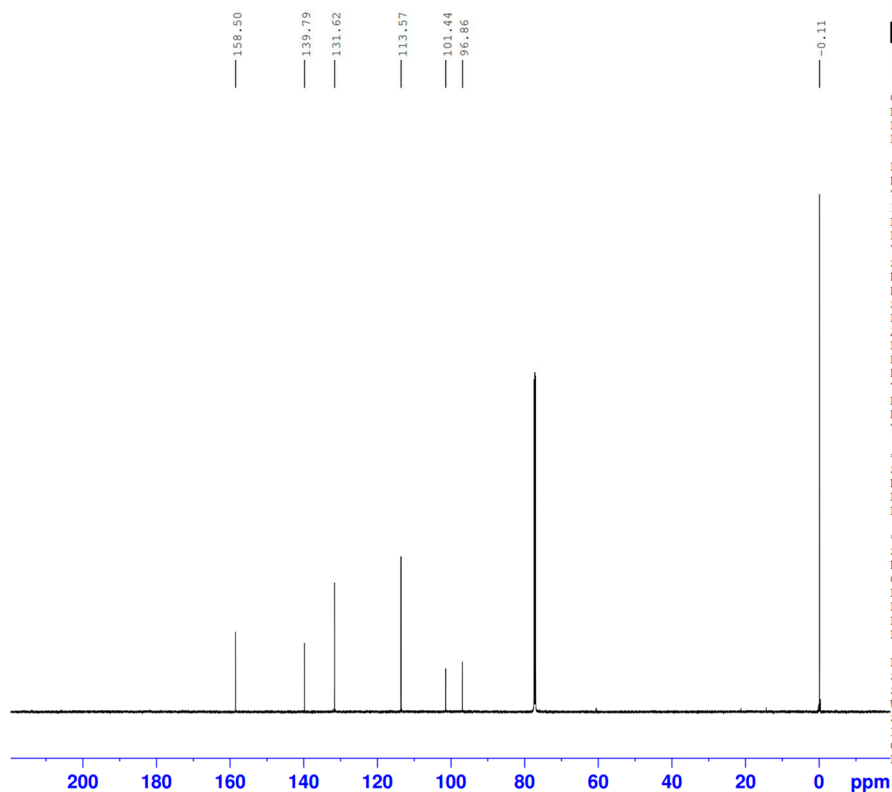


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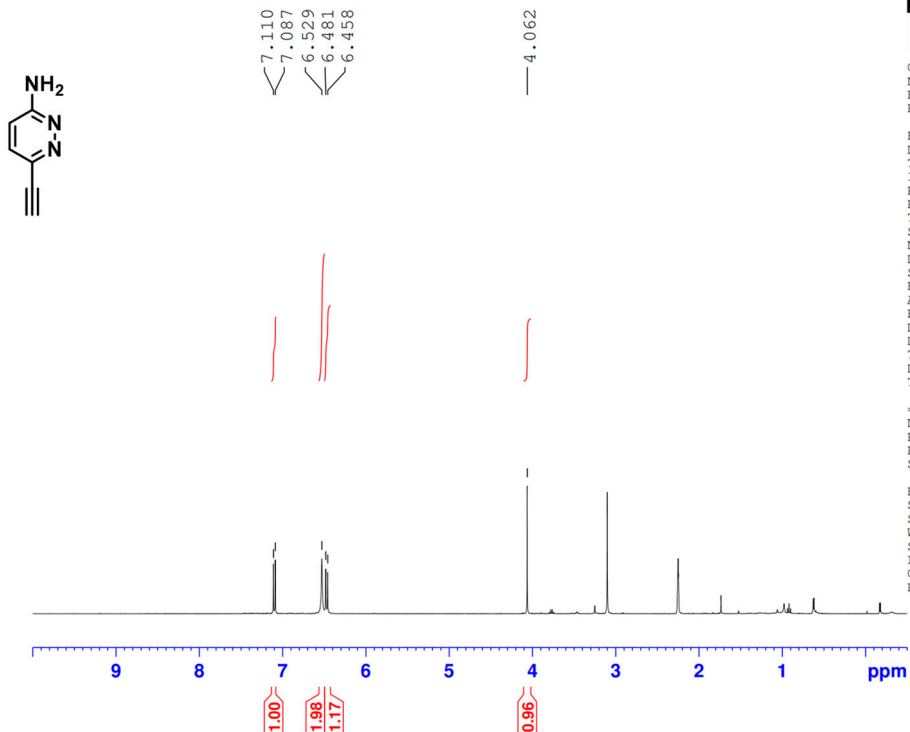
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Compound 12

GH422



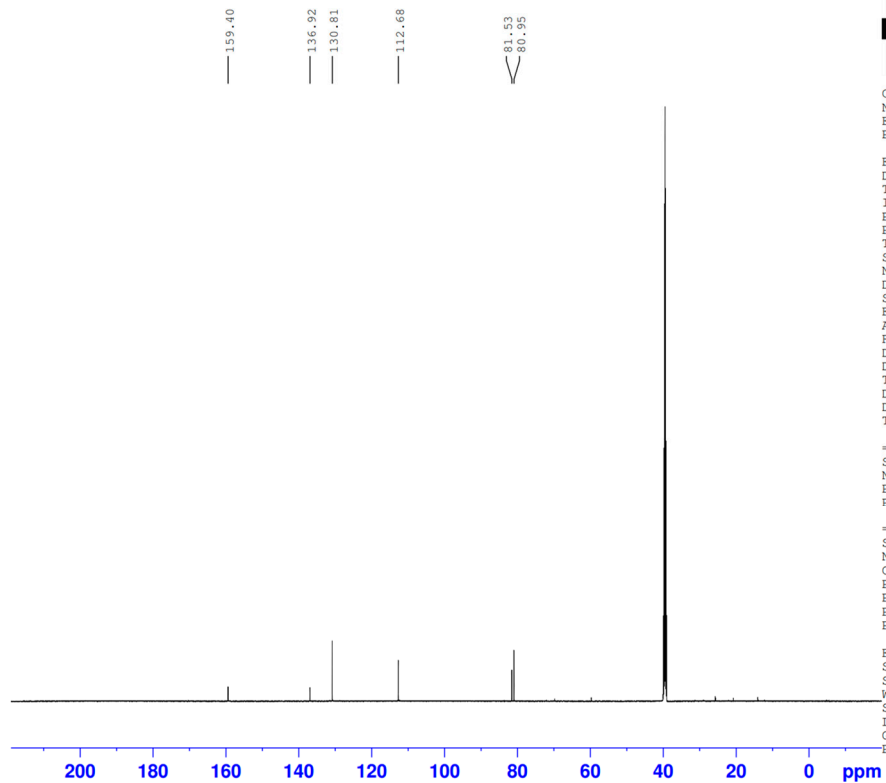
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GH422



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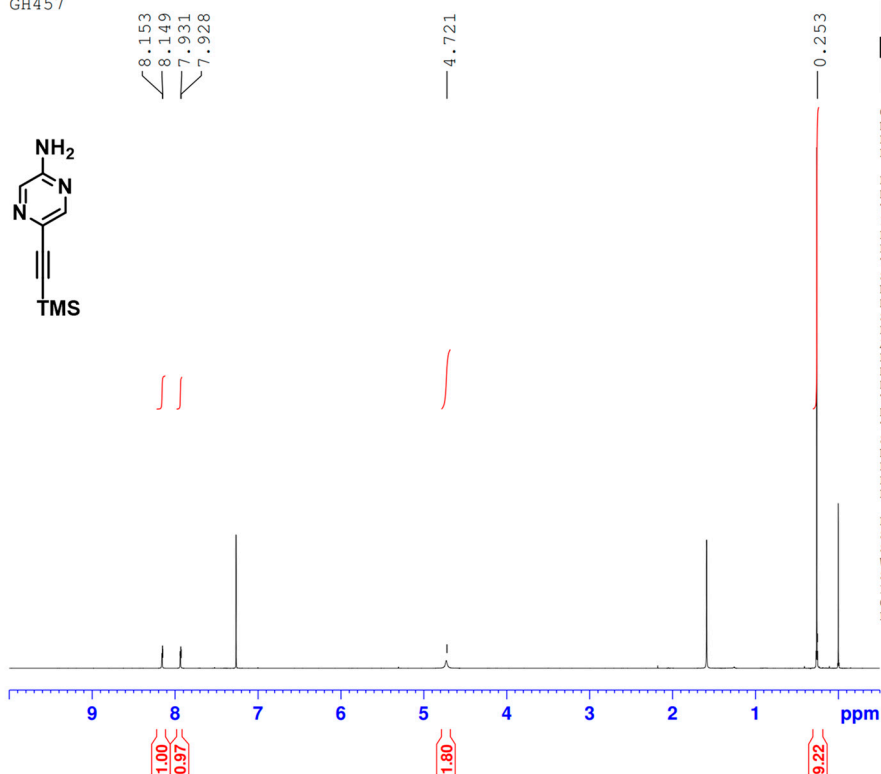
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Compound 14

