附錄一

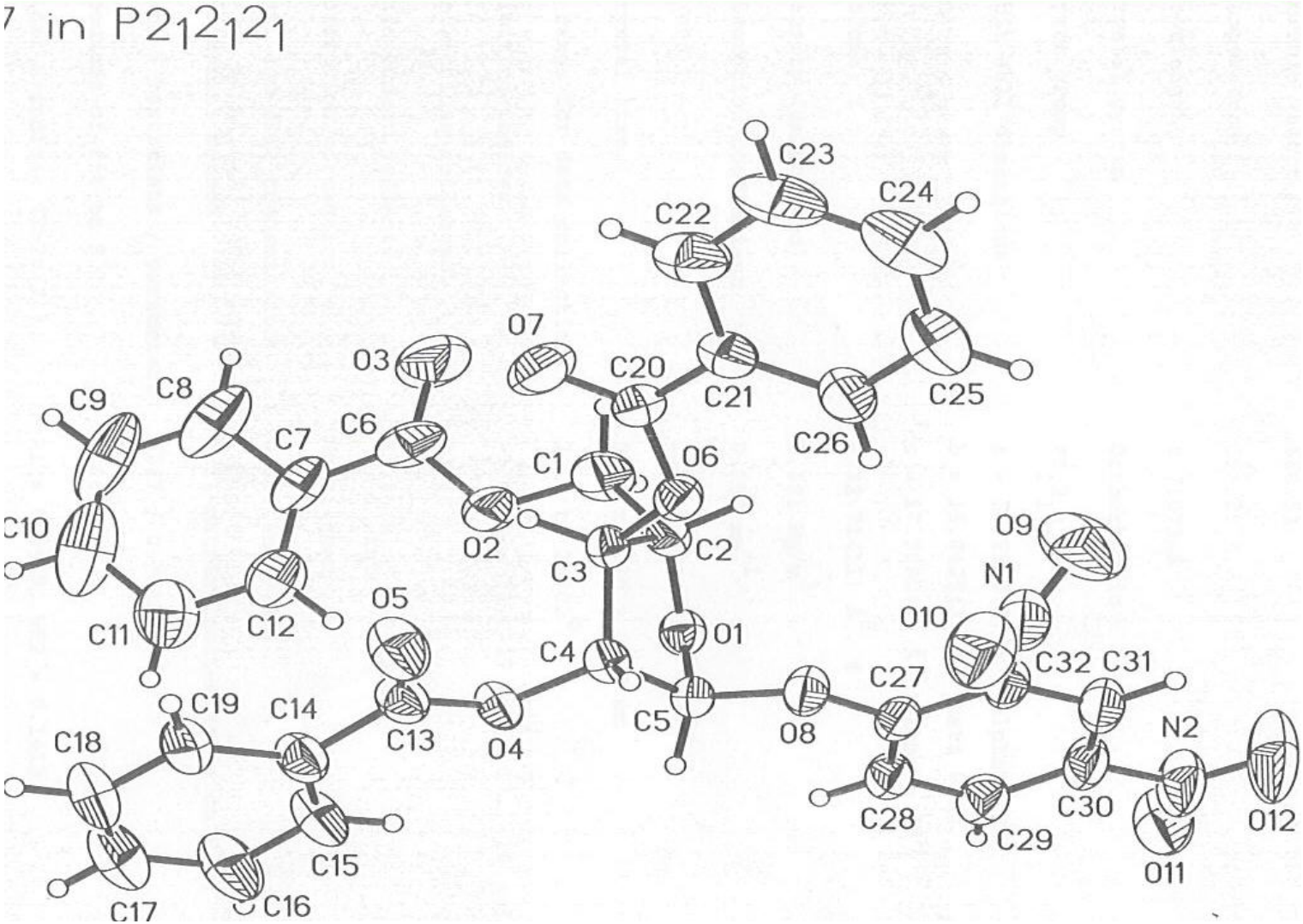

7 in P2₁2₁2₁
C23
C24
C22
O7
O3
C20
C21
C25
C9
C8
C6
C7
C26
C1
O6
C10
O2
C2
O9
C3
N1
O5
O10
C11
C12
O1
C4
C32
C31
C27
C19
C14
C5
O8
N2
C18
C13
O4
C30
O12
C28
C29
C15
O11
C17
C16

Table 1. Crystal data and structure refinement for IC9597.

