A novel bis(pinacolato)diboron-mediated N–O bond deoxygenative route to C6 benzotriazolyl purine nucleoside derivatives†

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O^6-(7-Azabenzotriazol-1-yl)-2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)inosine (9).

In a clean, dry, screw-cap reaction vial a mixture of 2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)inosine (200 mg, 0.327 mmol), (7-azabenzotriazol-1-yloxy) tripyrrolidinophosphonium hexaflurophosphate (PyAOP) (170.65 mg, 0.327 mg), and DBU (49 μL, 49.8 mmol) in anhydrous CH_3CN (2.8 mL) was stirred under a nitrogen atmosphere at room temperature, for 18 h. A second aliquot of PyAOP (170.65 mg, 0.327 mg) and DBU (49 μL, 49.8 mmol) were added and the stirring was continued at room temperature for 7 h. The mixture was diluted with EtOAc and washed with water containing a small amount of NaCl. The aqueous layer was back extracted with EtOAc and the combined organic layer was dried with anhydrous Na_2SO_4, filtered, and evaporated under reduced pressure. The crude material was purified by flash chromatography (SiO_2, elution with 20% and 30% EtOAc in hexanes) to give 124.3 mg (52% yield) of compound **9** as a white, fluffy solid. R_f (3:1 EtOAc in acetone) = 0.93. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.70 (d, J = 4.4 Hz, 1H, Ar-H), 8.59 (s, 1H, Ar-H), 8.48 (d, J = 8.3 Hz, 1H, Ar-H), 8.37 (s, 1H, Ar-H), 7.45 (dd, J = 4.4, 8.3 Hz, 1H, Ar-H), 6.13 (d, J = 3.9 Hz, 1H, H-1'), 4.57 (t, J = 3.9 Hz, 1H, H-2'), 4.35 (t, J = 4.4 Hz, 1H, H-3'), 4.18–4.16 (m, 1H, H-4'), 4.05 (dd, J = 3.1, 11.4 Hz, 1H, H-5'), 3.81 (dd, J = 1.5, 11.2 Hz, 1H, H-5'), 0.97, 0.93, and 0.83 (3s, 27H, *t*-Bu), 0.16, 0.15, 0.11, 0.10, 0.00, and –0.12 (6s, 18H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.1, 154.1, 151.9, 151.4, 144.0, 141.1, 135.3, 129.7, 121.0, 120.1, 89.2, 85.3, 76.6, 71.4, 62.2, 31.1, 26.3, 26.0, 25.9, 18.8, 18.3, 18.1, –4.1, –4.5, –4.56, –4.6, –5.1, –5.2. HRMS (ESI/TOF) calcd for $C_{33}H_{57}N_8O_5Si_3$ $[M + H]^+$ 729.3760, found 729.3773.

O^6-(7-Azabenzotriazol-1-yl)-3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyinosine (10).

As described for the synthesis of compound **9**, this reaction was carried out by the reaction of 3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyinosine (157.3 mg, 0.327 mmol) with PyAOP (341.3 mg, 0.655 mmol) and DBU (97.9 μL, 0.655 mmol) in anhydrous CH_3CN (2.8 mL), at room temperature over 25 h. Workup as described for compound **9** and purification by flash chromatography (SiO_2, elution with 30% EtOAc in hexanes) gave 130.4 mg (66% yield) of compound **10** as a white, fluffy solid. R_f (3:1 EtOAc in acetone) = 0.90. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.69 (d, J = 4.4 Hz, 1H, Ar-H), 8.51 (s, 1H, Ar-H), 8.48 (d, J = 8.3 Hz, 1H, Ar-H), 8.37 (s, 1H, Ar-H), 7.46 (dd, J = 4.4, 8.2 Hz, 1H, Ar-H), 6.53 (t, J = 6.4 Hz, 1H, H-1'), 4.63–4.60 (m, 1H, H-3'), 4.05–4.03 (m, 1H, H-4'), 3.90 (dd, J = 3.6, 11.5 Hz, 1H, H-5'), 3.79 (dd, J = 3.0, 11.2 Hz, 1H, H-5'), 2.61 (app quint, $J_{app} \sim$ 6.2 Hz, 1H, H-2'), 2.49 (ddd, J = 4.5, 5.9, 12.4 Hz, 1H, H-2'), 0.91 and 0.90 (2s, 18H, *t*-Bu), 0.10 (1s, 12H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.9, 153.6, 151.8, 151.2, 143.5, 140.9, 135.1, 129.6, 120.8, 119.9, 88.1, 85.1, 71.5, 62.6, 41.7, 26.0, 25.7, 18.4, 18.0, –4.6, –4.8, –5.4, –5.5. HRMS (ESI/TOF) calcd for $C_{27}H_{43}N_8O_4Si_2$ $[M + H]^+$ 599.2946, found 599.2947.

O^6-(6-Chlorobenzotriazol-1-yl)-2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)inosine (11).

As described for the synthesis of compound **9**, this reaction was carried out by the reaction of 2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)inosine (508.3 mg, 0.832 mmol) with (6-chloro-benzotriazol-1*H*-yloxy)trispyrrolidinophosphonium hexafluorophosphate (PyClocK) (923.3 mg, 1.664 mmol) and DBU (248 μL, 1.664 mmol) in anhydrous CH_3CN (7 mL), at room temperature over 23 h. Workup as described for compound **9** and purification by flash chromatography (SiO_2, elution with 10% EtOAc in hexanes) gave 349 mg (55% yield) of compound **11** as a white, fluffy solid. R_f (3:1 EtOAc in acetone) = 0.95. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 (s, 1H, Ar-H), 8.41 (s, 1H, Ar-H), 8.06 (d, J = 8.7 Hz, 1H, Ar-H), 7.49 (s,

1H, Ar-H), 7.42 (d, *J* = 9.3 Hz, 1H, Ar-H), 6.16 (d, *J* = 4.4 Hz, 1H, H-1'), 4.58 (t, *J* = 4.4 Hz, 1H, H-2'), 4.34 (t, *J* = 4.1 Hz, 1H, H-3'), 4.19–4.17 (m, 1H, H-4'), 4.05 (dd, *J* = 3.2, 11.5 Hz, 1H, H-5'), 3.82 (dd, *J* = 2.0, 11.7 Hz, 1H, H-5'), 0.97, 0.93, and 0.82 (3s, 27H, *t*-Bu), 0.17, 0.16, 0.11, 0.10, 0.00, and –0.16 (6s, 18H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.7, 153.9, 151.3, 144.0, 142.0, 135.3, 129.5, 126.1, 121.5, 109.9, 108.5, 88.8, 85.3, 76.4, 71.4, 62.1, 26.0, 25.8, 25.6, 18.5, 18.0, 17.8, –4.4, –4.7, –4.8, –5.0, –5.4, –5.5. HRMS (ESI/TOF) calcd for $C_{34}H_{56}ClN_7O_5Si_3Na$ $[M + Na]^+$ 784.3231, found 784.3220.

O^6-(6-Chlorobenzotriazol-1-yl)-3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyinosine (12).

As described for the synthesis of compound **9**, this reaction was carried out by the reaction of 3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyinosine (400 mg, 0.832 mmol) with PyClocK (923.3 mg, 1.66 mmol) and DBU (248 μL, 1.66 mmol) in CH_3CN (7 mL), at room temperature over 23 h. Workup as described for compound **9** and purification by flash chromatography (SiO_2, elution with 20% EtOAc in hexanes) gave 392.4 mg (74% yield) of compound **12** as a white, fluffy solid. R_f (3:1 EtOAc in acetone) = 0.95. ^1H NMR (500 MHz, $CDCl_3$): δ 8.54 (s, 1H, Ar-H), 8.41 (s, 1H, Ar-H), 8.05 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.48 (d, *J* = 1.0 Hz, 1H, Ar-H), 7.41 (dd, *J* = 1.4, 9.2 Hz, 1H, Ar-H), 6.54 (t, *J* = 6.1 Hz, 1H, H-1'), 4.65–4.63 (m, 1H, H-3'), 4.04–4.06 (m, 1H, H-4'), 3.91 (dd, *J* = 3.7, 11.5 Hz, 1H, H-5'), 3.80 (dd, *J* = 2.7, 11.4 Hz, 1H, H-5'), 2.64 (app quint, $J_{app} \sim$ 6.2 Hz, 1H, H-2'), 2.51 (ddd, *J* = 4.6, 5.9, 13.1 Hz, 1H, H-2'), 0.92 and 0.91 (2s, 18H, *t*-Bu), 0.10 (1s, 12H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.8, 153.7, 151.3, 143.7, 142.0, 135.4, 129.5, 126.2, 121.6, 119.9, 108.6, 88.2, 85.1, 71.6, 62.6, 41.7, 26.0, 25.7, 18.4, 18.0, –4.6, –4.8, –5.4, –5.5. HRMS (ESI/TOF) calcd for $C_{28}H_{42}ClN_7O_4Si_2Na$ $[M + Na]^+$ 654.2423, found 654.2418.

O^6-(6-Chlorobenzotriazol-1-yl)-2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)guanosine (13).

As described in the synthesis of compound **9**, this reaction was carried out by the reaction of 2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)guanosine (300 mg, 0.479 mmol) with PyClocK (531.8 mg, 0.958 mmol) and DBU (143 μL, 0.958 mmol) in CH_3CN (4 mL), at room temperature over 20 h. Workup as described for compound **9** and purification by flash chromatography (SiO_2, elution with 10% EtOAc in hexanes) gave 162.0 mg (43% yield) of compound **13** as a pale yellow, fluffy solid. R_f (10% EtOAc in hexanes) = 0.17. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (s, 1H, Ar-H), 8.02 (d, J = 8.2 Hz, 1H, Ar-H), 7.49 (s, 1H, Ar-H), 7.39 (dd, J = 1.7, 9.3 Hz, 1H, Ar-H), 5.94 (d, J = 4.4 Hz, 1H, H-1'), 4.96 (s, 2H, NH_2), 4.44 (t, J = 4.4 Hz, 1H, H-2'), 4.28 (t, J = 3.9 Hz, 1H, H-3'), 4.13–4.11 (m, 1H, H-4'), 3.98 (dd, J = 2.7, 11.6 Hz, 1H, H-5'), 3.79 (dd, J = 2.2, 11.5 Hz, 1H, H-5'), 0.96, 0.90, and 0.81 (3s, 27H, *t*-Bu), 0.15, 0.14, 0.09, 0.05, –0.02, and –0.12 (6s, 18H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.2, 158.5, 156.0, 142.0, 140.5, 135.1, 129.5, 126.0, 121.4, 113.2, 108.7, 88.0, 85.3, 76.6, 71.7, 62.4, 26.1, 25.8, 25.7, 18.6, 18.1, 17.9, –4.3, –4.6, –4.8, –4.9, –5.3, –5.4. HRMS (ESI/TOF) calcd for $C_{34}H_{58}ClN_8O_5Si_3$ [M + H]$^+$ 777.3521, found 777.3524.

O^6-(6-Chlorobenzotriazol-1-yl)-3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyguanosine (14).

As described in the synthesis of compound **9**, this reaction was carried out by the reaction of 3',5'-di-*O*-(*t*-butyldimethylsilyl)-2'-deoxyguanosine (300 mg, 0.605 mmol) with PyClocK (671 mg, 1.21 mmol) and DBU (181 μL, 1.21 mmol) in CH_3CN (5 mL), at room temperature over 22 h. Workup as described for compound **9** and purification by flash chromatography (SiO_2, elution with 20% EtOAc in hexanes) gave 211.6 mg (54% yield) of compound **14** as a white, fluffy solid. R_f (20% EtOAc in hexanes) = 0.40. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 (s,

1H, Ar-H), 8.01 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.50 (d, *J* = 1.0 Hz, 1H, Ar-H), 7.39 (dd, *J* = 1.7, 9.5 Hz, 1H, Ar-H), 6.34 (t, *J* = 6.4 Hz, 1H, H-1'), 4.83 (br s, 2H, NH_2), 4.62–4.59 (m, 1H, H-3'), 4.01–3.99 (m, 1H, H-4'), 3.84 (dd, *J* = 3.9, 11.2 Hz, 1H, H-5'), 3.77 (dd, *J* = 2.7, 11.5 Hz, 1H, H-5'), 2.57 (app quint, $J_{app} \sim 6.3$ Hz, 1H, H-2'), 2.40 (ddd, *J* = 4.3, 6.0, 12.9 Hz, 1H, H-2'), 0.92 and 0.91 (2s, 18H, *t*-Bu), 0.10, 0.095, and 0.09 (3s, 12H, $SiCH_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.2, 158.4, 155.8, 142.0, 140.4, 135.1, 129.5, 126.1, 121.4, 113.4, 108.7, 87.9, 84.1, 71.7, 62.7, 41.2, 26.0, 25.7, 18.4, 18.0, –4.6, –4.8, –5.4, –5.5. HRMS (ESI/TOF) calcd for $C_{28}H_{44}ClN_8O_4Si_2$ $[M + H]^+$ 647.2707, found 647.2693.