GH457

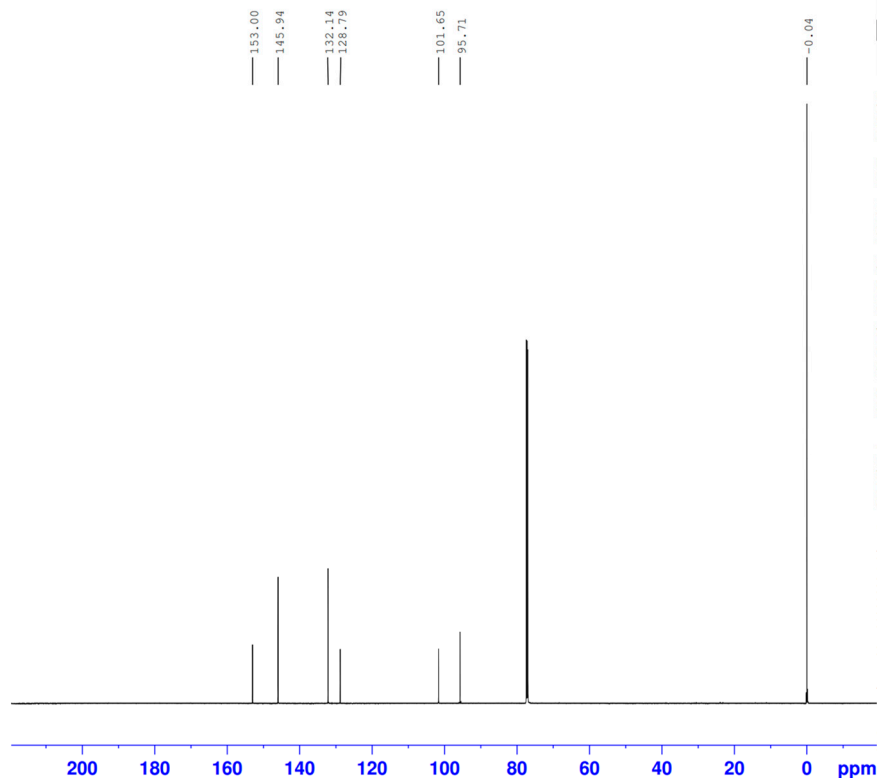


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GH457



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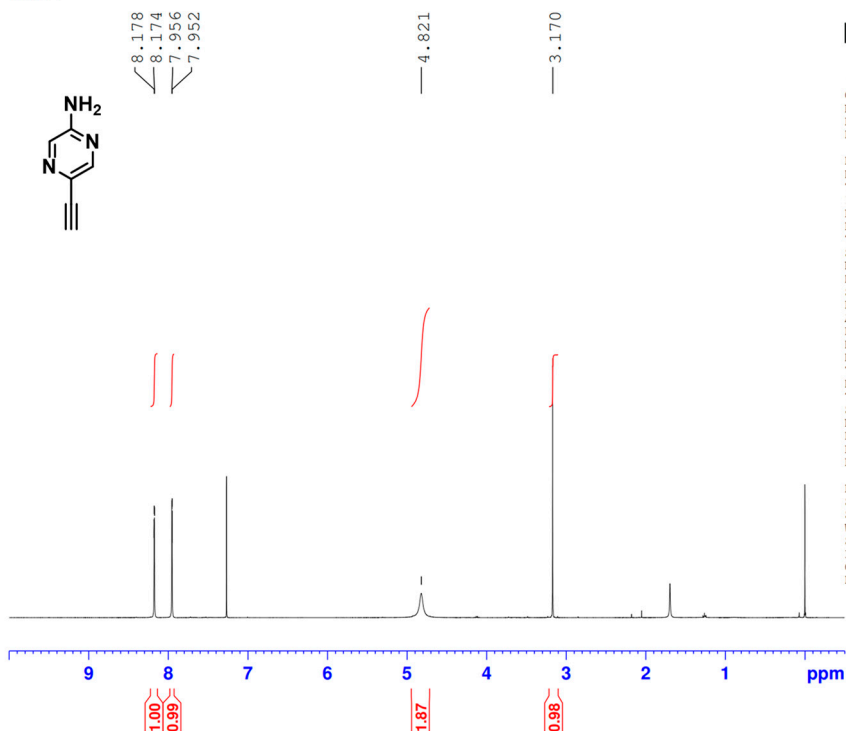
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Compound 15

GH477

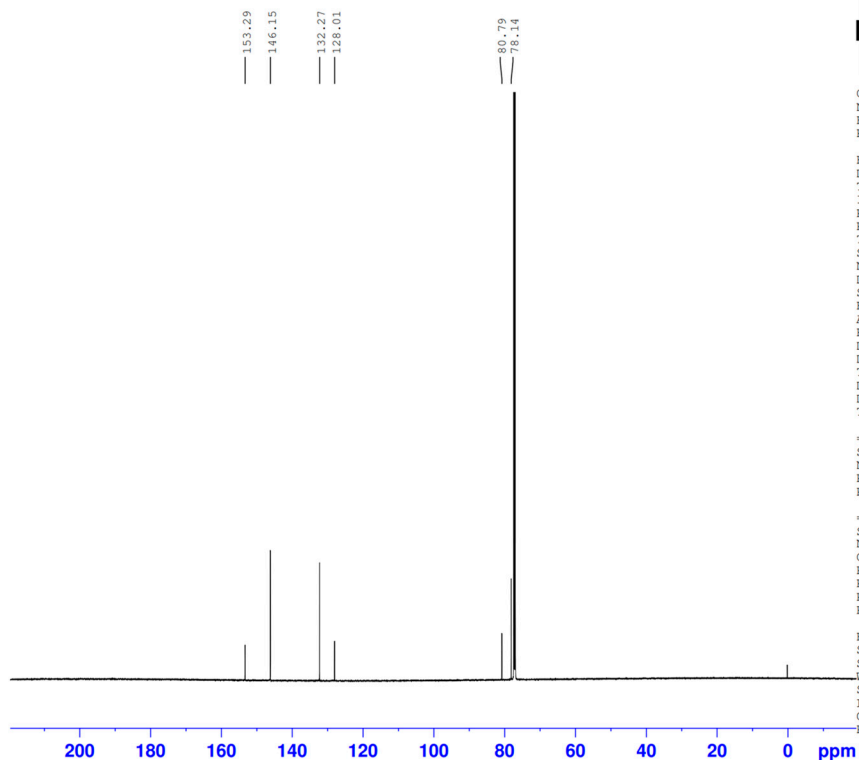


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GH477



Current Data Parameters
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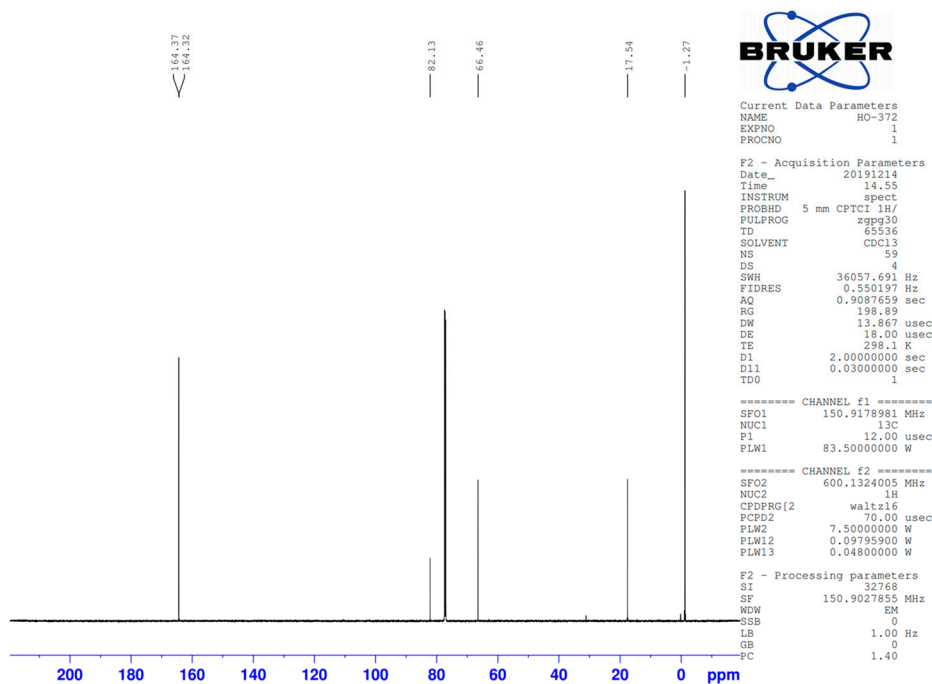
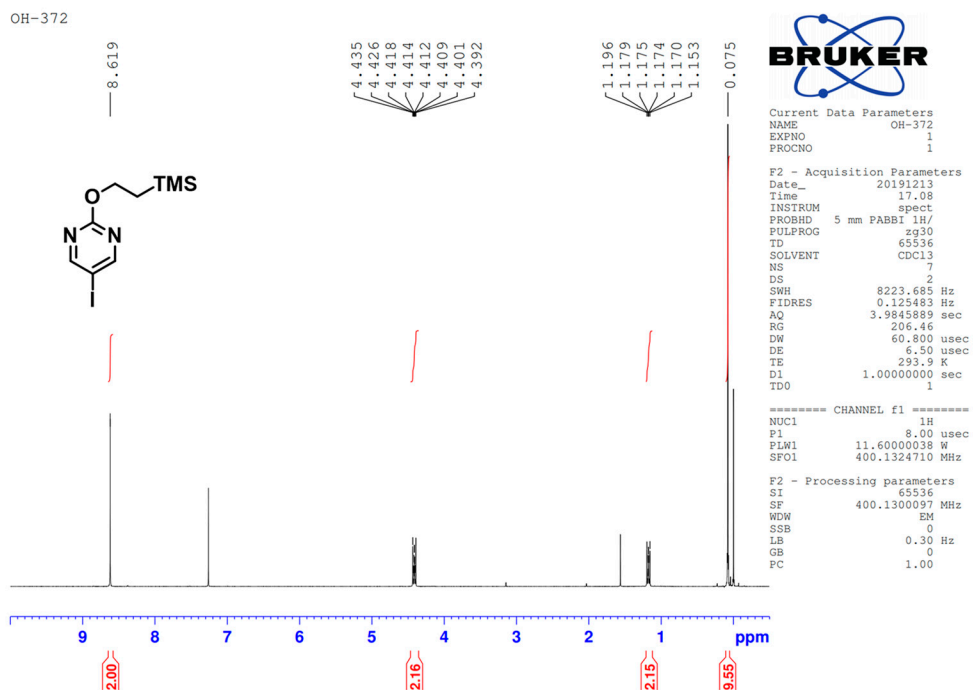
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INSTRUM spect
PROBHD 5 mm CPTCI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 613
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 198.89
DW 13.867 usec
DE 18.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 150.9178981 MHz
NUC1 13C
P1 12.00 usec
PLW1 83.50000000 W