Identification code	ic9597
Diffractometer used	Nonius KappaCCD
Empirical formula	$C_{32}H_{24}N_2O_{12}$
Formula weight	628.53
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 11.2970(2) Å alpha = 90° b = 15.0420(3) Å beta = 90° c = 17.7880(4) Å gamma = 90°
Volume, Z	3022.71(11) $Å^3$, 4
Density (calculated)	1.381 Mg/m^3
Absorption coefficient	0.107 mm^{-1}
F(000)	1304
Crystal size	0.30 x 0.20 x 0.10 mm
θ range for data collection	2.14 to 25.02°
Limiting indices	$-13 \le h \le 13$, $-17 \le k \le 17$, $-19 \le l \le 21$
Reflections collected	13688
Independent reflections	5328 (R_{int} = 0.0598)
Absorption correction	Multi-scan
Max. and min. transmission	0.990 and 0.934
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5287 / 0 / 416
Goodness-of-fit on F^2	1.004
Final R indices [I>2σ(I)]	R1 = 0.0569, wR2 = 0.1413
R indices (all data)	R1 = 0.1149, wR2 = 0.1838
Absolute structure parameter	0(2)
Extinction coefficient	0.017(2)
Largest diff. peak and hole	0.358 and -0.189 $eÅ^{-3}$

Table 2. Bond lengths [Å] and angles [°] for 9597.

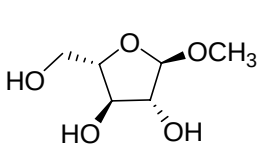
O(1)-C(5)	1.382(5)	O(1)-C(2)	1.447(5)
O(2)-C(6)	1.325(6)	O(2)-C(1)	1.439(6)
O(3)-C(6)	1.178(7)	O(4)-C(13)	1.342(5)
O(4)-C(4)	1.441(5)	O(5)-C(13)	1.188(5)
O(6)-C(20)	1.334(5)	O(6)-C(3)	1.444(5)
O(7)-C(20)	1.210(5)	O(8)-C(27)	1.355(5)
O(8)-C(5)	1.435(5)	O(9)-N(1)	1.153(6)
O(10)-N(1)	1.252(6)	O(11)-N(2)	1.217(7)
O(12)-N(2)	1.207(6)	N(1)-C(32)	1.458(7)
N(2)-C(30)	1.469(6)	C(1)-C(2)	1.494(7)
C(2)-C(3)	1.525(6)	C(3)-C(4)	1.519(5)
C(4)-C(5)	1.504(6)	C(6)-C(7)	1.464(8)
C(7)-C(12)	1.352(8)	C(7)-C(8)	1.396(8)
C(8)-C(9)	1.408(13)	C(9)-C(10)	1.337(14)
C(10)-C(11)	1.365(12)	C(11)-C(12)	1.416(9)
C(13)-C(14)	1.485(7)	C(14)-C(19)	1.389(6)
C(14)-C(15)	1.390(6)	C(15)-C(16)	1.365(7)
C(16)-C(17)	1.393(9)	C(17)-C(18)	1.371(9)
C(18)-C(19)	1.368(8)	C(20)-C(21)	1.475(6)
C(21)-C(26)	1.371(6)	C(21)-C(22)	1.388(7)
C(22)-C(23)	1.388(9)	C(23)-C(24)	1.357(9)
C(24)-C(25)	1.363(9)	C(25)-C(26)	1.382(7)
C(27)-C(28)	1.374(6)	C(27)-C(32)	1.393(6)
C(28)-C(29)	1.388(6)	C(29)-C(30)	1.378(7)
C(30)-C(31)	1.355(7)	C(31)-C(32)	1.363(6)