2-Bromo-6-(2,3-dibromopropoxy)-2',3',5'-tri-*O*-(*t*-butyldimethylsilyl)inosine (17). Compound **17** (26.8 mg, 7% yield) was obtained as a byproduct in the synthesis of **16,** as a white, fluffy solid. R_f (20% EtOAc in hexanes) = 0.59. ^1H NMR (500 MHz, $CDCl_3$): δ 8.27 and 8.25 (2s, 2H, Ar-H), 6.00 (d, *J* = 4.4 Hz, 1H, H-1'), 5.99 (d, *J* = 4.4 Hz, 1H, H-1'), 5.01 (d, *J* = 4.4 Hz, 2H, OCH_2), 4.69 (s, 1H, H-2'), 4.57 (d, *J* = 5.9 Hz, 1H, CH), 4.34 (s, 1H, H-3'), 4.16–4.13 (m, 1H, H-4'), 4.04 (dd, *J* = 4.6, 11.4 Hz, 1H, H-5'), 3.95–3.3 (m, 2H, CH), 3.81 (dd, *J* = 3.0, 11.7 Hz, 1H, H-5'), 0.96, 0.95, 0.84, and 0.83 (4s, 27H, *t*-Bu), 0.154, 0.15, 0.145, 0.142, 0.13, 0.12, 0.002, –0.001, –0.15, –0.16 (10s, 18H, $SiCH_3$). HRMS (ESI/TOF) calcd for $C_{31}H_{57}Br_3N_4O_5Si_3Na$ $[M + Na]^+$ 909.1079, found 909.1093.

Note. Two purinyl-H and two H-1' resonances were observed in ^1H NMR spectrum of **17**, plausibly due to presence of the C2 chloro analogue that can be formed when these reactions are conducted in CH_2Cl_2. Correspondingly, two purinyl-H resonances (at δ = 8.24 and 8.22 ppm) and two H-1' resonances (doublets at δ = 5.98 ppm, *J* = 3.9 Hz, and δ = 5.97

ppm, J = 4.4 Hz) were also observed in desired compound **16** for the same reason. Data for pure **16** are provided in the paper and herein.

1-[(5,6-Dichloro-1*H*-benzotriazol-1-yl)oxy]-*N,N,N'N'*-tetramethylphosphanediamine (36).

R_f (50% EtOAc in hexanes) = 0.38. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.33 (s, 1H, Ar-H), 8.15 (s, 1H, Ar-H), 2.73 and 2.71 (2s, 12H, CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.5, 135.2, 133.9, 129.5, 120.3, 115.0, 36.7, 36.5. ^{31}P NMR (202 MHz, $CDCl_3$): δ 14.63 (relative to 85% aq. H_3PO_4 as external standard). HRMS (ESI/TOF) calcd for $C_{10}H_{14}Cl_2N_5OPNa$ $[M + Na]^+$ 344.0205, found 344.0206.

Reduction of 6-(6-chlorobenzotriazol-1-yl)-9-[2,3,5-tri-*O*-(*t*-butyldimethylsilyl)-β-D-ribofuranosyl]purine (27b).

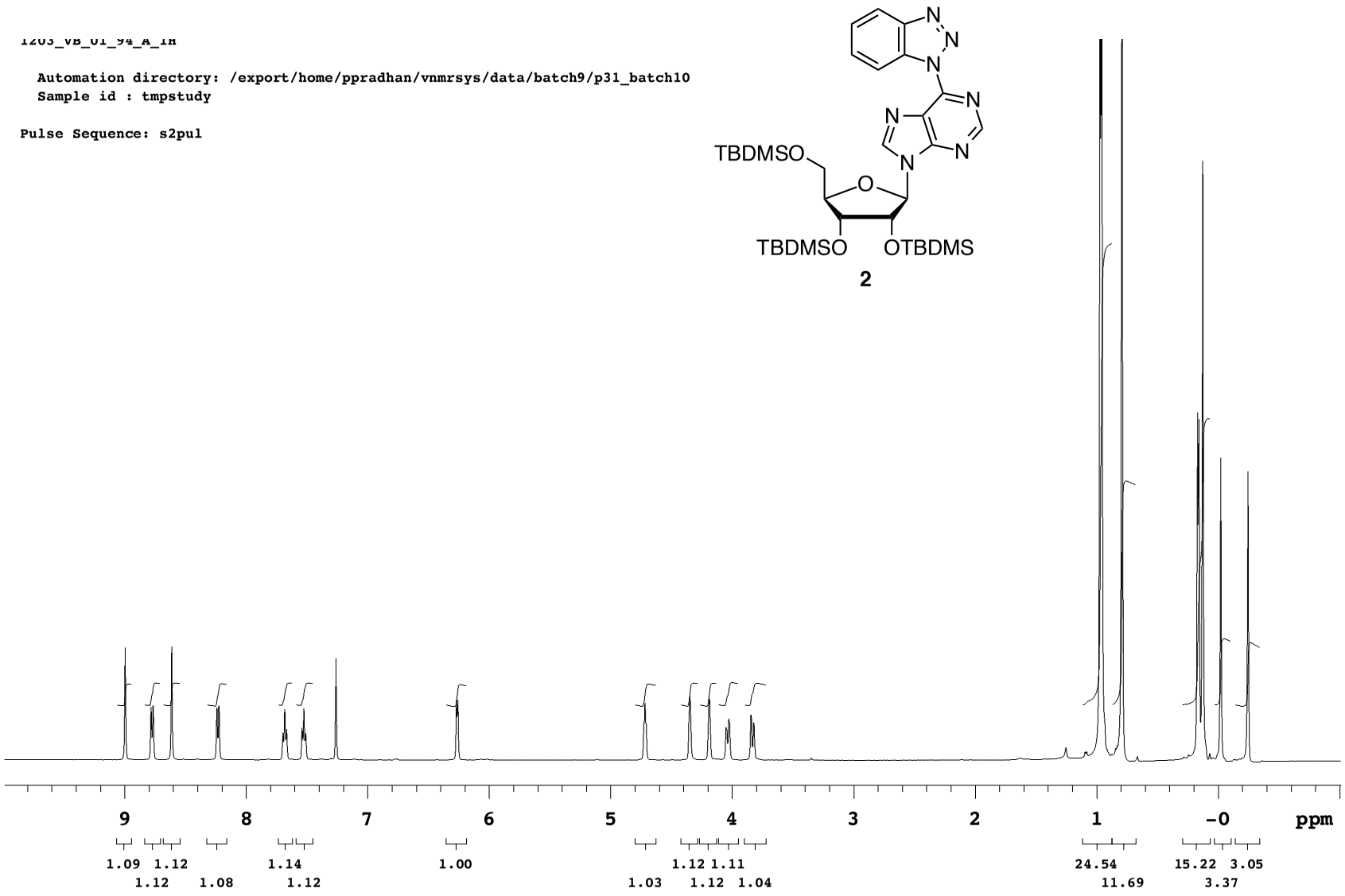
In a clean, dry 5 mL round-bottomed flask, equipped with a stirring bar, a solution of 6-(6-chlorobenzotriazol-1-yl) nucleoside **27b** (20.0 mg, 26.8 μmol) in anhydrous MeOH (2.0 mL) was prepared. To this was added 10% w/w Pd/C (20.0 mg, 100% wt. equivalent) and Et_3N (7.5 μL, 53.6 μmol). The flask was evacuated and filled with hydrogen gas, and the process was repeated five times. Finally, the mixture was vigorously stirred under a balloon filled with hydrogen gas, for 5 h at room temperature. The mixture was filtered through Celite and the filtrate was evaporated to dryness. The crude material was purified by preparative TLC (500 μm, 20 x 20 cm SiO_2 plate eluted with 30% EtOAc in hexanes) to give 10.3 mg (54% yield) of benzotriazolyl compound **1** as an off-white, oily material. R_f (30% EtOAc in hexanes) = 0.71. An uncharacterized purple, oily product (6.6 mg) was also isolated in this reaction. R_f (30% EtOAc in hexanes) = 0.48.

Reduction of 6-(5-chlorobenzotriazol-1-yl)-9-[3,5-di-*O*-(*t*-butyldimethylsilyl)-2-deoxy-β-D-ribofuranosyl]purine (28a).

As described for the reduction of **27b**, this reduction was carried out by the addition of 10% w/w Pd/C (1.0 mg, 10% wt. equivalent) and Et_3N (3.0 μL, 19.4 μmol) to a solution of **28a** (10.0 mg, 16.2 μmol) in anhydrous MeOH (1.0 mL), over 2 h at room temperature, under a balloon filled with hydrogen gas. The mixture was filtered through Celite and the filtrate was evaporated to dryness. The crude material was purified by preparative TLC (500 μm, 20 x 20 cm SiO_2 plate eluted with 30% EtOAc in hexanes) to give 6.2 mg (66% yield) of benzotriazolyl compound **5** as an off-white solid. R_f (30% EtOAc in hexanes) = 0.33.

Reduction of 6-(6-chlorobenzotriazol-1-yl)-9-[3,5-di-*O*-(*t*-butyldimethylsilyl)-2-deoxy-β-D-ribofuranosyl]purine (28b).