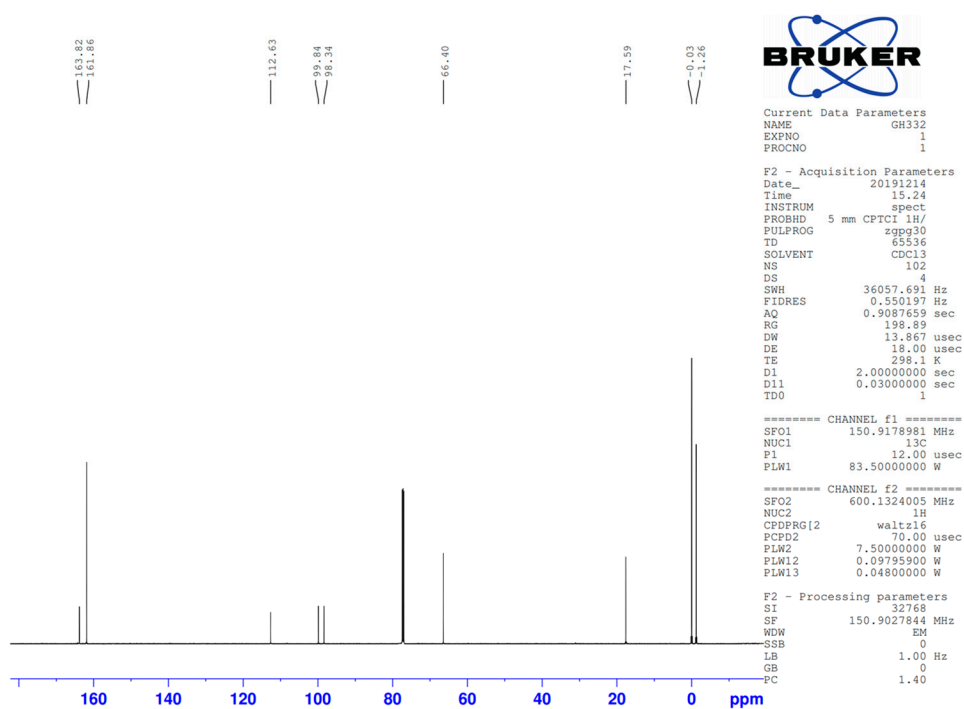
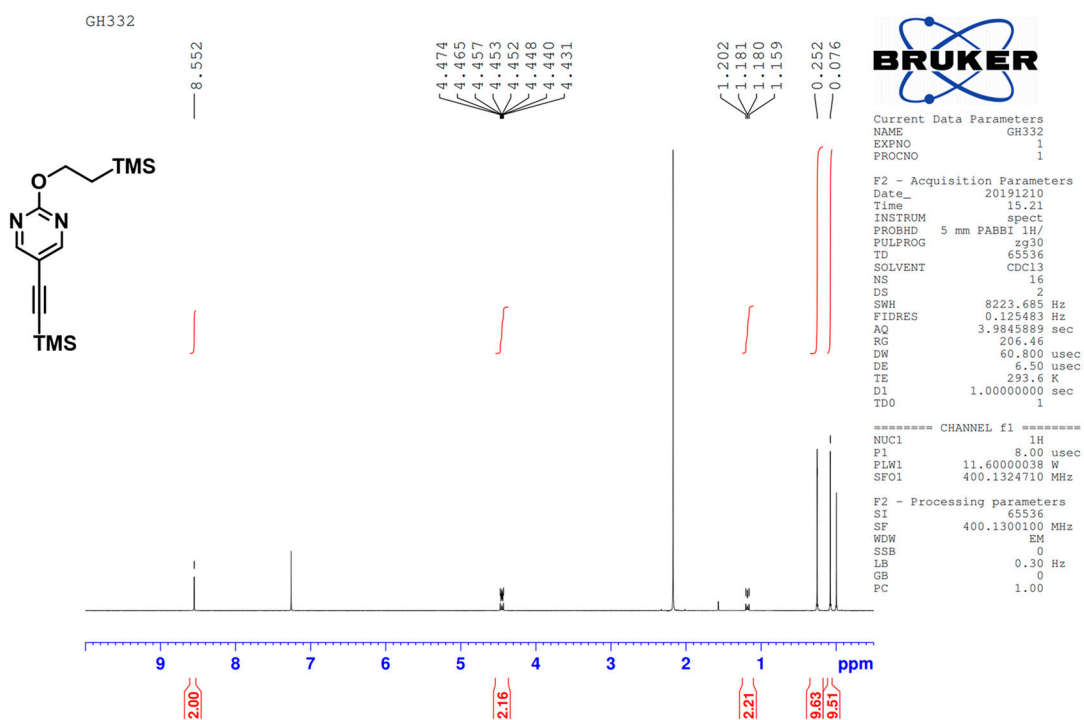
===== CHANNEL f2 =====
SF02 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 7.50000000 W
PLW12 0.09795900 W
PLW13 0.04800000 W

F2 - Processing parameters
SI 32768
SF 150.9027840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

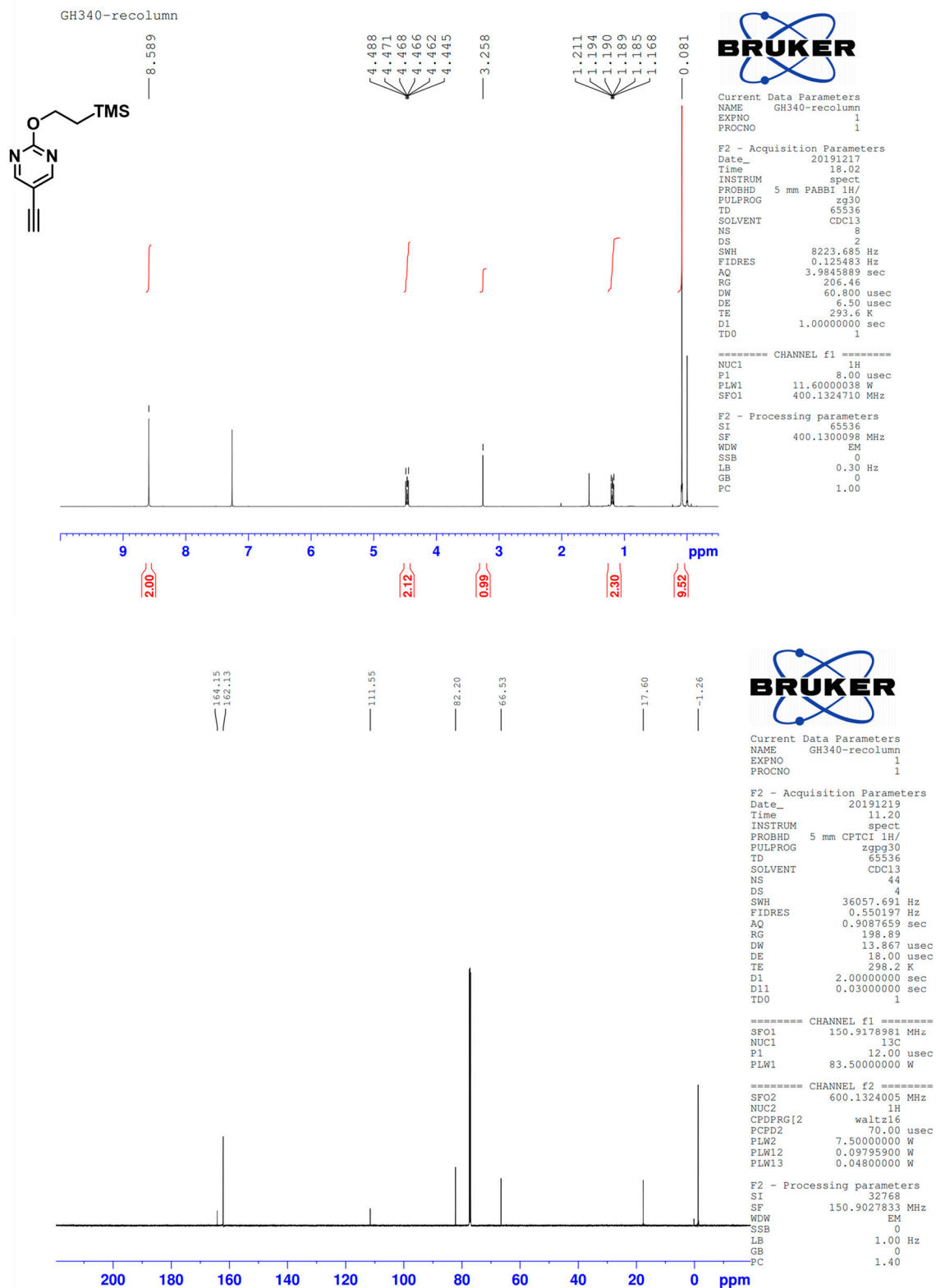
Compound 17



Compound 18

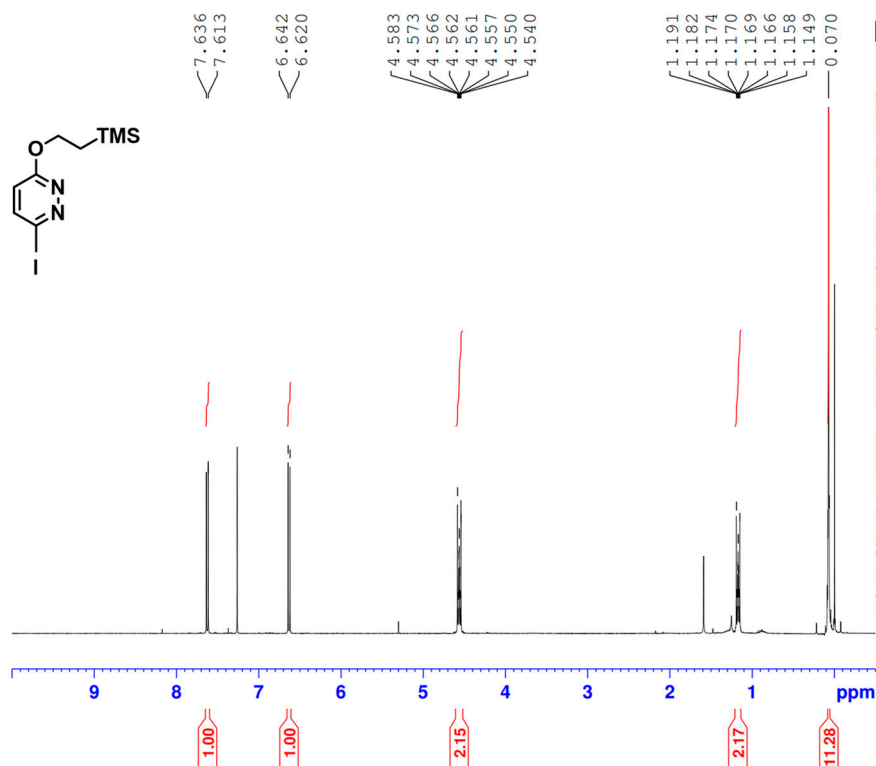


Compound 19



Compound 21

GH350

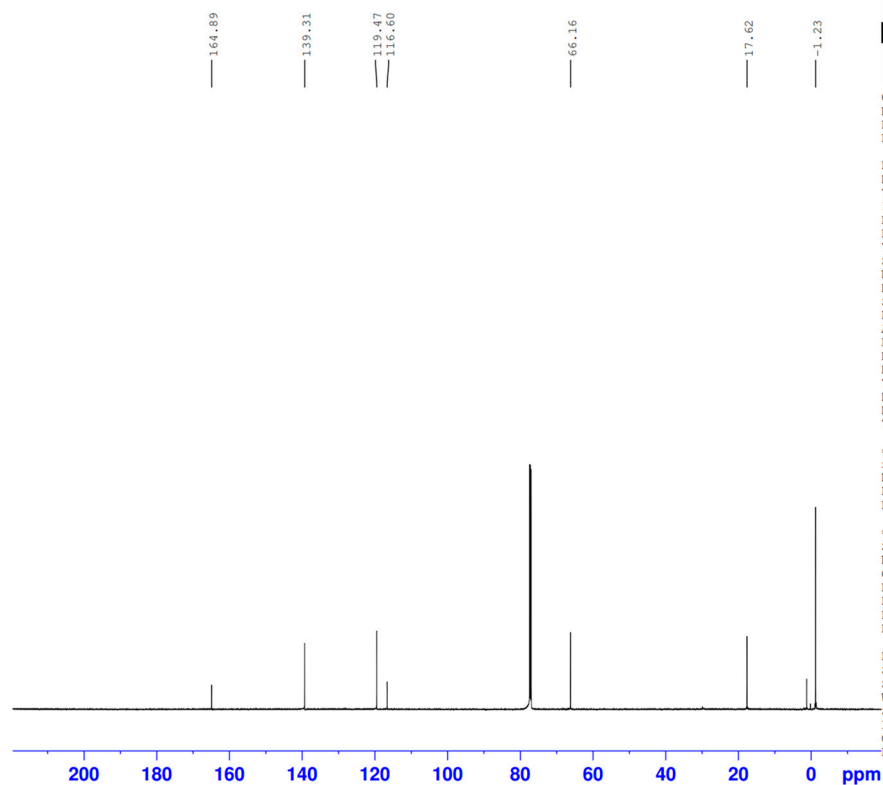


Current Data Parameters
NAME GH350
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191221
Time 16.30
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 139.07
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PLW1 11.60000038 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME GH350
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200109
Time 15.21
INSTRUM spect
PROBHD 5 mm CPTCI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 258
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 198.89
DW 13.867 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