C(5)-O(1)-C(2)	107.3(3)	C(6)-O(2)-C(1)	118.3(4)
C(13)-O(4)-C(4)	117.5(3)	C(20)-O(6)-C(3)	118.7(3)
C(27)-O(8)-C(5)	118.6(3)	O(9)-N(1)-O(10)	121.5(6)
O(9)-N(1)-C(32)	120.0(6)	O(10)-N(1)-C(32)	118.2(6)
O(12)-N(2)-O(11)	123.2(5)	O(12)-N(2)-C(30)	117.7(5)
O(11)-N(2)-C(30)	119.0(5)	O(2)-C(1)-C(2)	109.4(4)
O(1)-C(2)-C(1)	110.0(4)	O(1)-C(2)-C(3)	105.7(3)
C(1)-C(2)-C(3)	115.5(4)	O(6)-C(3)-C(4)	108.2(3)
O(6)-C(3)-C(2)	110.5(3)	C(4)-C(3)-C(2)	104.8(3)
O(4)-C(4)-C(5)	103.6(3)	O(4)-C(4)-C(3)	112.2(3)
C(5)-C(4)-C(3)	102.9(3)	O(1)-C(5)-O(8)	111.0(3)
O(1)-C(5)-C(4)	106.3(3)	O(8)-C(5)-C(4)	105.3(3)
O(3)-C(6)-O(2)	120.6(6)	O(3)-C(6)-C(7)	124.9(6)
O(2)-C(6)-C(7)	114.4(5)	C(12)-C(7)-C(8)	119.2(7)
C(12)-C(7)-C(6)	123.0(5)	C(8)-C(7)-C(6)	117.7(7)
C(7)-C(8)-C(9)	119.8(9)	C(10)-C(9)-C(8)	118.5(8)
C(9)-C(10)-C(11)	123.9(10)	C(10)-C(11)-C(12)	116.8(9)
C(7)-C(12)-C(11)	121.6(6)	O(5)-C(13)-O(4)	123.0(4)
O(5)-C(13)-C(14)	125.9(4)	O(4)-C(13)-C(14)	111.0(4)
C(19)-C(14)-C(15)	119.5(5)	C(19)-C(14)-C(13)	119.0(5)
C(15)-C(14)-C(13)	121.5(4)	C(16)-C(15)-C(14)	121.0(5)
C(15)-C(16)-C(17)	118.4(6)	C(18)-C(17)-C(16)	121.4(6)
C(19)-C(18)-C(17)	119.8(5)	C(18)-C(19)-C(14)	120.0(6)
O(7)-C(20)-O(6)	121.6(4)	O(7)-C(20)-C(21)	125.5(4)
O(6)-C(20)-C(21)	112.9(4)	C(26)-C(21)-C(22)	118.4(5)
C(26)-C(21)-C(20)	122.6(4)	C(22)-C(21)-C(20)	118.9(5)
C(23)-C(22)-C(21)	120.2(6)	C(24)-C(23)-C(22)	120.0(6)
C(23)-C(24)-C(25)	120.5(6)	C(24)-C(25)-C(26)	119.9(6)
C(21)-C(26)-C(25)	120.9(5)	O(8)-C(27)-C(28)	124.7(4)
O(8)-C(27)-C(32)	116.6(4)	C(28)-C(27)-C(32)	118.7(4)
C(27)-C(28)-C(29)	120.0(4)	C(30)-C(29)-C(28)	118.8(5)
C(31)-C(30)-C(29)	122.2(4)	C(31)-C(30)-N(2)	118.8(5)
C(29)-C(30)-N(2)	118.9(5)	C(30)-C(31)-C(32)	118.3(4)

C(31)-C(32)-C(27)	121.8(4)	C(31)-C(32)-N(1)	118.2(4)
C(27)-C(32)-N(1)	120.0(4)		

Symmetry transformations used to generate equivalent atoms:

附錄二



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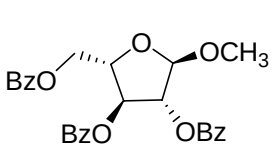

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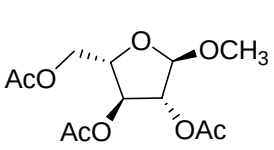

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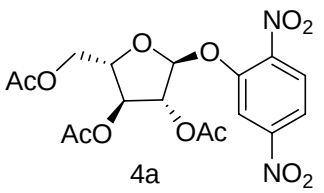