As described in the reduction of **27b**, this reduction was carried out by the addition of 10% w/w Pd/C (20.0 mg, 100% wt. equivalent) and Et_3N (9.0 μL, 64.9 μmol) to a solution of **28b** (20.0 mg, 32.4 μmol) in anhydrous MeOH (2.0 mL), over 5 h at room temperature, under balloon filled with hydrogen gas. The mixture was filtered through Celite and the filtrate was evaporated to dryness. The crude material was purified by preparative TLC (500 μm, 20 x 20 cm SiO_2 plate eluted with 30% EtOAc in hexanes) to give 9.6 mg (51% yield) of benzotriazolyl compound **5** as an off-white, fluffy solid. R_f (30% EtOAc in hexanes) = 0.45. An uncharacterized purple, oily product (3.2 mg) was also isolated in this reaction. R_f (30% EtOAc in hexanes) = 0.20.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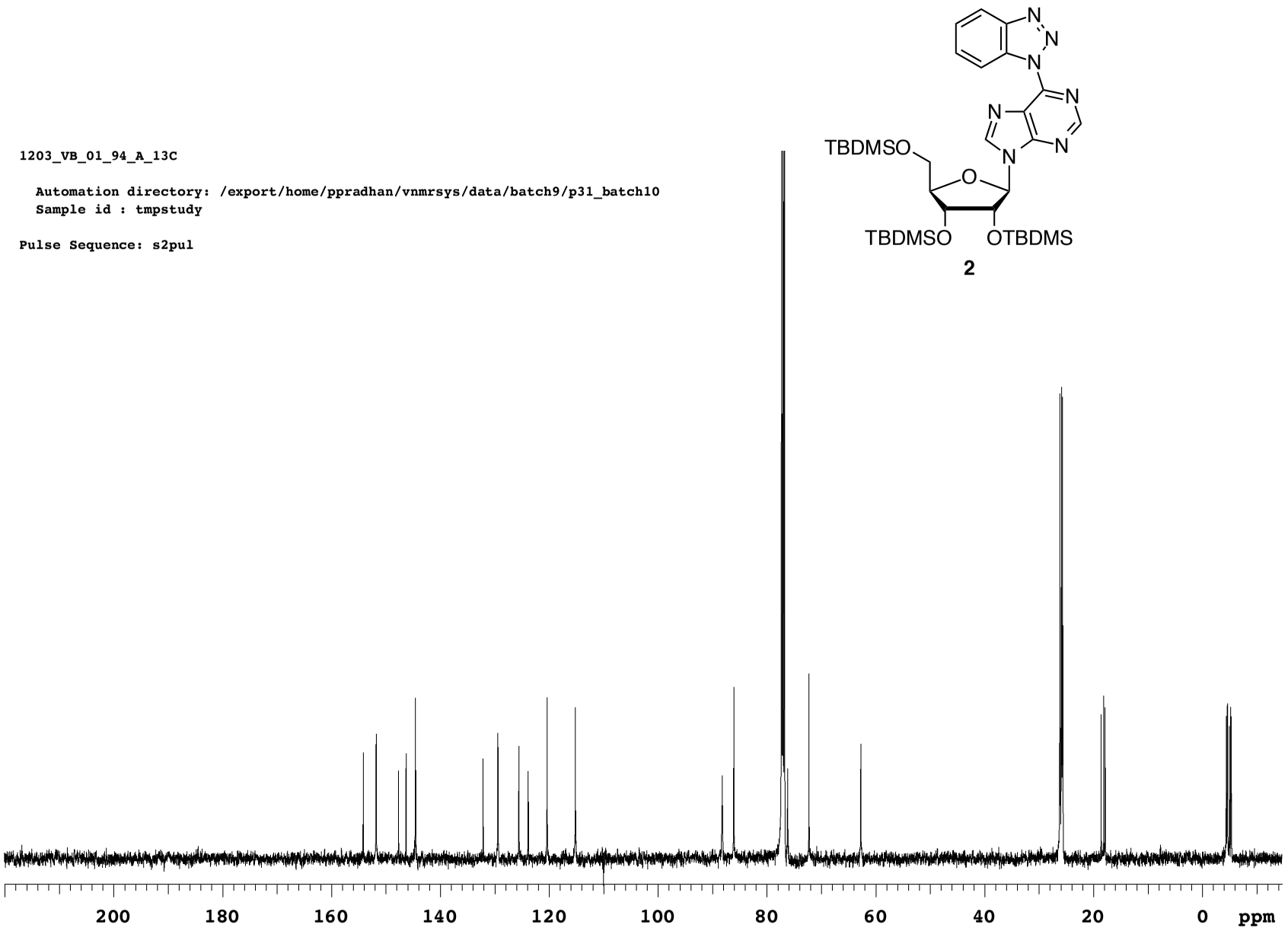
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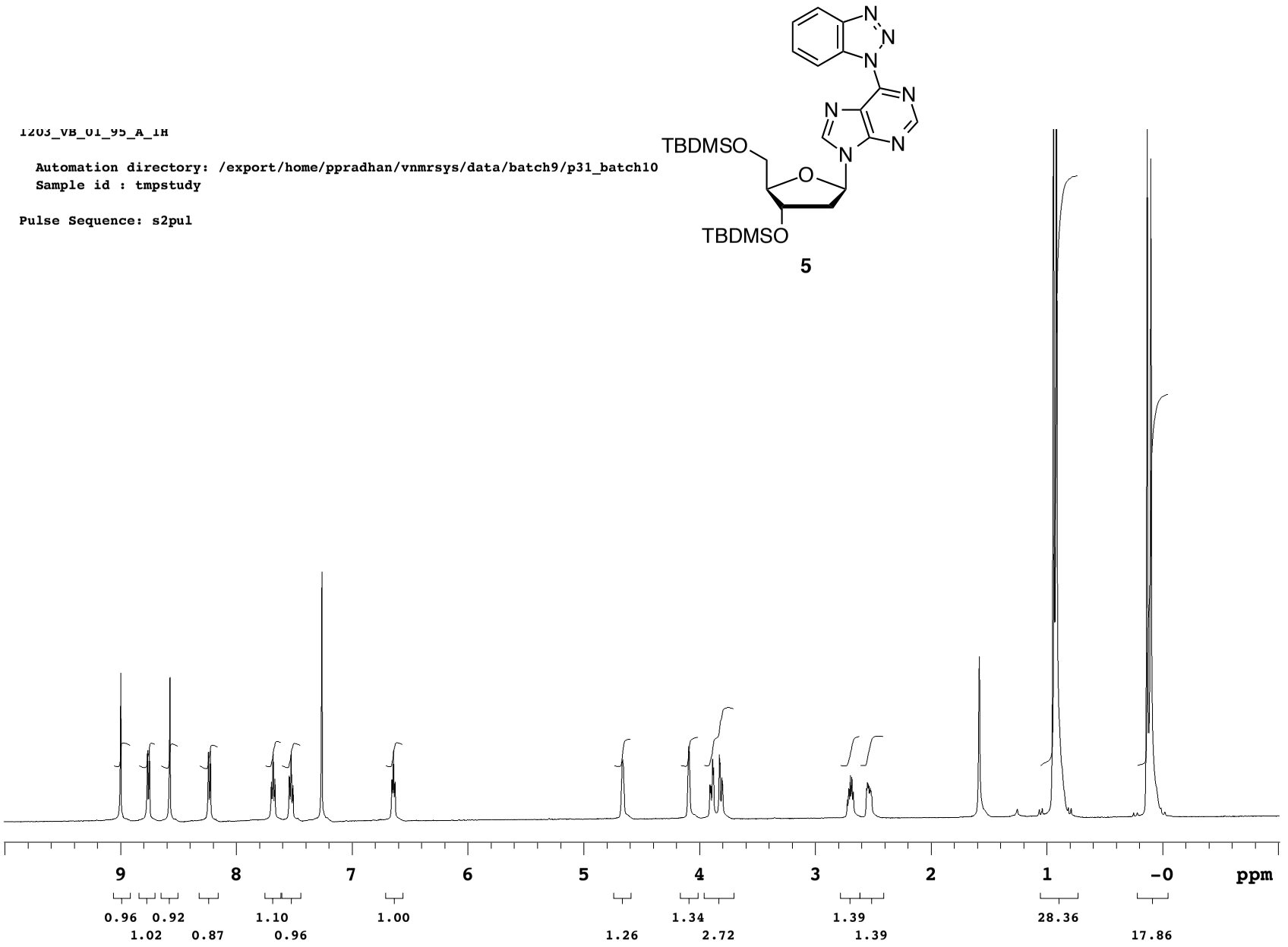
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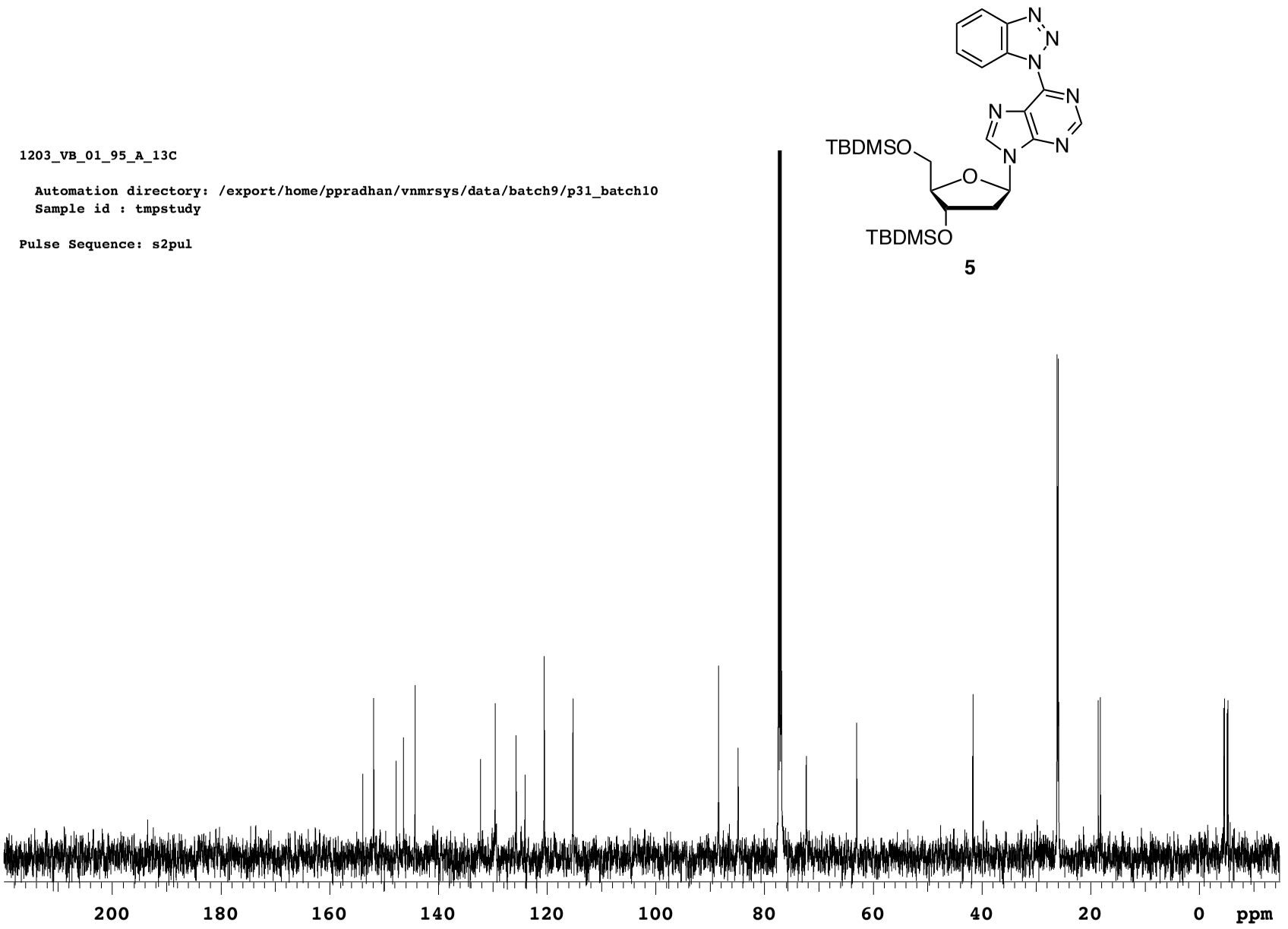
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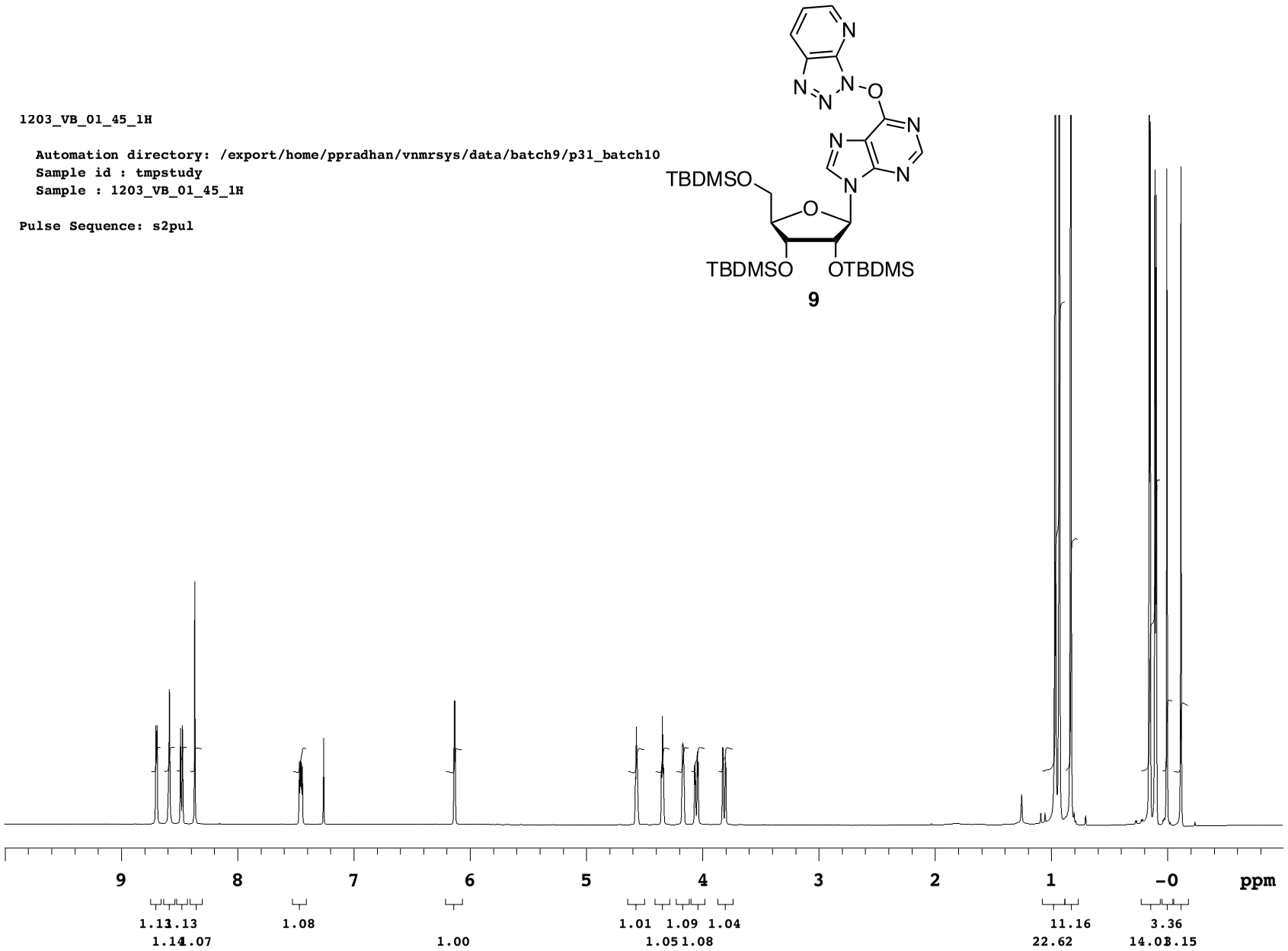