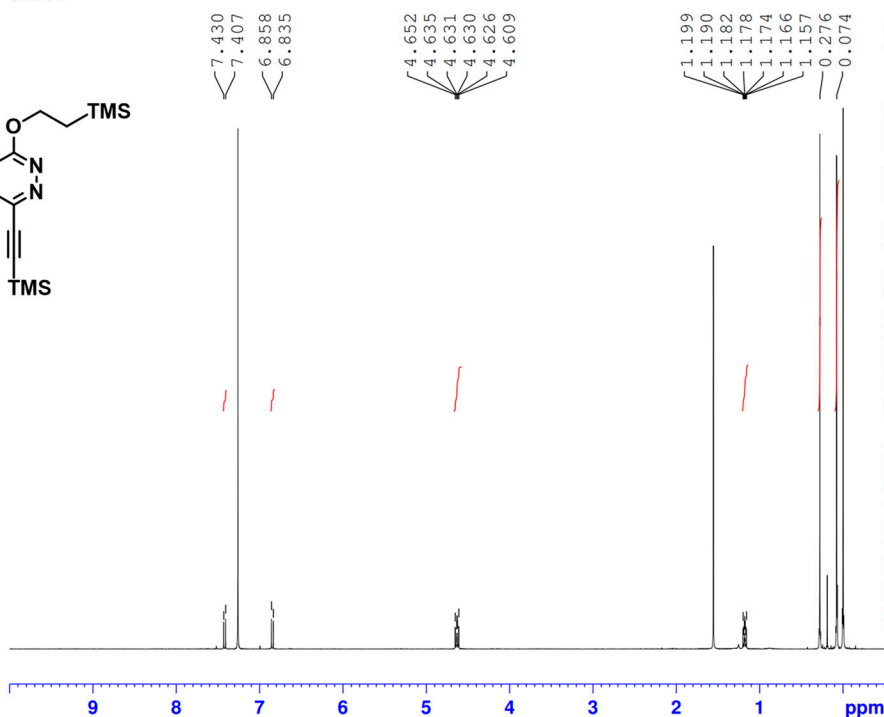
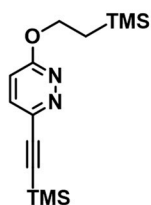
===== CHANNEL f1 =====
SFO1 150.9178981 MHz
NUC1 13C
P1 12.00 usec
PLW1 83.50000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 7.50000000 W
PLW12 0.09795900 W
PLW13 0.04800000 W

F2 - Processing parameters
SI 32768
SF 150.9027841 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 22

GH362

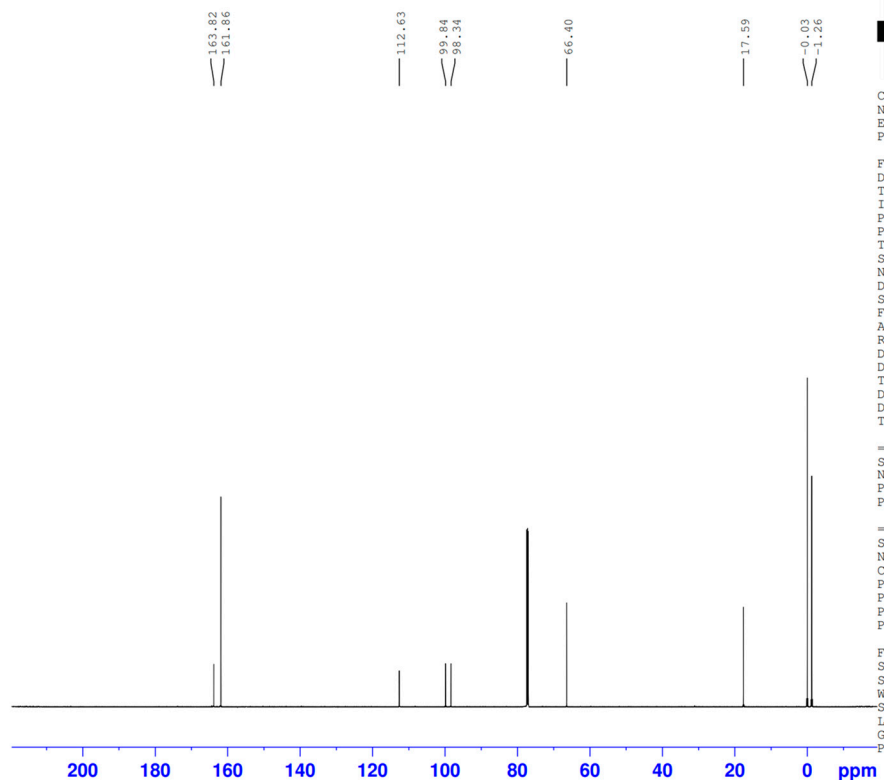


Current Data Parameters
NAME GH362
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191228
Time 15.26
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 206.46
DW 60.800 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PLW1 11.6000038 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME GH332
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 15.24
INSTRUM spect
PROBHD 5 mm CPTCI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 198.89
DW 13.867 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

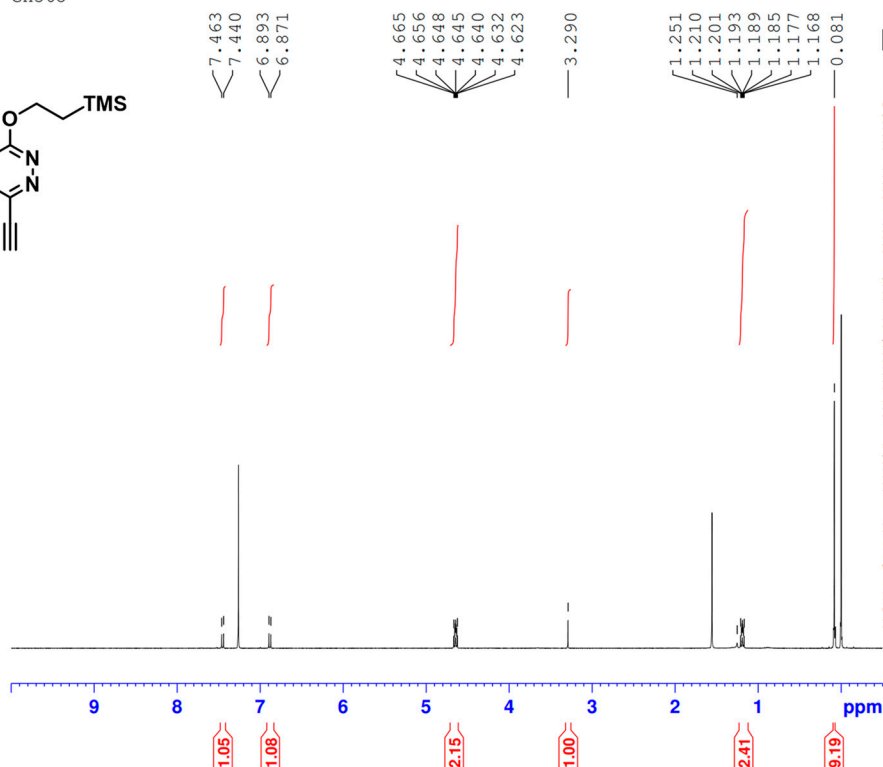
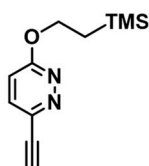
===== CHANNEL f1 =====
SFO1 150.9178981 MHz
NUC1 13C
P1 12.00 usec
PLW1 83.5000000 W

===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
PCPD2 waltz16
PLW2 7.5000000 W
PLW12 0.09795900 W
PLW13 0.04800000 W

F2 - Processing parameters
SI 32768
SF 150.9027844 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 23

GH365

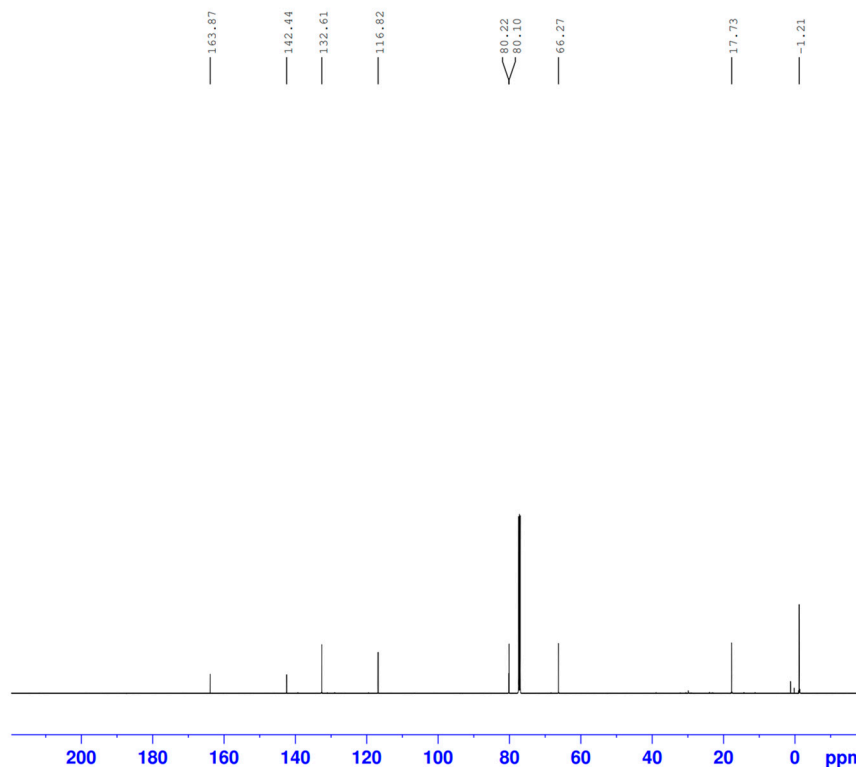


Current Data Parameters
 NAME GH365
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200103
 Time 12.35
 INSTRUM spect
 PROBHD 5 mm PABBI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 206.46
 DW 60.800 usec
 DE 6.50 usec
 TE 293.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PLW1 11.60000038 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME GH365
 EXPNO 1
 PROCNO 1