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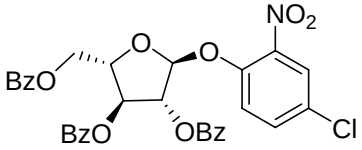

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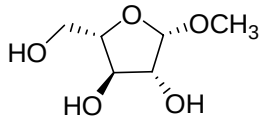

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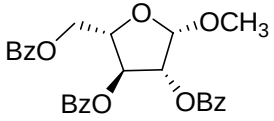

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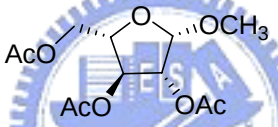

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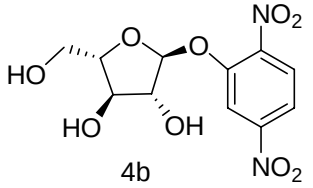

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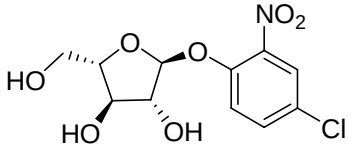

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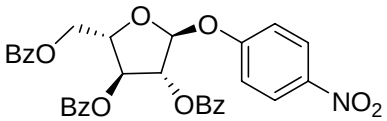

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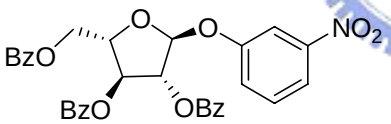
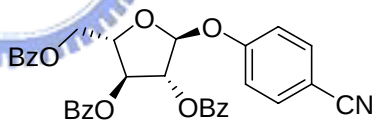
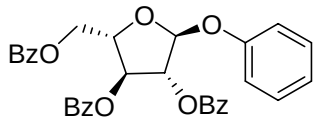


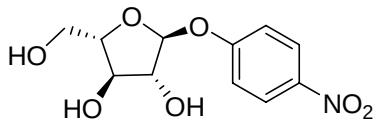
7a



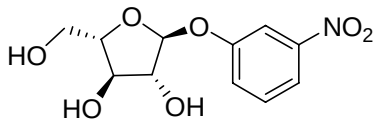
8a



9a



6b



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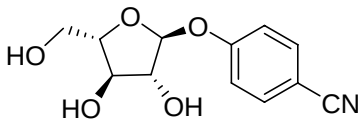
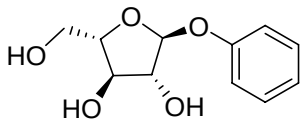