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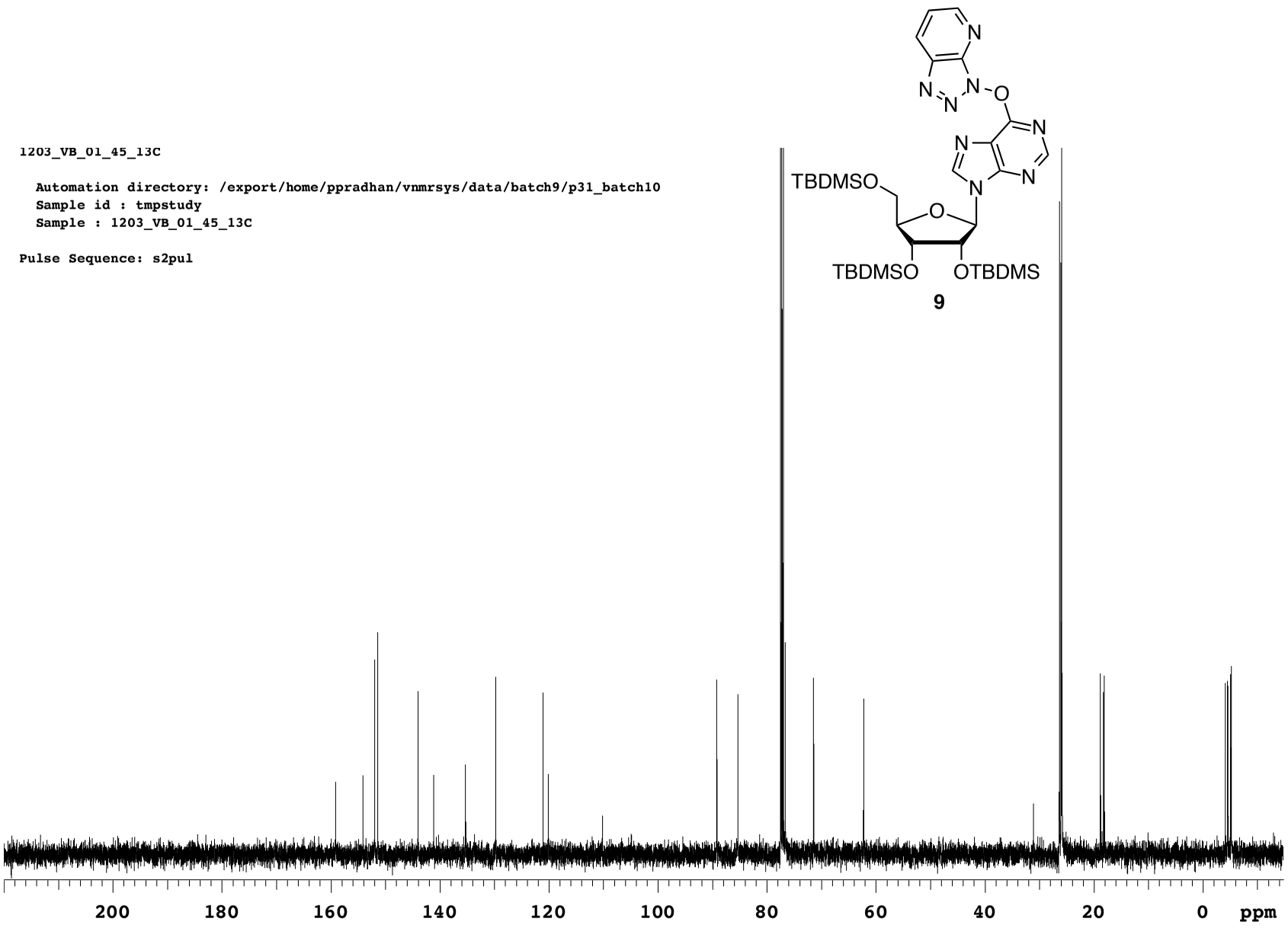
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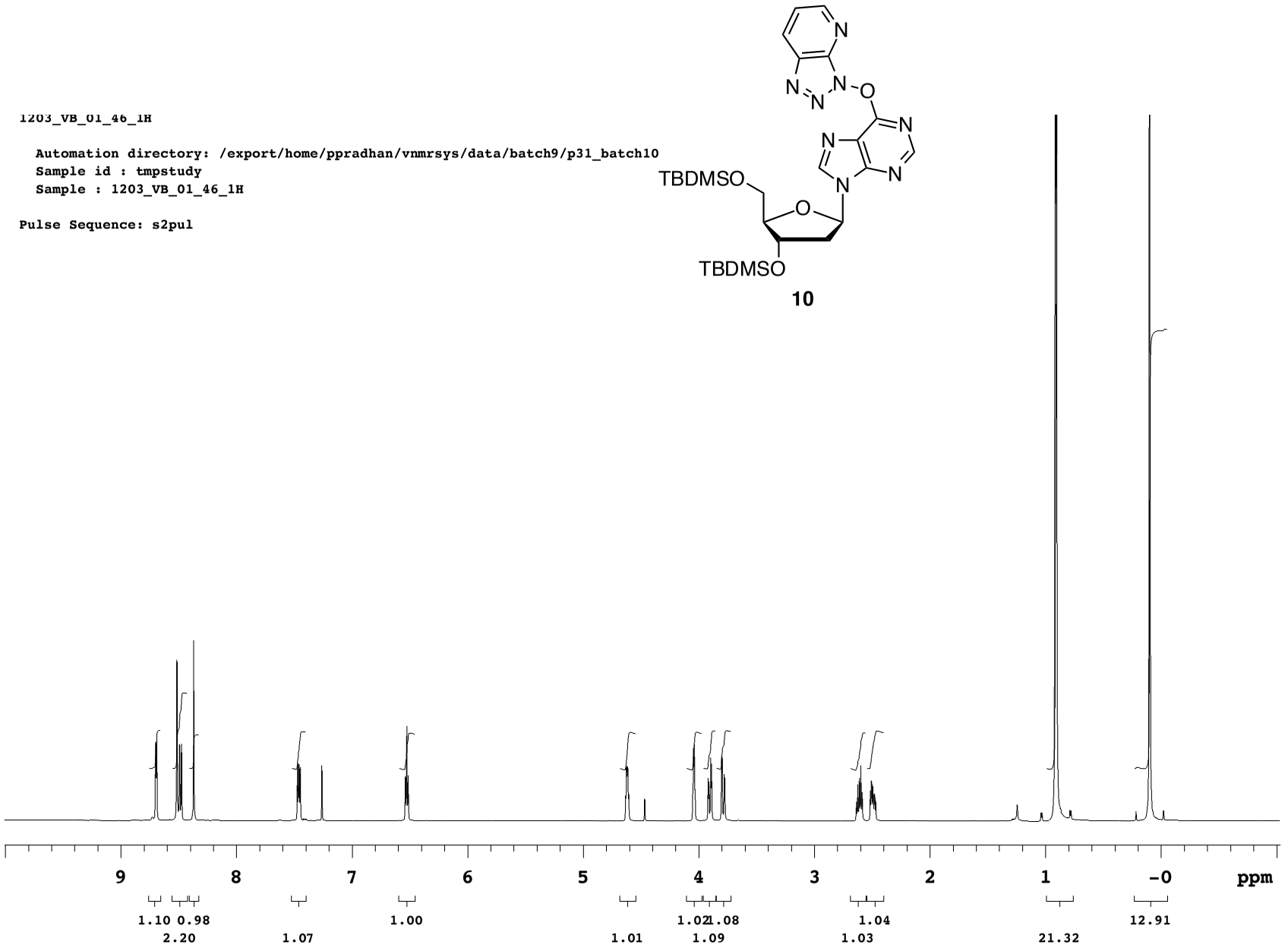
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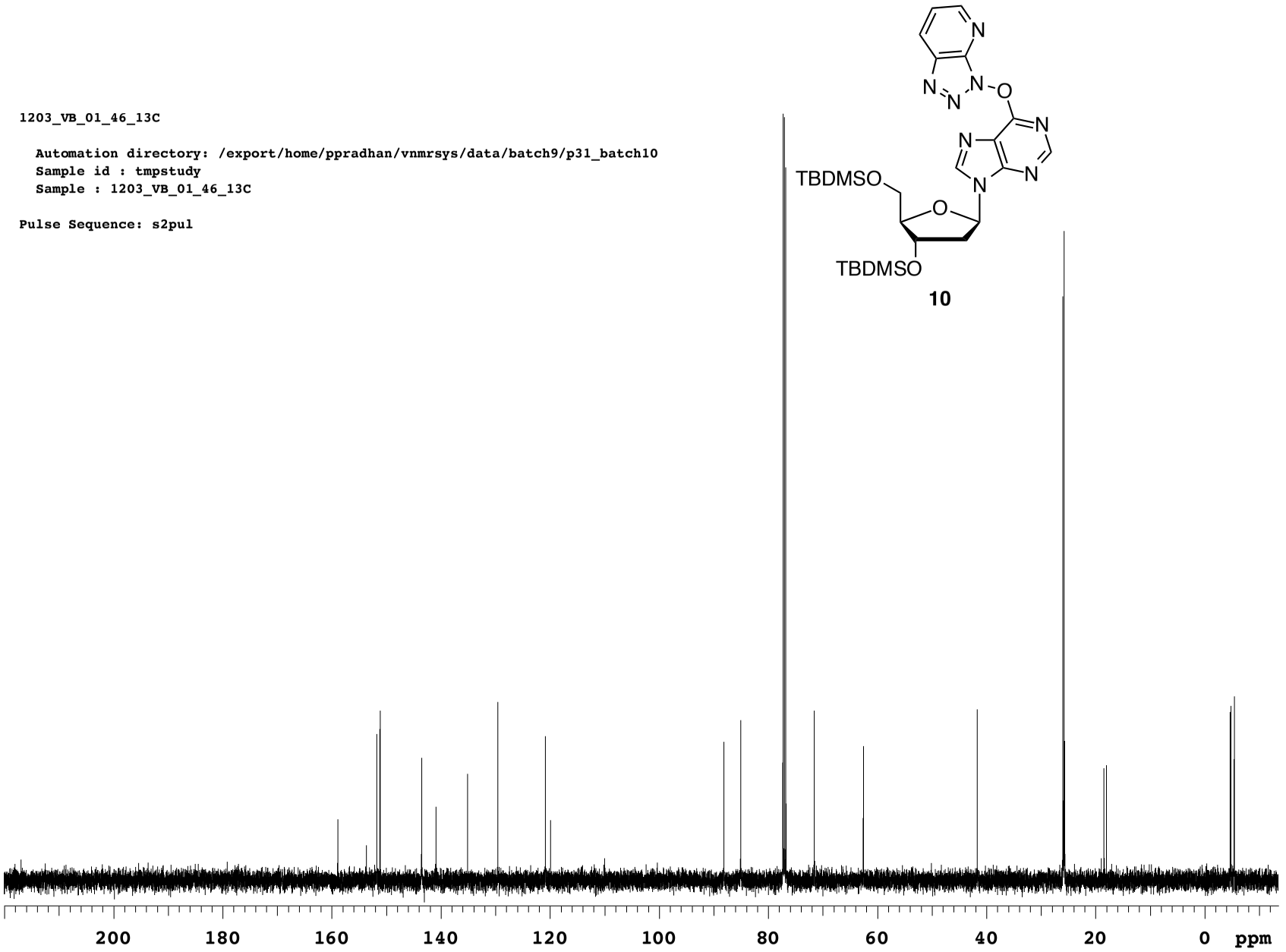
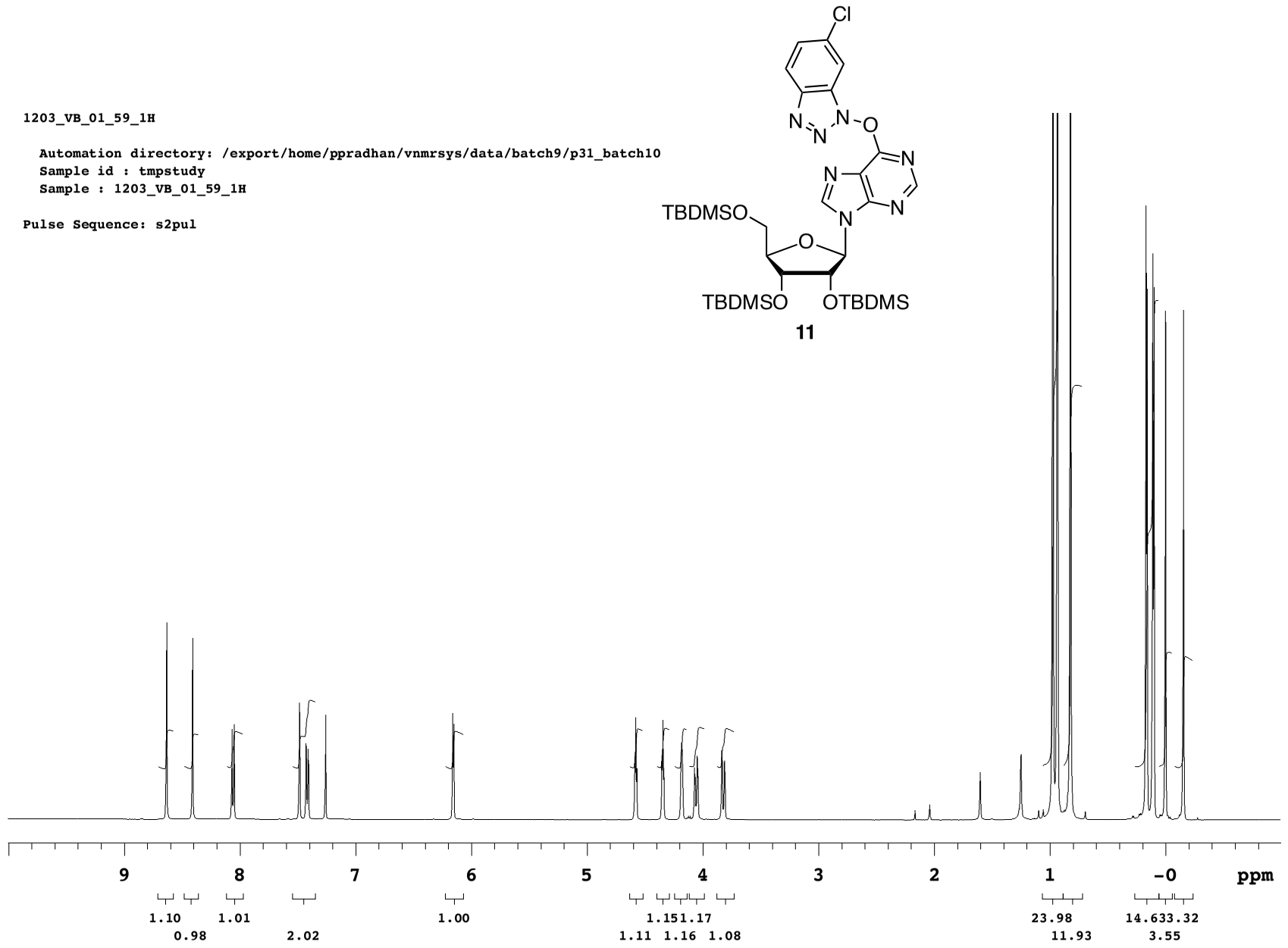
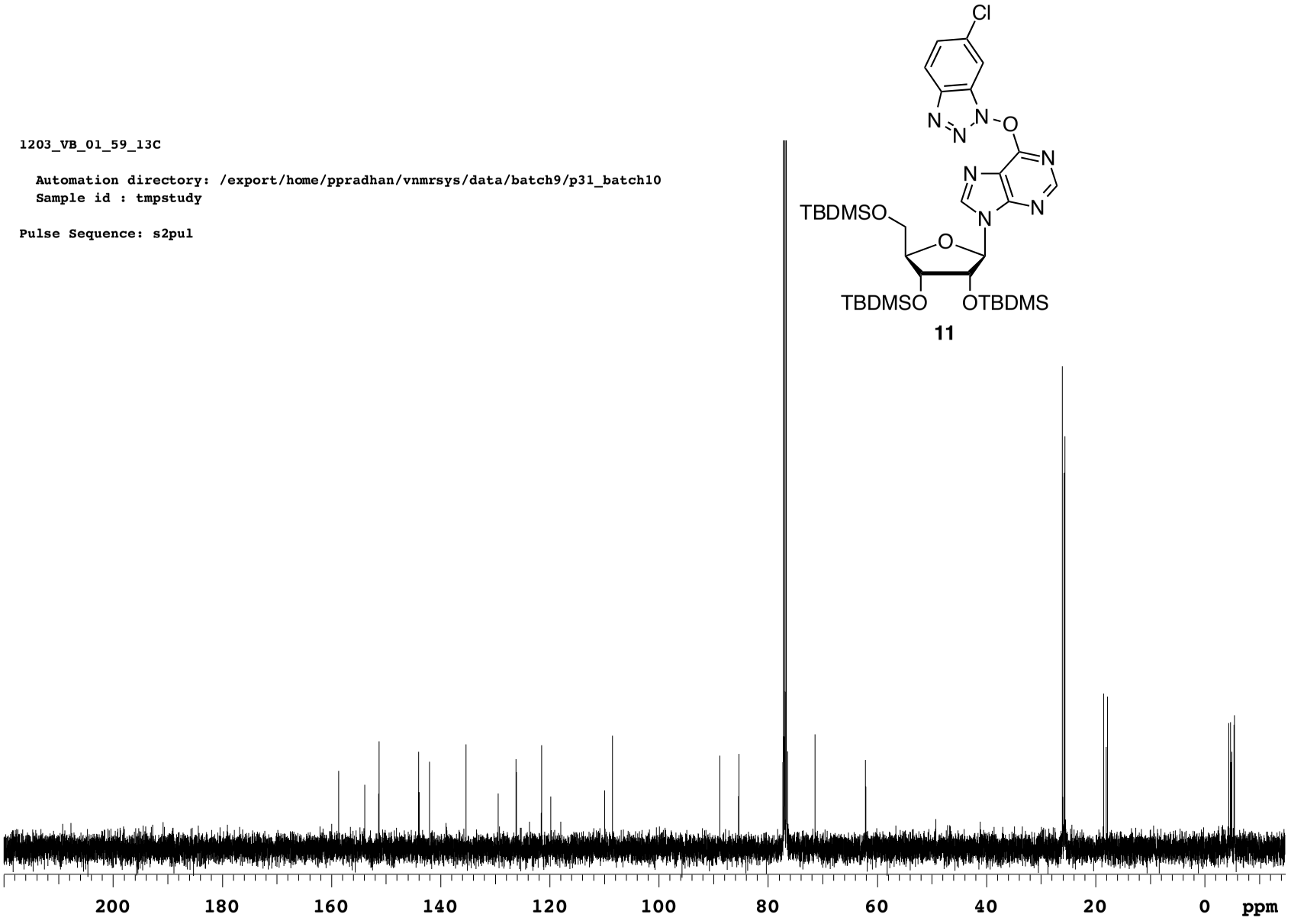
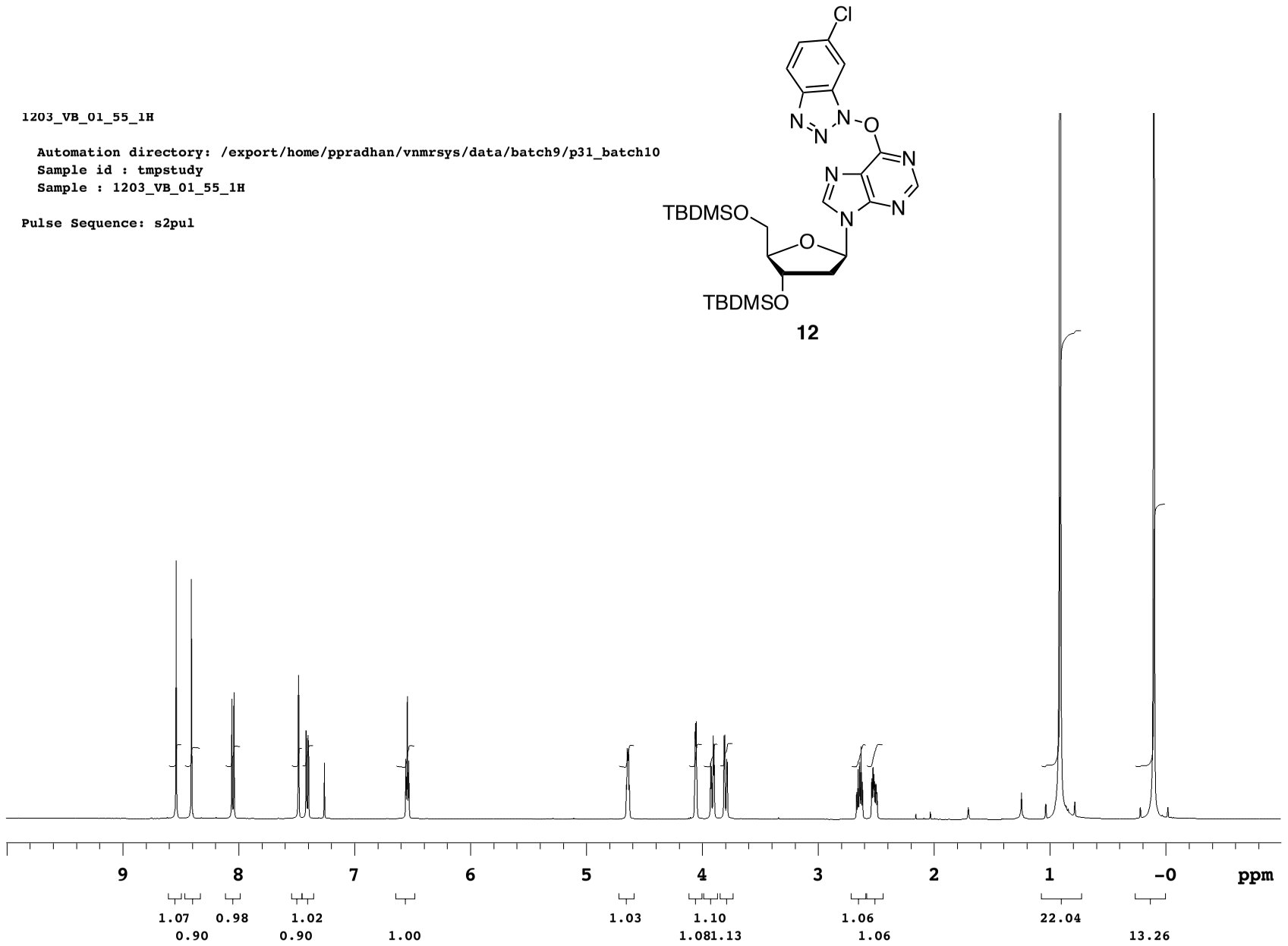
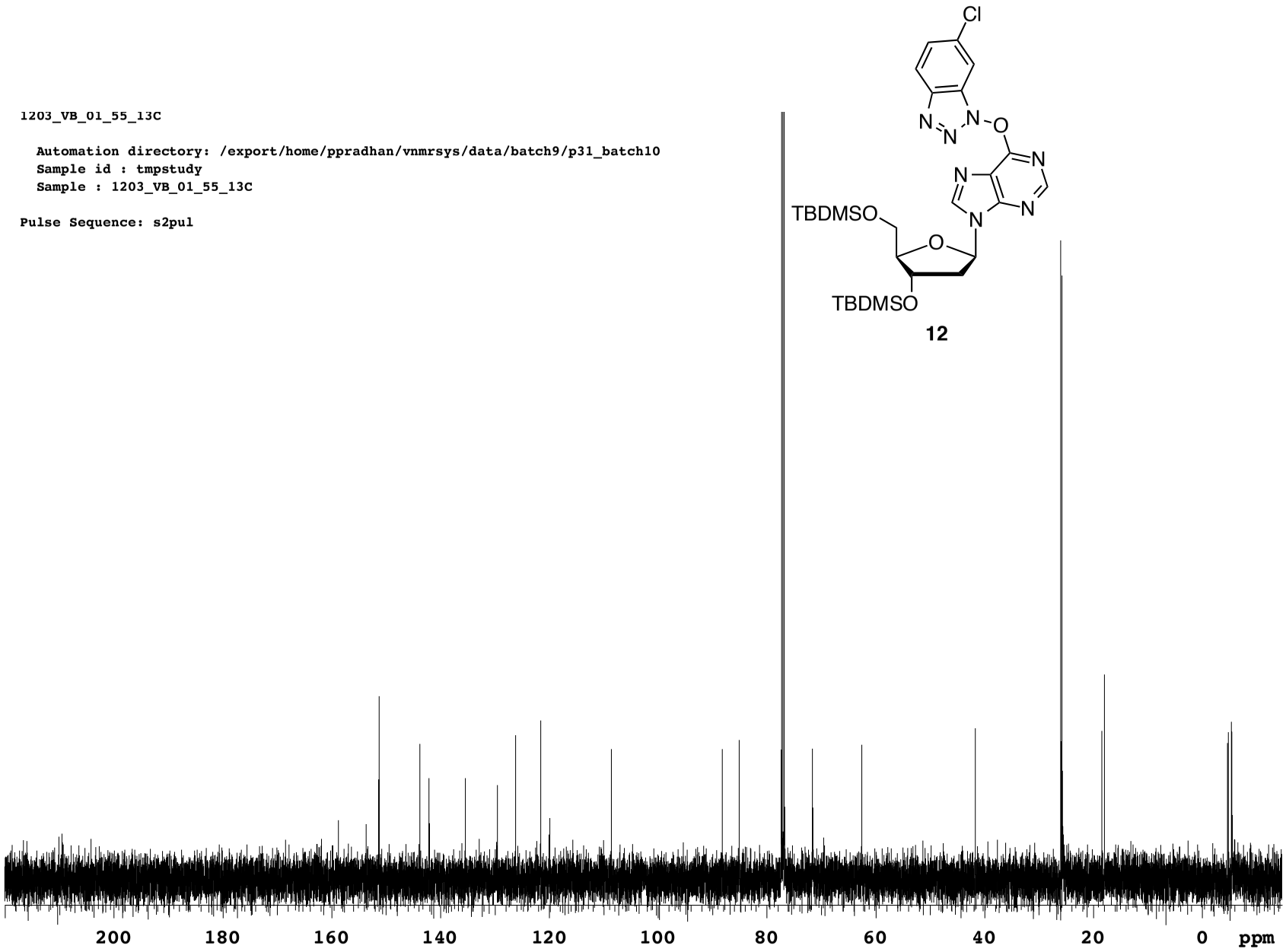
Sample : 1203_VB_01_46_1H
Pulse Sequence: s2pul
TBDMSO
TBDMSO
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.10 0.98
2.20
1.07
1.00
1.01
1.02 1.08
1.09
1.04
1.03
21.32
12.91