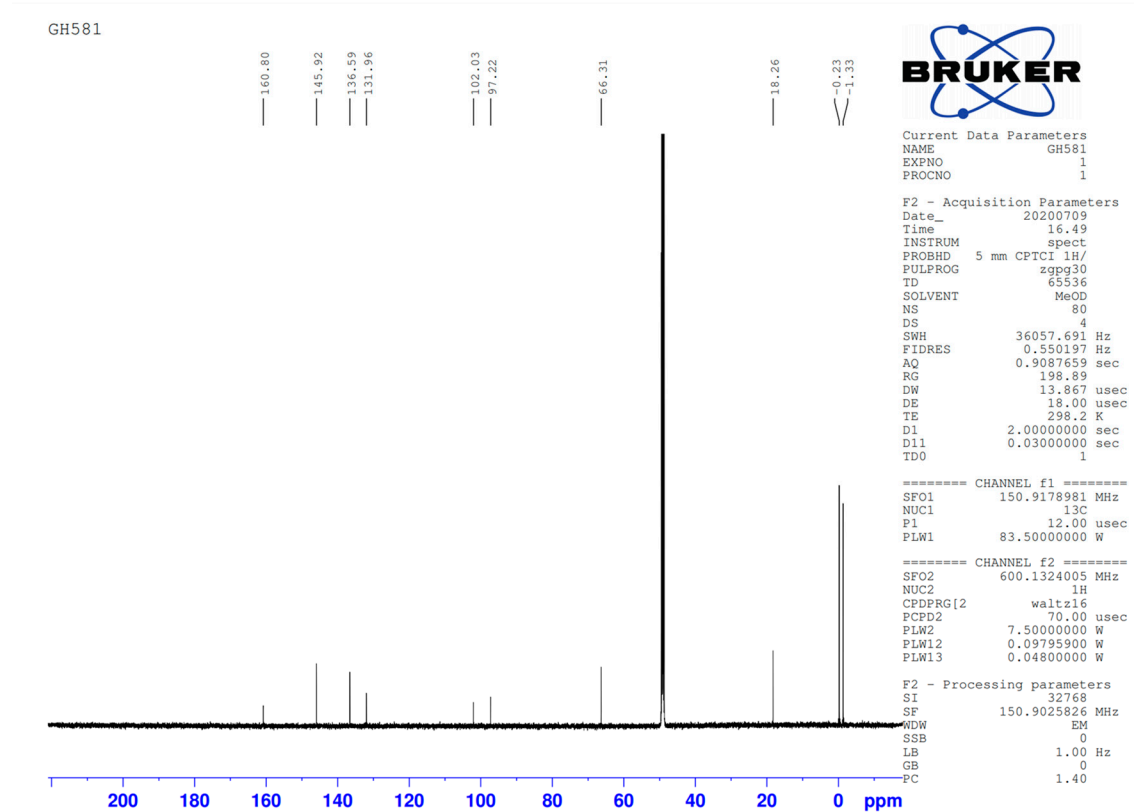
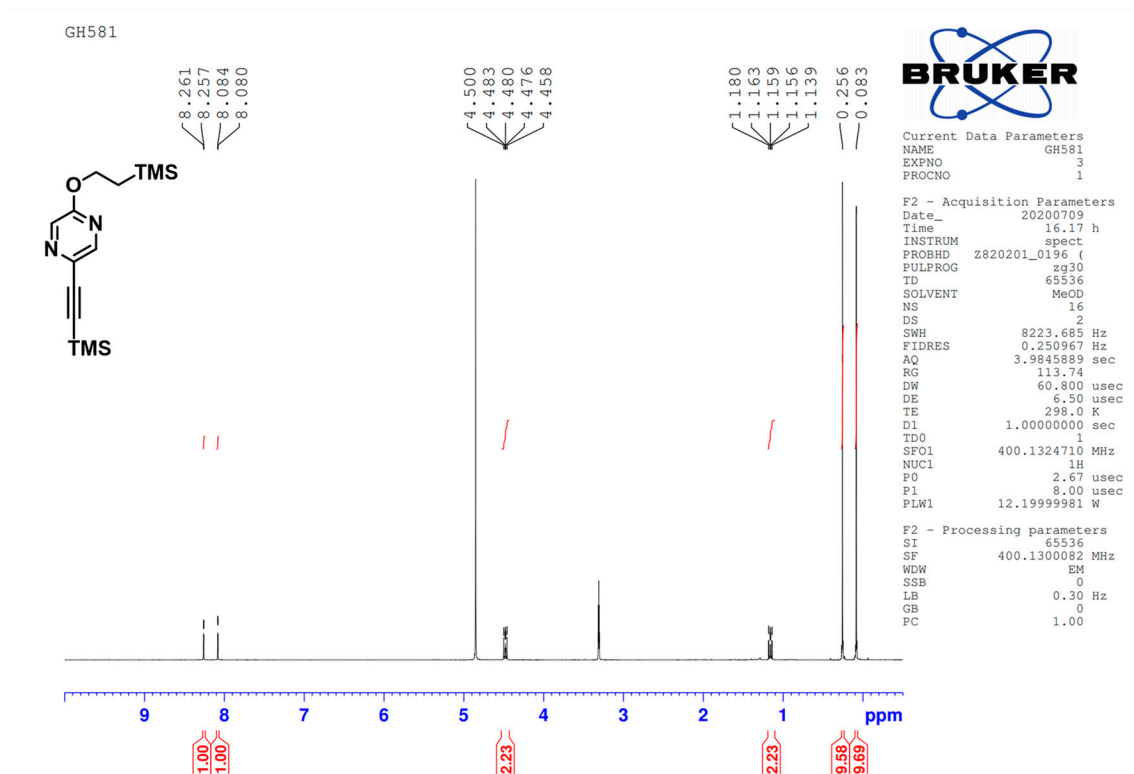
F2 - Acquisition Parameters
 Date_ 20200109
 Time 15.40
 INSTRUM spect
 PROBHD 5 mm CPTCI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 258
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 198.89
 DW 13.867 usec
 DE 18.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178981 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 83.50000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 7.50000000 W
 PLW12 0.09795900 W
 PLW13 0.04800000 W

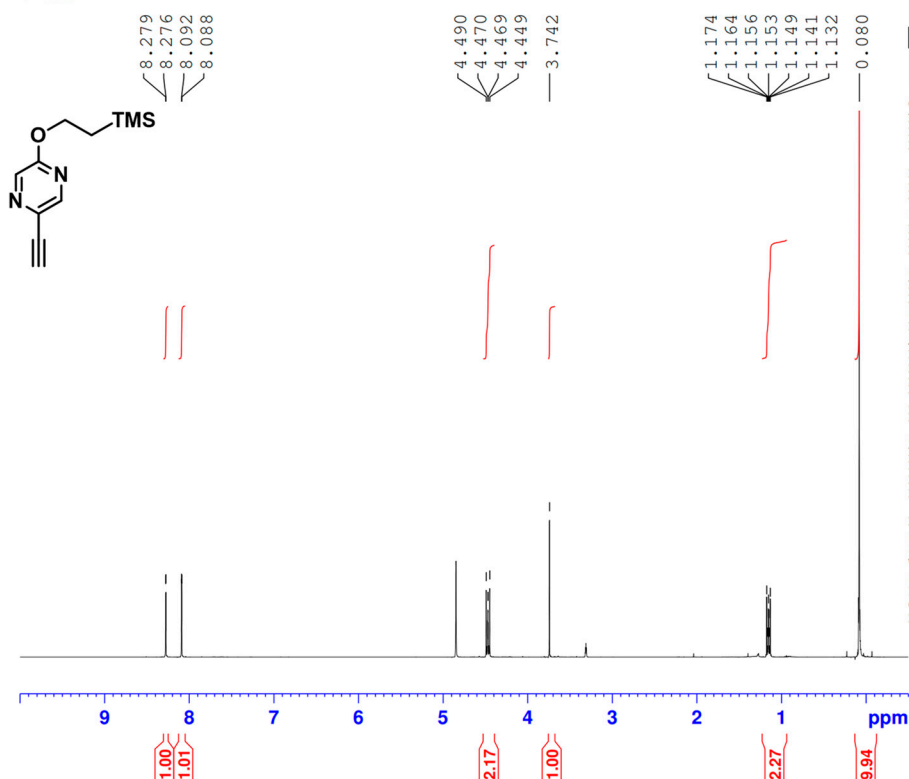
F2 - Processing parameters
 SI 32768
 SF 150.9027830 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Compound 27



Compound 28

GH589

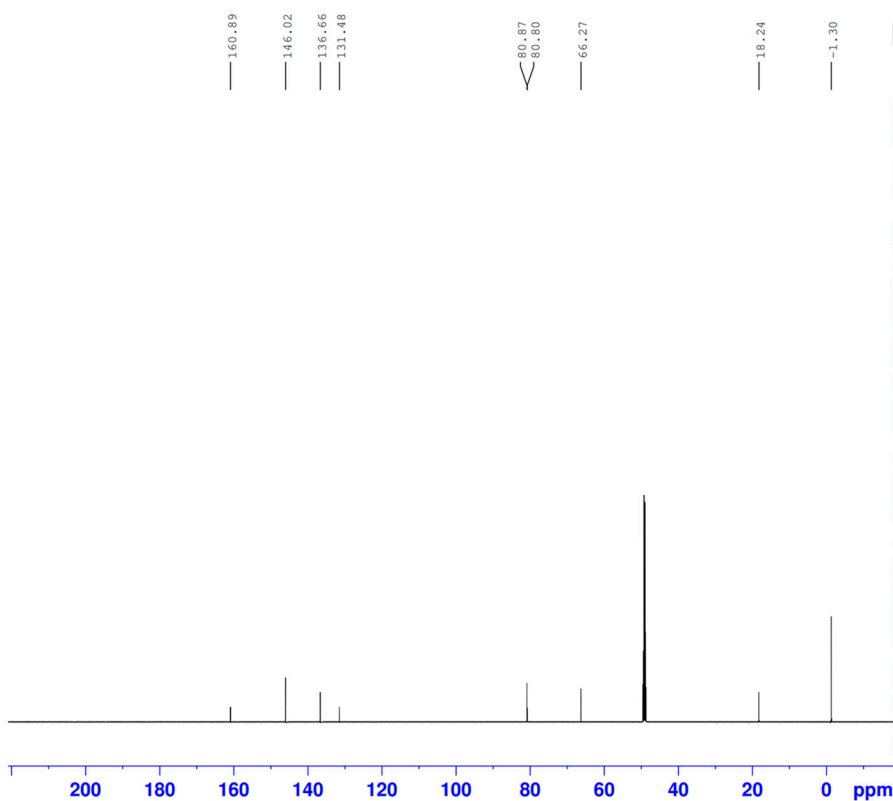


Current Data Parameters
 NAME GH589
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200709
 Time 16.26 h
 INSTRUM spect
 PROBHD Z820201_0196 (zg30)
 PULPROG 65536
 TD 16
 SOLVENT MeOD
 NS 2
 DS 8223.685 Hz
 SWH 0.250967 Hz
 FIDRES 3.9845889 sec
 AQ 33.3
 RG 60.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1324710 MHz
 NUC1 1H
 PO 2.67 usec
 P1 8.00 usec
 PLW1 12.19999981 W