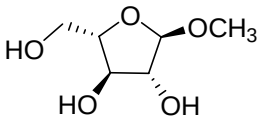
8b



9b

附錄三

化合物 1a


HO
O
OCH3
HO
OH

chen 050113 OCH3
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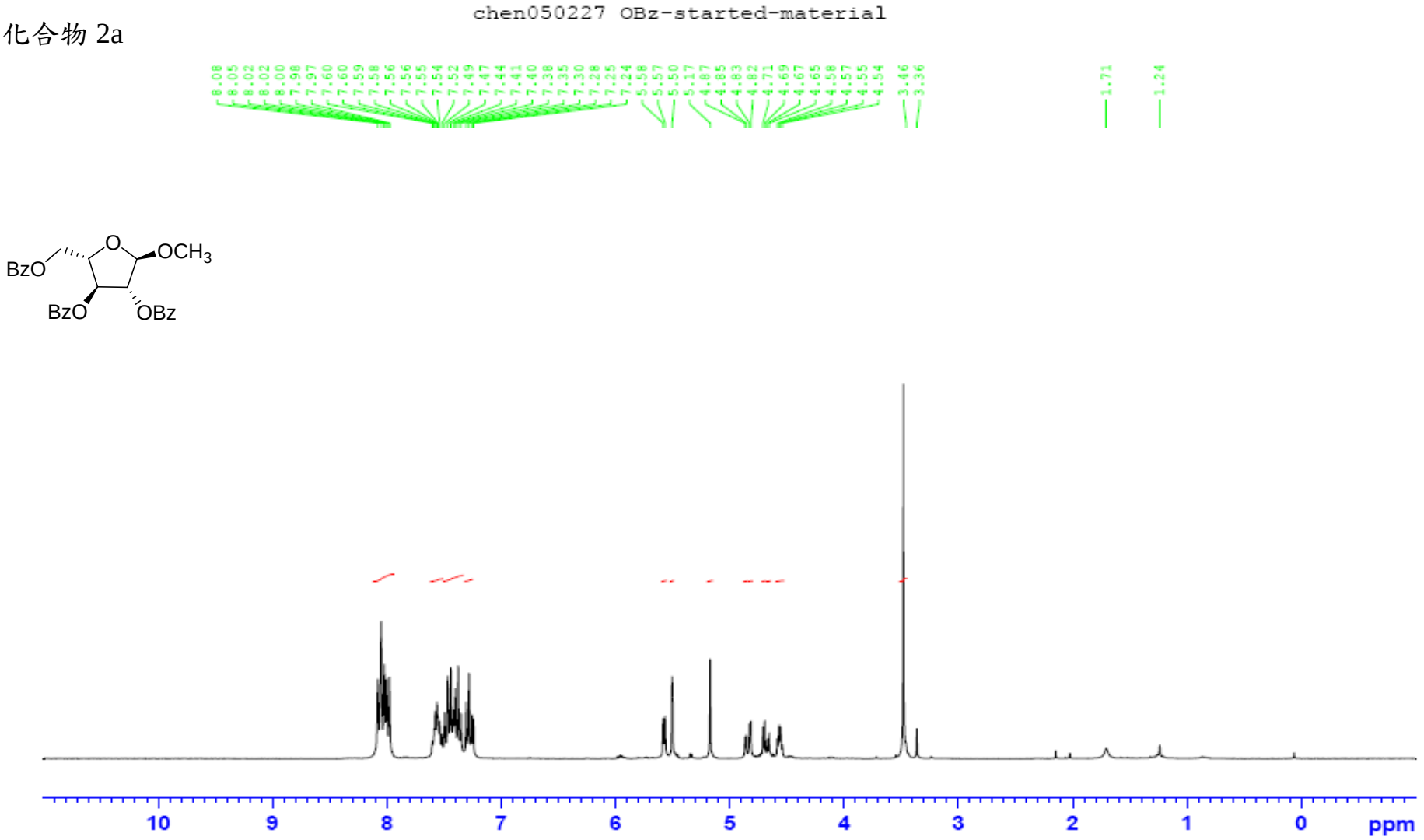