1203_VB_01_46_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_46_13C
Pulse Sequence: s2pul
TBDMSO
TBDMSO
10
200
180
160
140
120
100
80
60
40
20
0
ppm

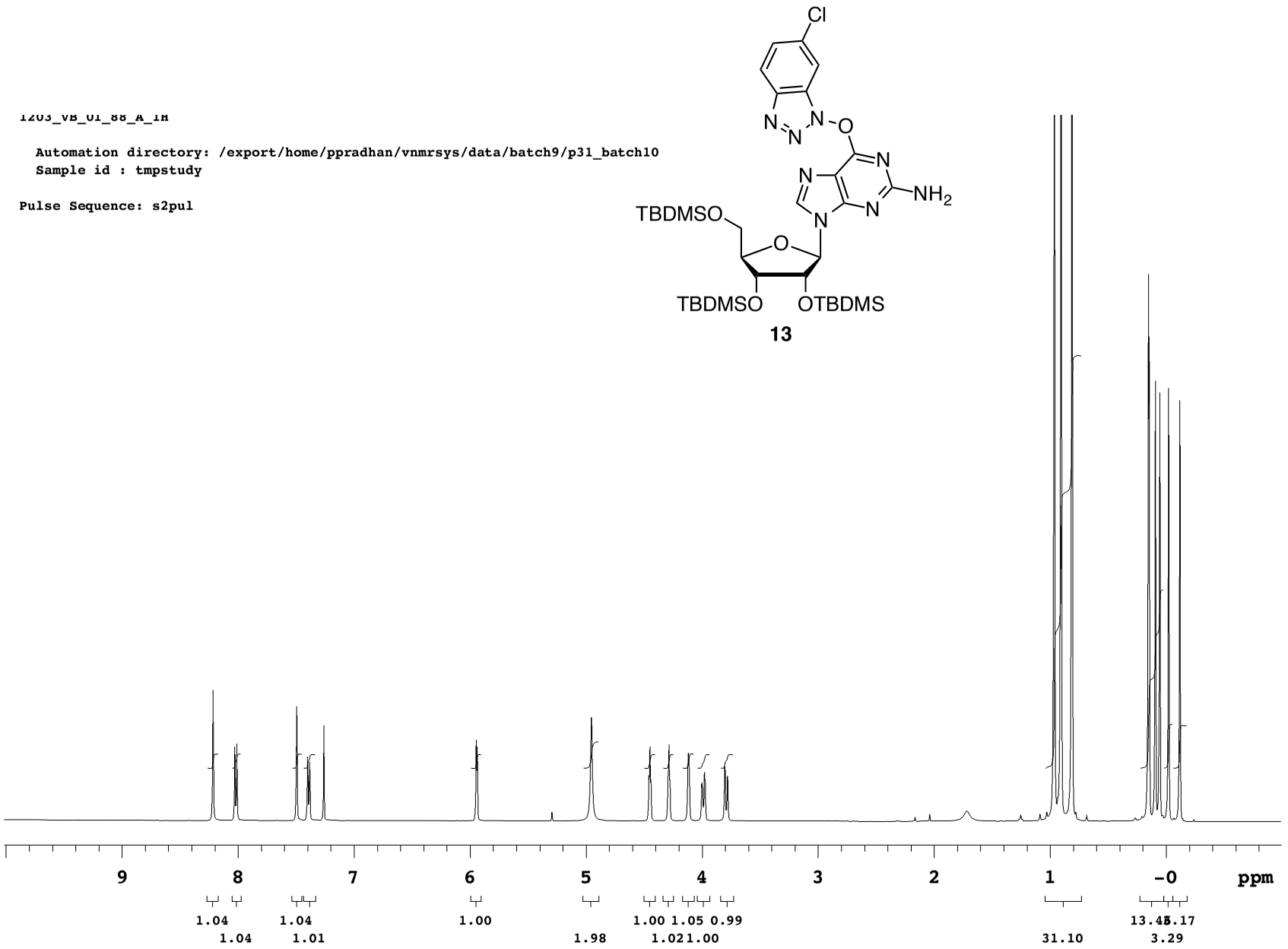

1203_VB_01_59_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_59_1H
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
11
9
8
7
6
5
4
3
2
1
-0
ppm
1.10
0.98
1.01
2.02
1.00
1.11
1.15
1.16
1.17
1.08
23.98
11.93
14.63
3.55
3.32

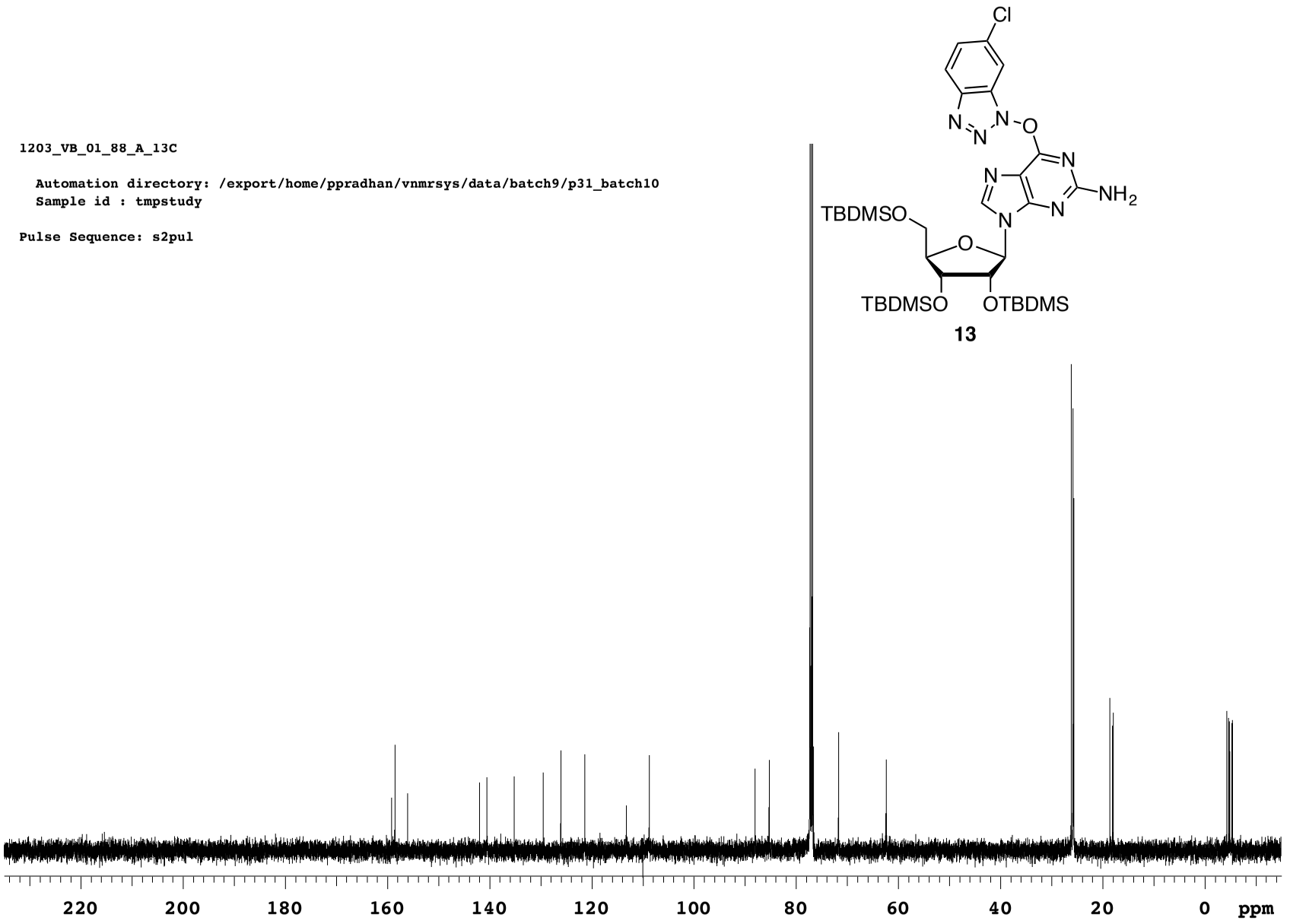

1203_VB_01_59_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
11
200
180
160
140
120
100
80
60
40
20
0
ppm