F2 - Processing parameters
 SI 65536
 SF 400.1300074 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

GH589



Current Data Parameters
 NAME GH589
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200709
 Time 16.40
 INSTRUM spect
 PROBHD 5 mm CPTCI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 14
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 198.89
 DW 13.867 usec
 DE 18.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

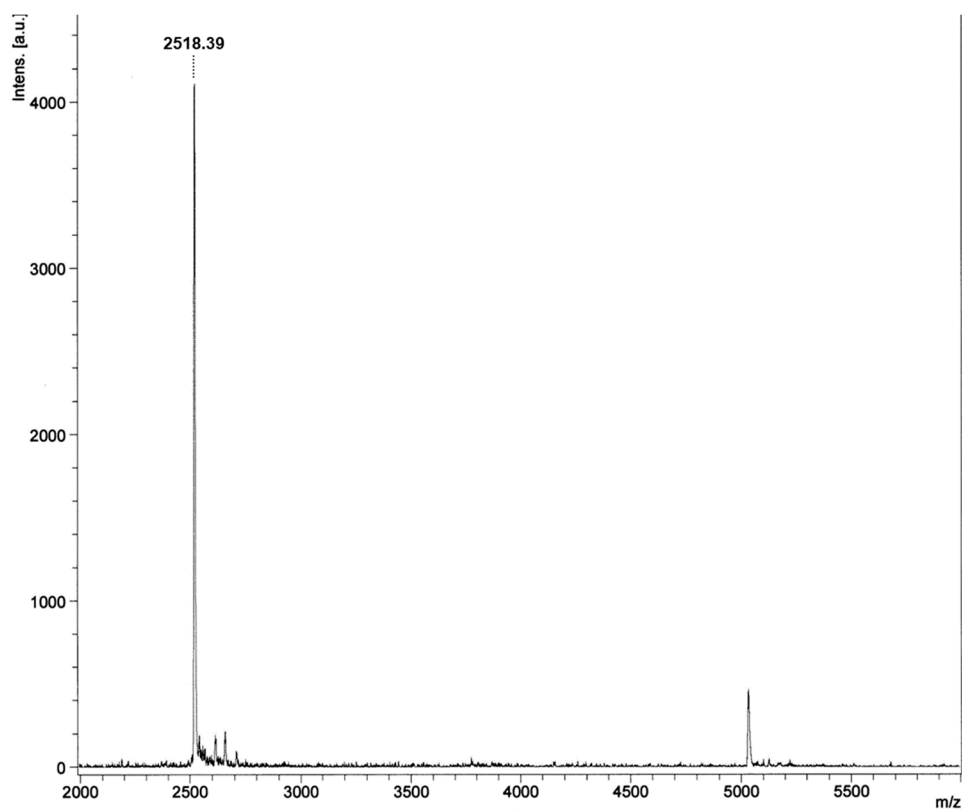
===== CHANNEL f1 =====
 SFO1 150.9178981 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 83.50000000 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 70.00 usec
 PLW2 7.50000000 W
 PLW12 0.09795900 W
 PLW13 0.04800000 W

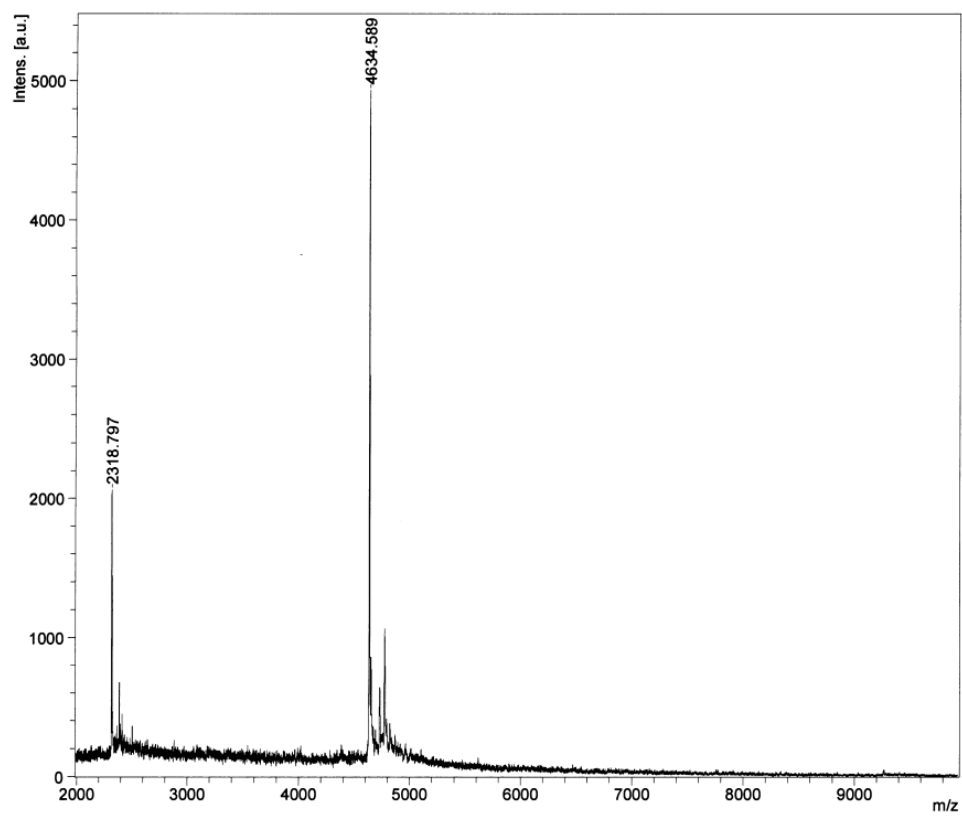
F2 - Processing parameters
 SI 32768
 SF 150.9025879 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5. MALDI-TOF MS charts of the synthesized ODNs