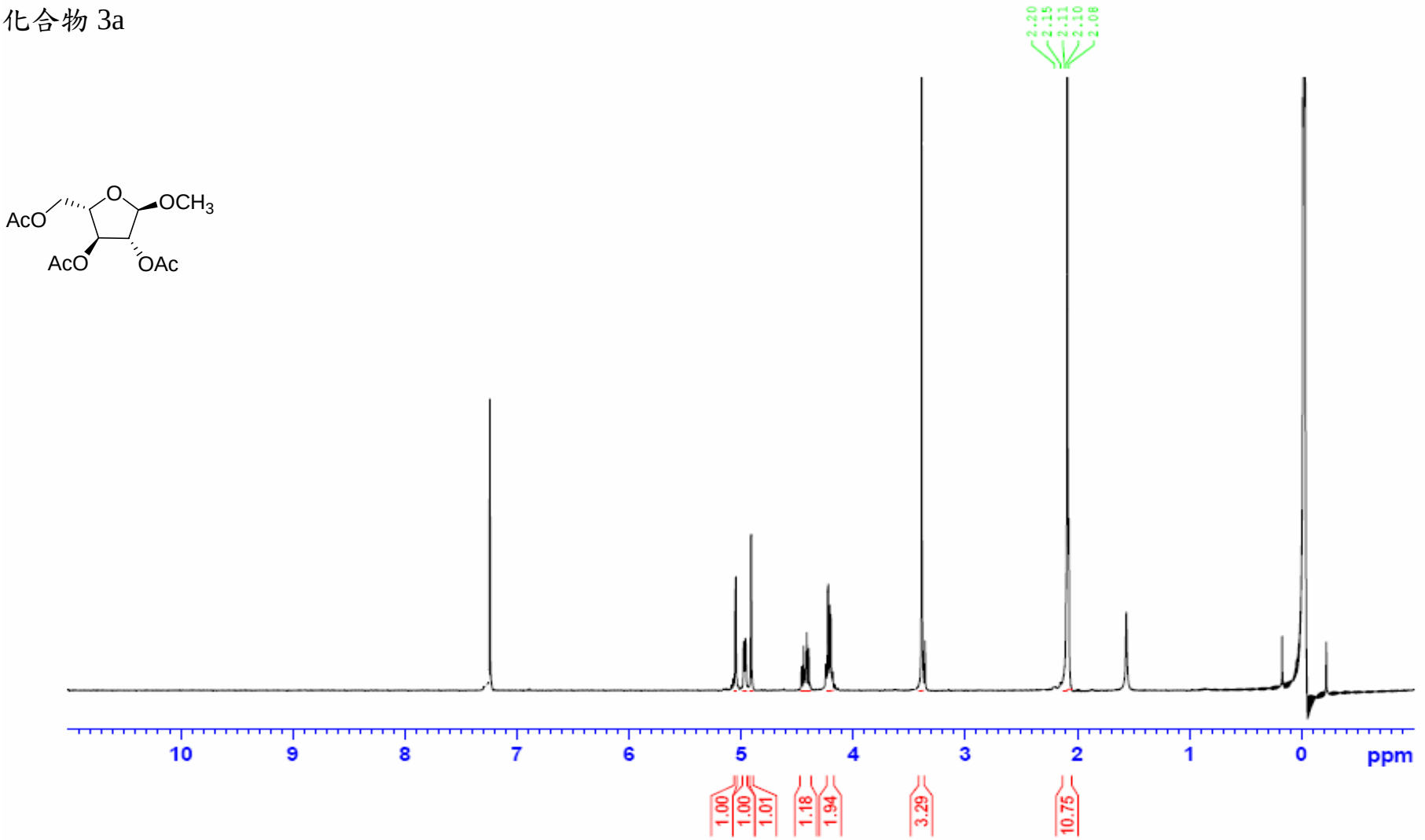
4.81
3.95
3.94
3.93
3.93
3.92
3.91
3.90
3.84
3.83
3.82
3.81
3.73
3.71
3.69
3.67
3.61
3.59
3.57
3.55
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.87
0.92
1.00
0.98
2.89