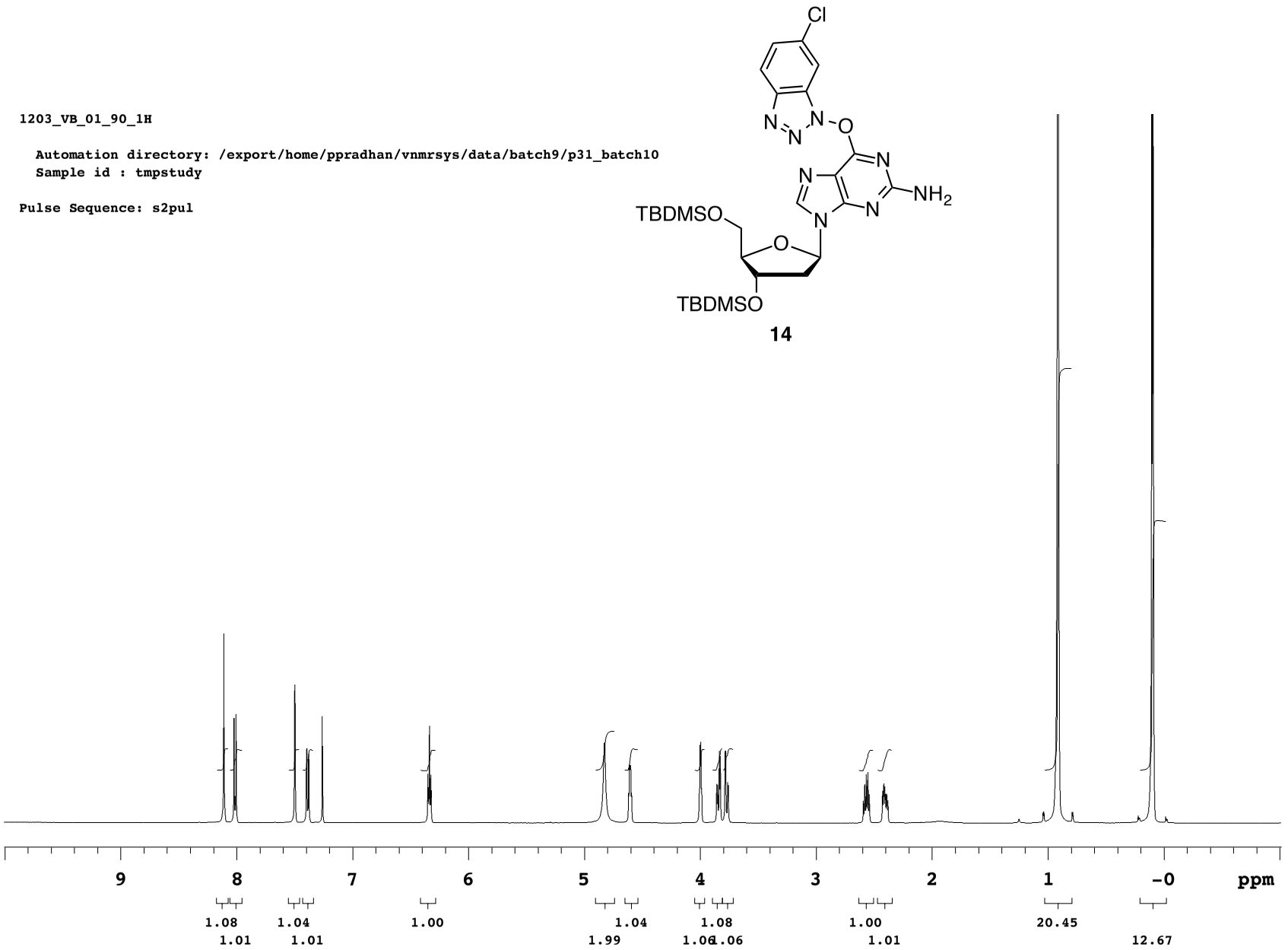

1203_VB_01_55_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_55_1H
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
TBDMSO
O
TBDMSO
12
9
8
7
6
5
4
3
2
1
-0
ppm
1.07
0.90
0.98
1.02
0.90
1.00
1.03
1.10
1.08
1.13
1.06
1.06
22.04
13.26

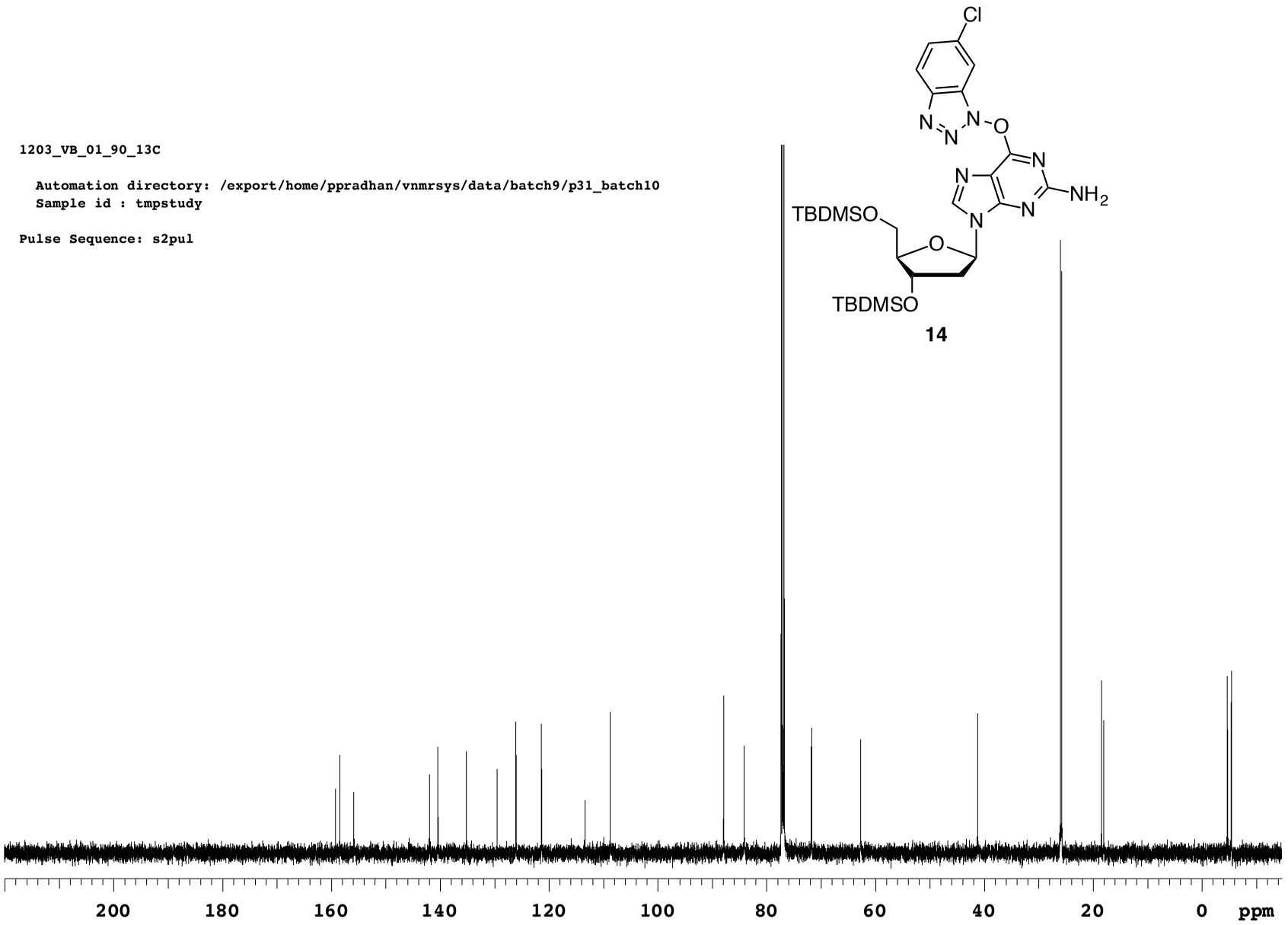

1203_VB_01_55_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_55_13C
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
TBDMSO
O
TBDMSO
200
180
160
140
120
100
80
60
40
20
0
ppm