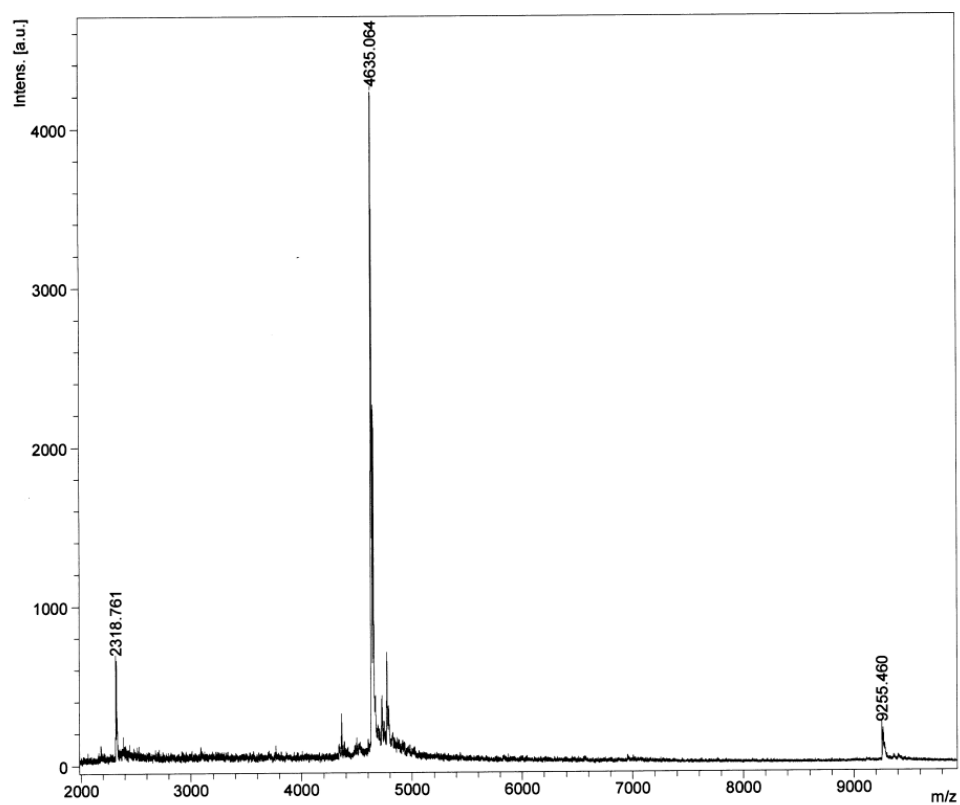
ODN1-^NPu1



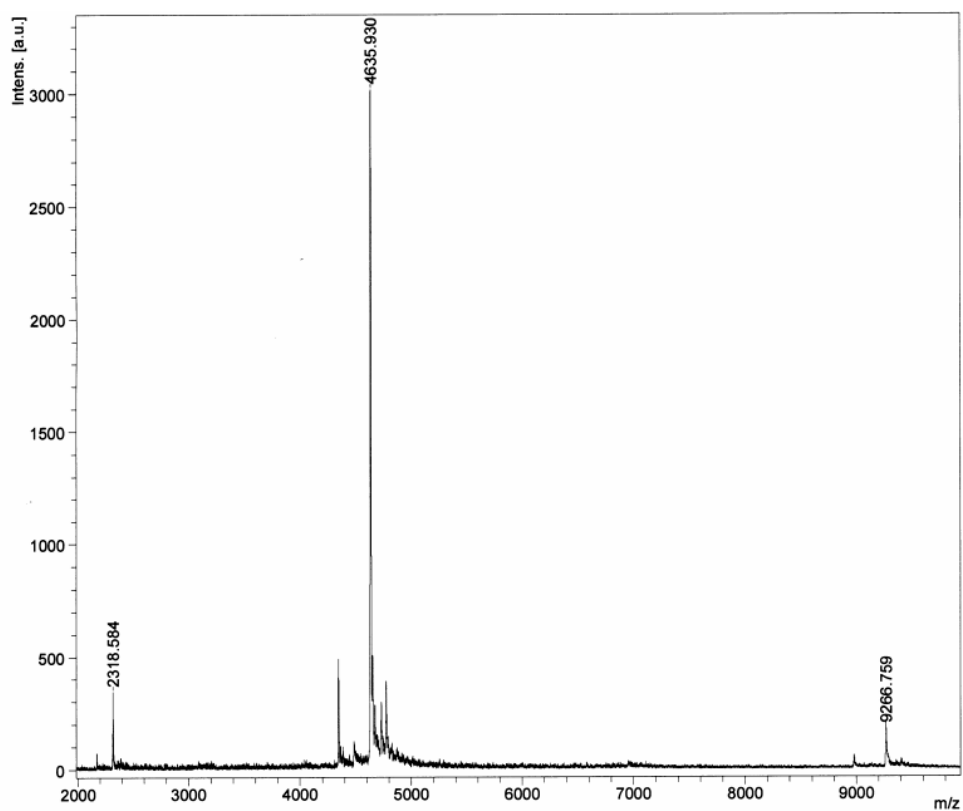
ODN3-^NPu1



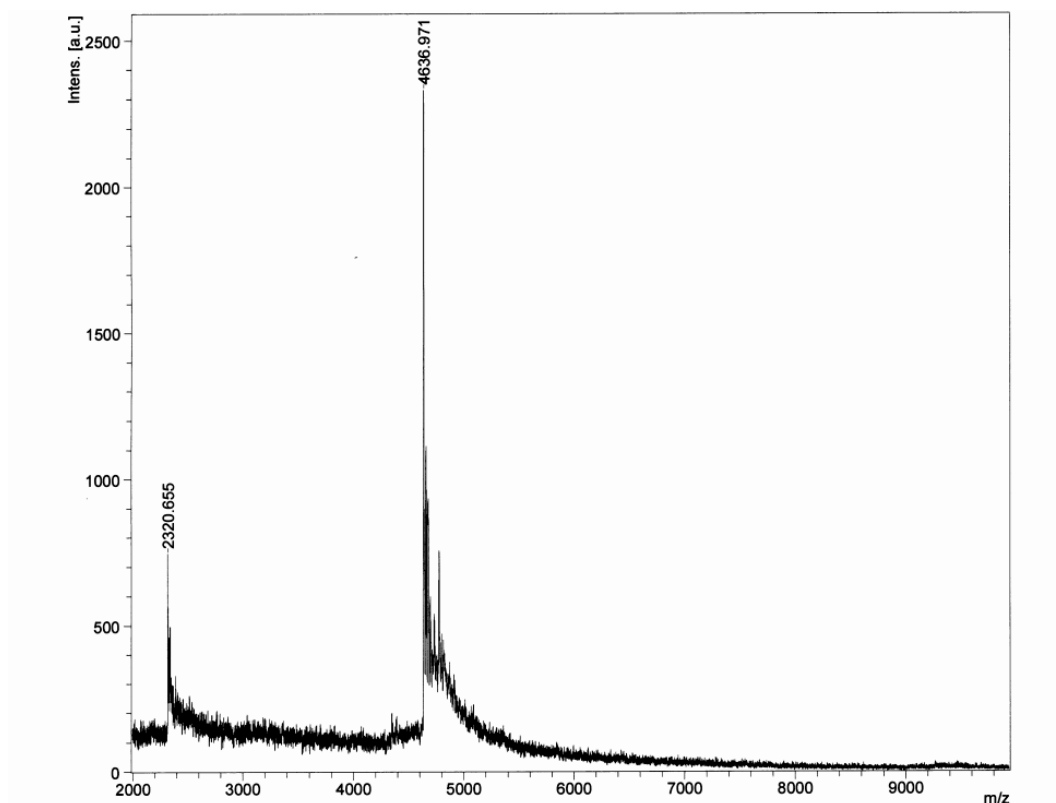
ODN3-^NPu2



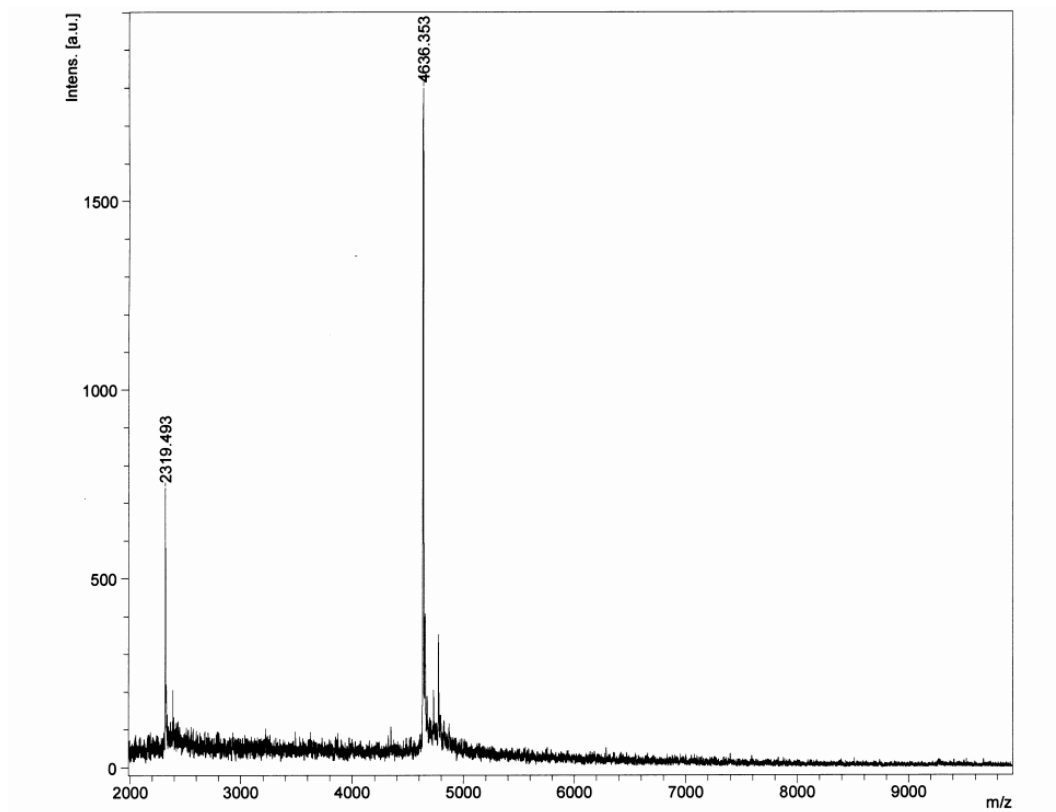
ODN3-^NPu3



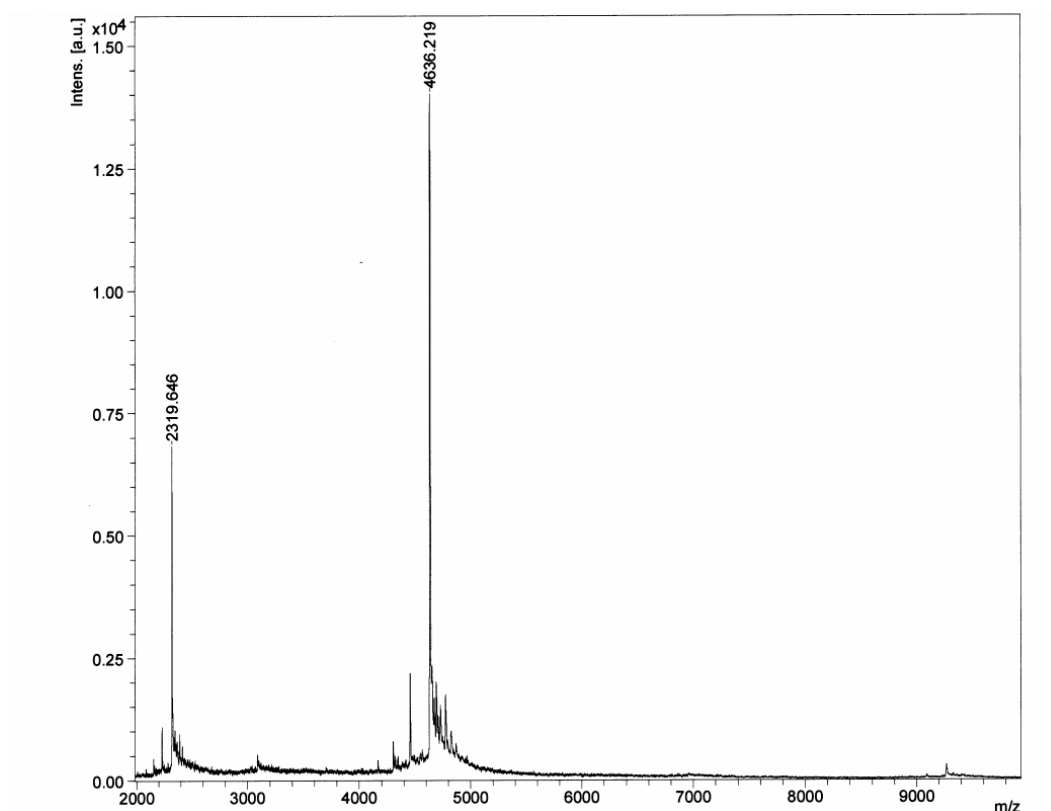
ODN3-⁰Pu1