化合物 2a


chen050227 OBz-started-material
8.08
8.05
8.02
8.02
8.00
7.98
7.97
7.60
7.60
7.59
7.58
7.56
7.56
7.55
7.54
7.52
7.49
7.47
7.44
7.41
7.40
7.38
7.35
7.30
7.28
7.25
7.24
5.58
5.57
5.50
5.17
4.87
4.85
4.83
4.82
4.71
4.69
4.67
4.65
4.58
4.57
4.55
4.54
3.46
3.36
1.71
1.24
BzO
OCH3
BzO
OBz
10
9
8
7
6
5
4
3
2
1
0
ppm

化合物 3a


AcO
O
OCH3
AcO
OAc
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2.11
2.10
2.08
10
9
8
7
6
5
4
3
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1
0
ppm
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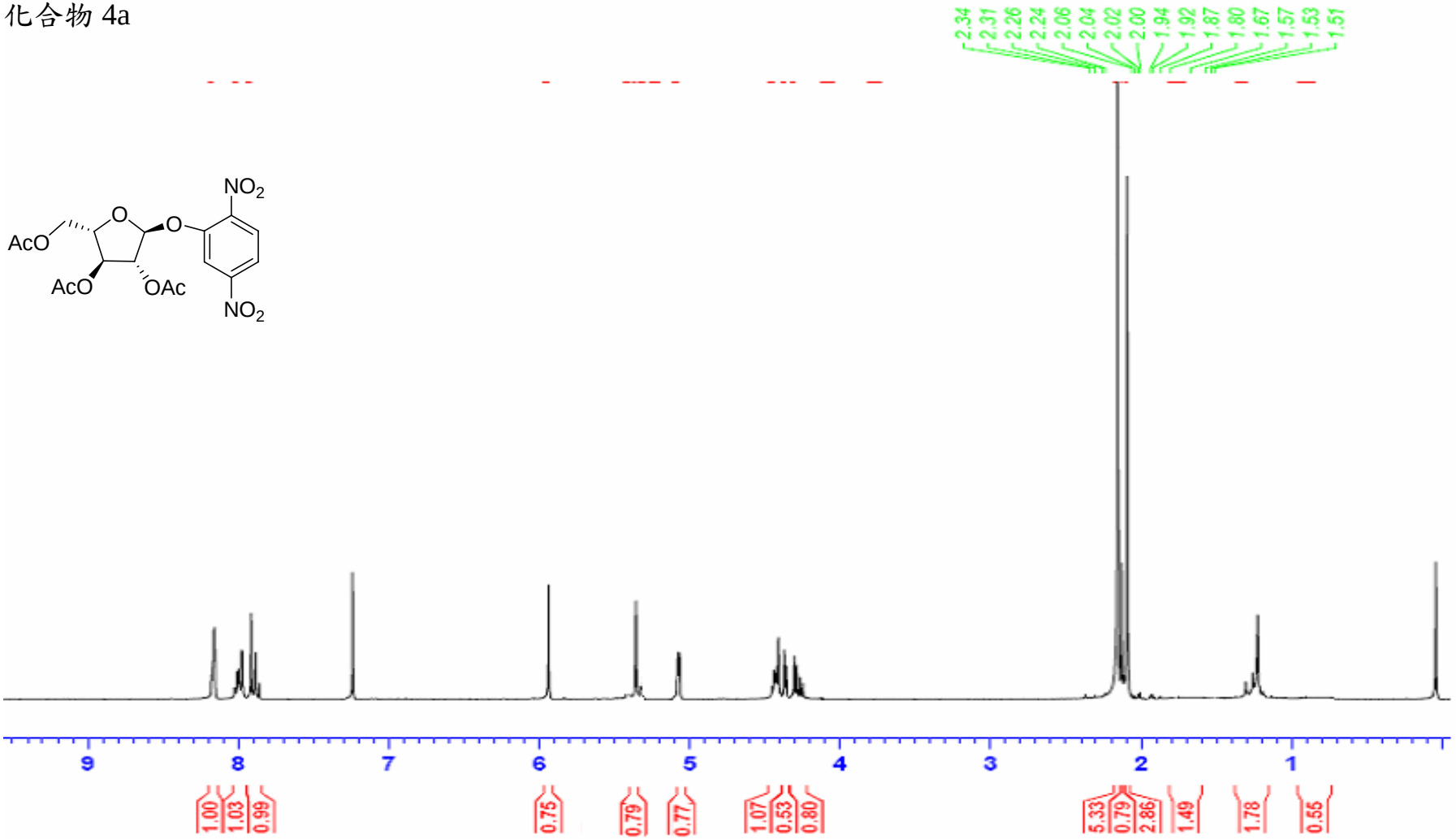
1.00
1.01
1.18
1.94
3.29
10.75