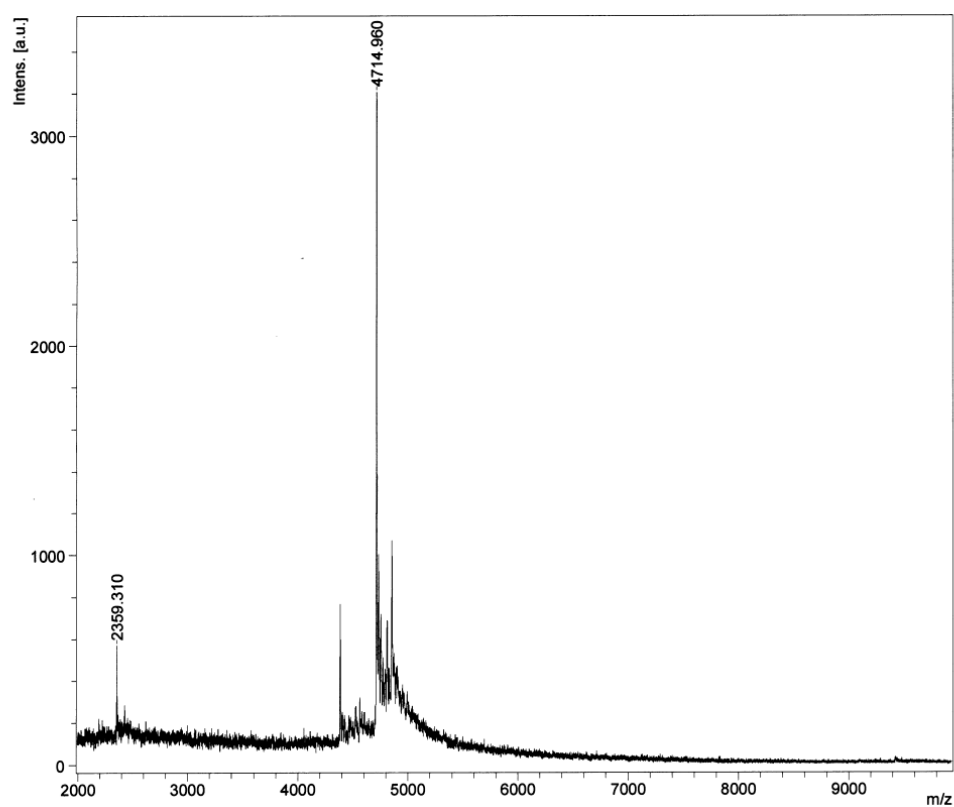
ODN3-⁰Pu2



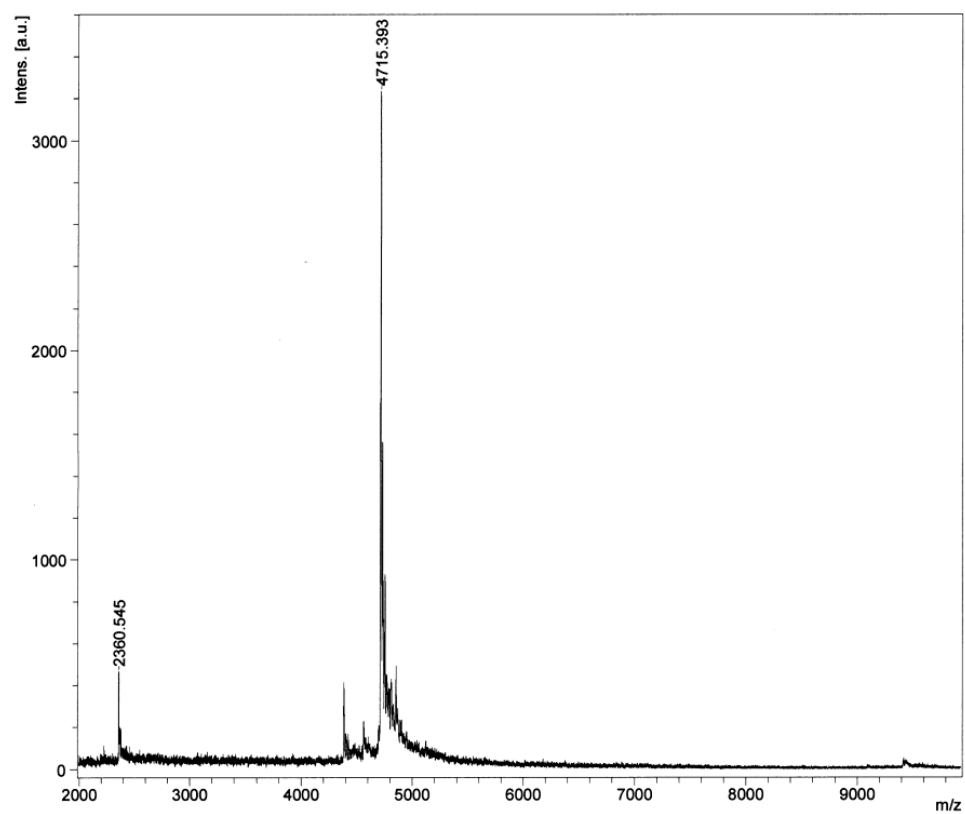
ODN3-⁰Pu3



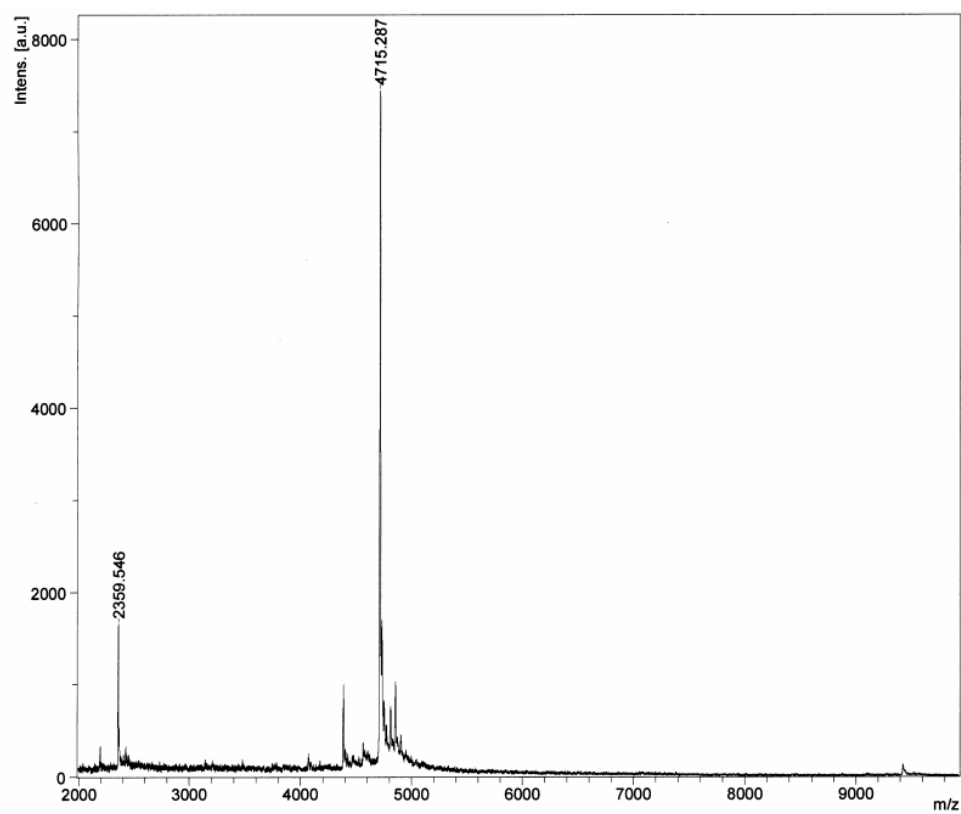
ODN4-^NPu1



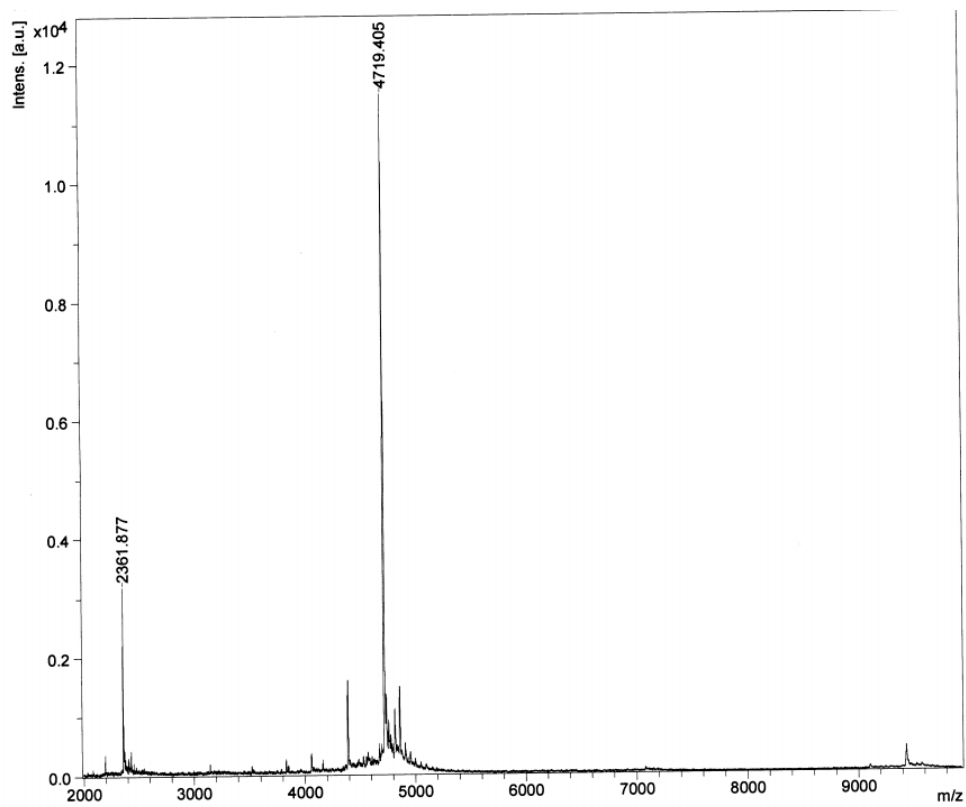
ODN4-^NPu2



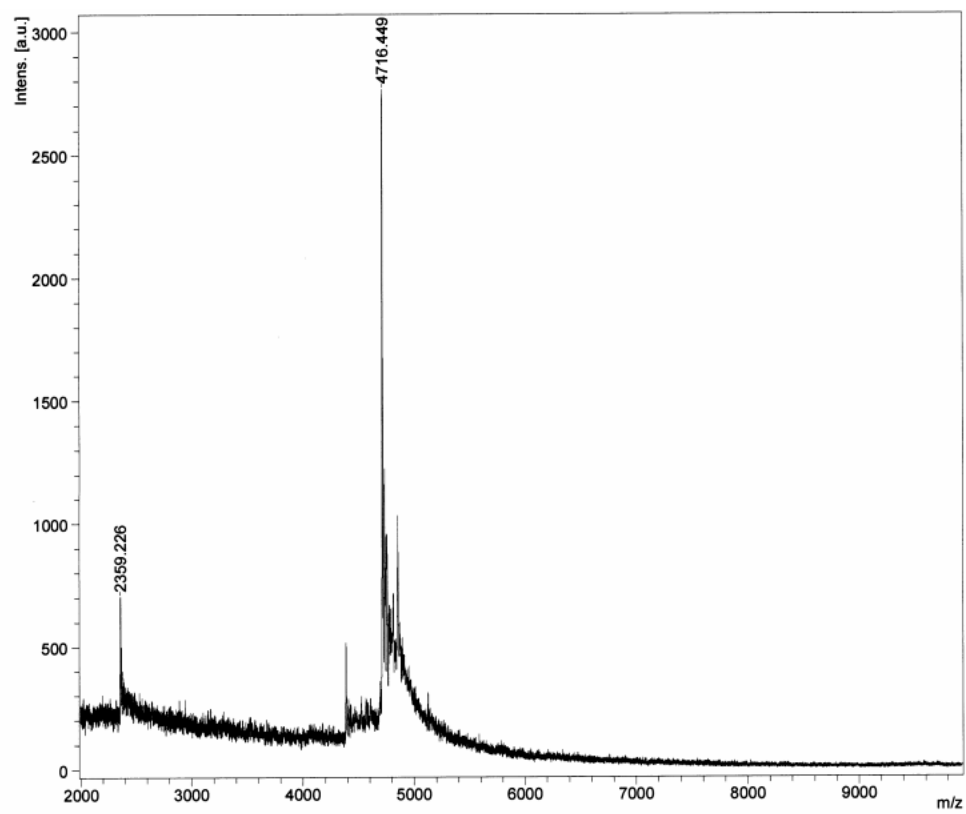
ODN4-^NPu3



ODN4-⁰Pu1



ODN4-⁰Pu2



ODN4-⁰Pu3