化合物 4a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2.02
2.00
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1.92
1.87
1.80
1.67
1.57
1.53
1.51
NO2
O
O
AcO
AcO
OAc
NO2
9
8
7
6
5
4
3
2
1
1.00
1.03
0.99
0.75
0.79
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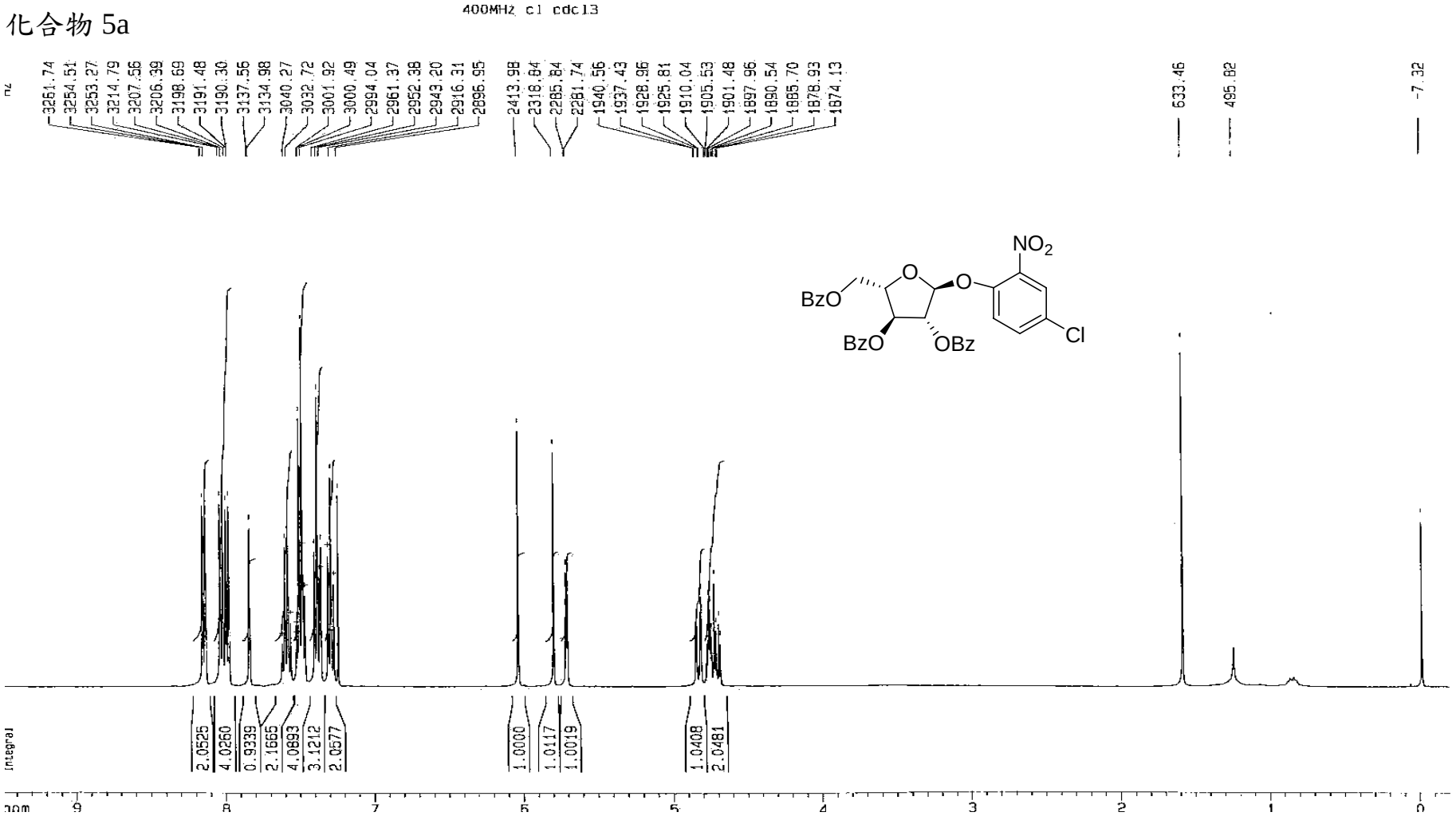
0.53
0.80
5.33
0.79
2.86
1.49
1.78
0.55

化合物 5a


400MHz cl cdcl3
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3207.56
3206.39
3198.69
3191.48
3190.30
3137.56
3134.98
3040.27
3032.72
3001.92
3000.49
2994.04
2961.37
2952.38
2943.20
2916.31
2896.95
2413.98
2316.84
2285.84
2281.74
1940.56
1937.43
1928.96
1925.81
1910.04
1905.53
1901.48
1897.96
1890.54
1885.70
1878.93
1874.13
633.46
495.82
7.32
NO2
O
O
BzO
BzO
OBz
Cl
Integral
2.0525
4.0260
0.9339
2.1665
4.0893
3.1212
2.0577
1.0000
1.0117
1.0019
1.0408
2.0481
ppm
9
8
7
6
5
4
3
2
1
0