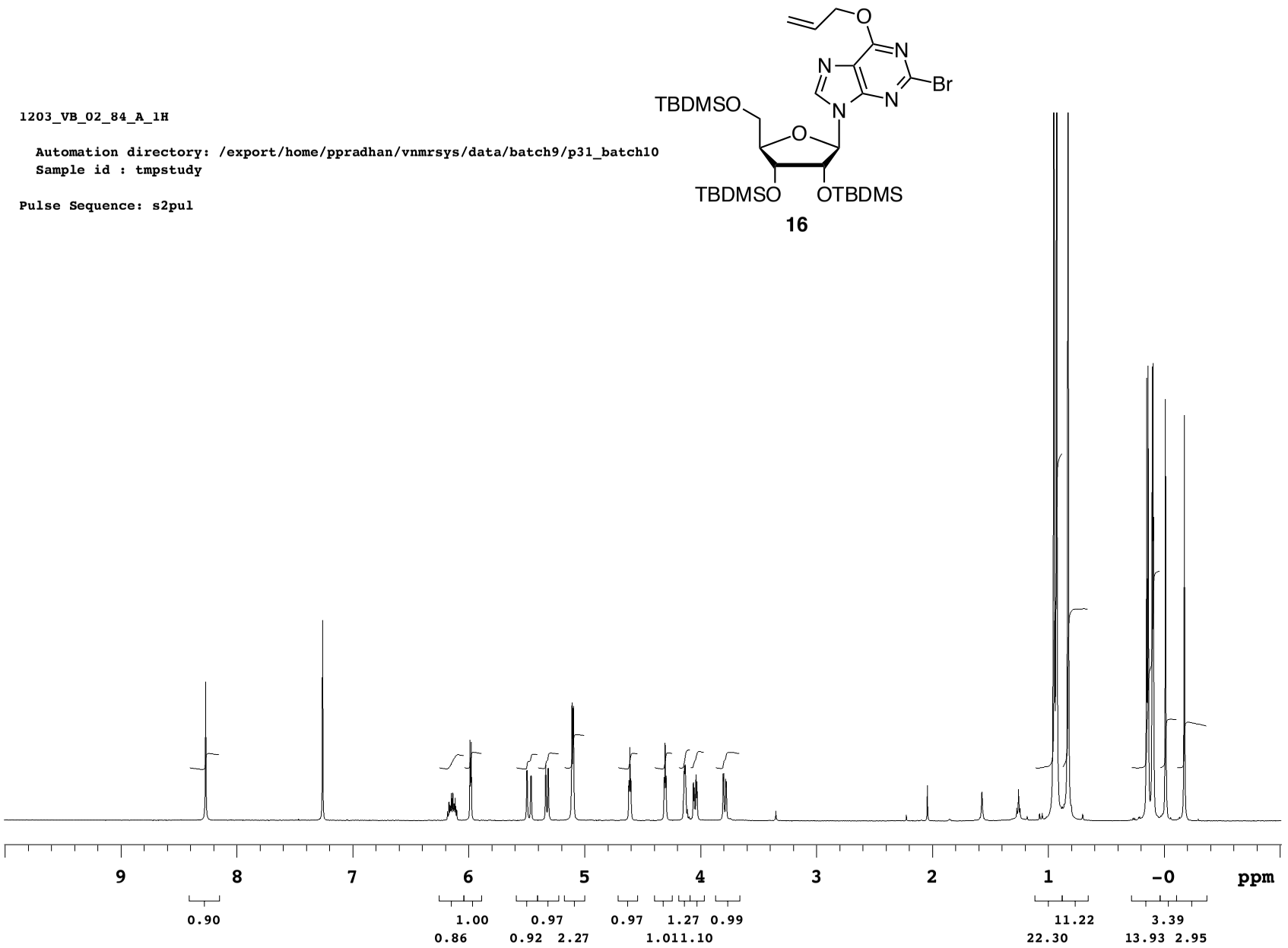
12

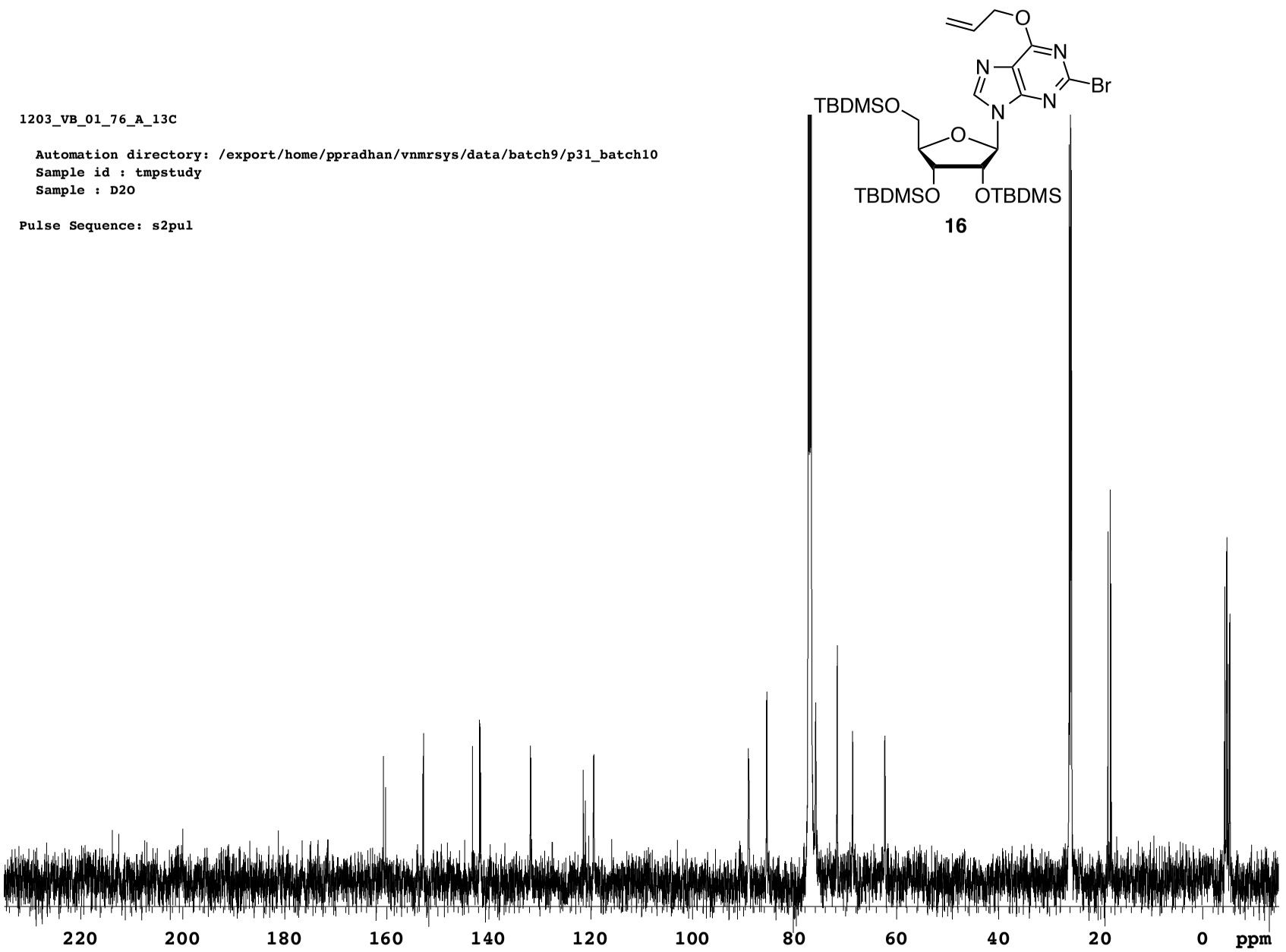

1203_vb_01_88_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
NH2
N
TBDMSO
O
TBDMSO
OTBDMS
13
9
8
7
6
5
4
3
2
1
-0
ppm
1.04
1.04
1.04
1.01
1.00
1.98
1.00
1.05
0.99
1.02
1.00
31.10
13.45
5.17
3.29

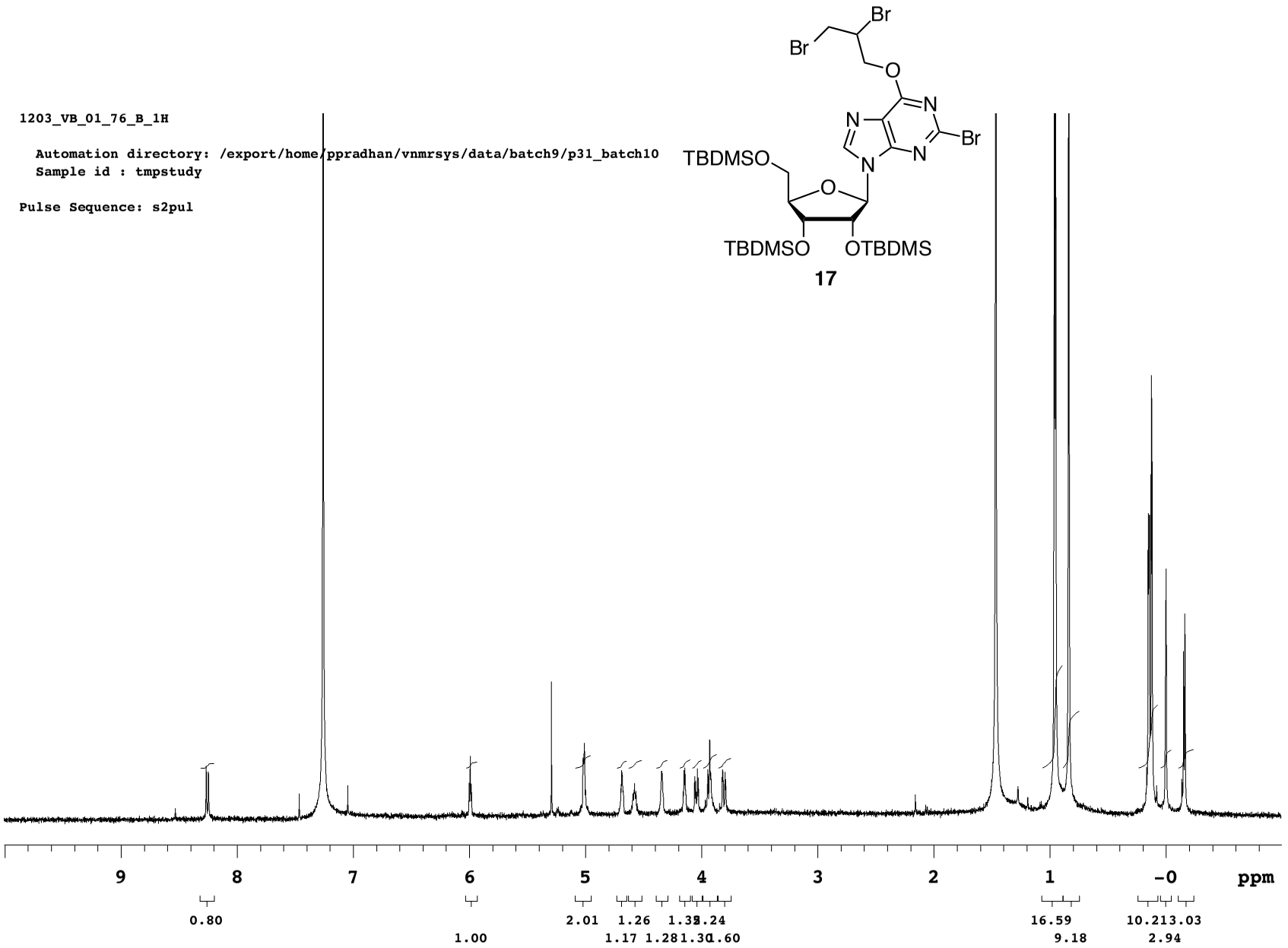

1203_VB_01_88_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
NH2
TBDMSO
O
TBDMSO
OTBDMS
13
220
200
180
160
140
120
100
80
60
40
20
0
ppm

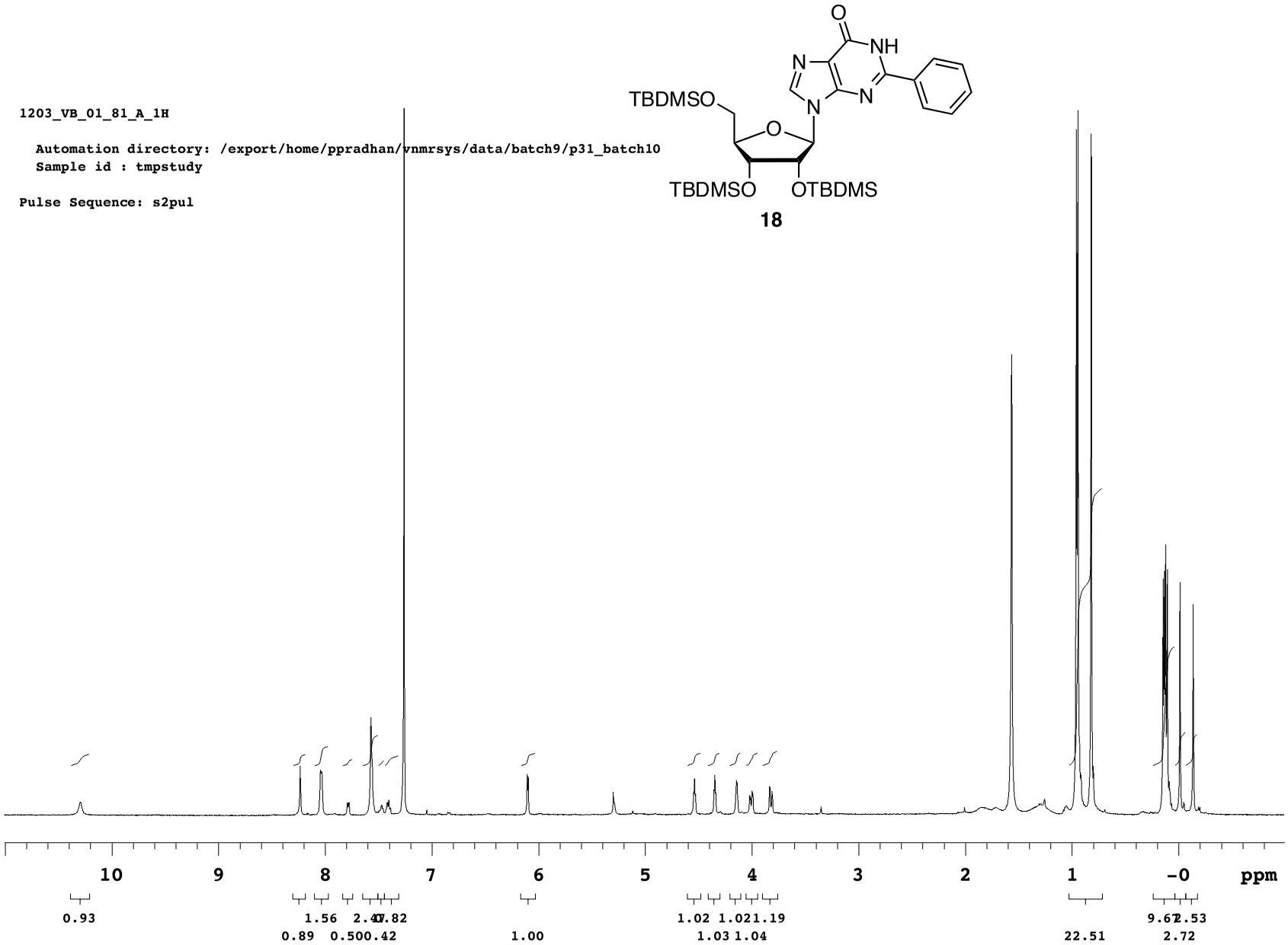

1203_VB_01_90_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
NH2
N
TBDMSO
O
TBDMSO
14
9
8
7
6
5
4
3
2
1
-0
ppm
1.08
1.01
1.04
1.01
1.00
1.04
1.99
1.08
1.06
1.06
1.00
1.01
20.45
12.67

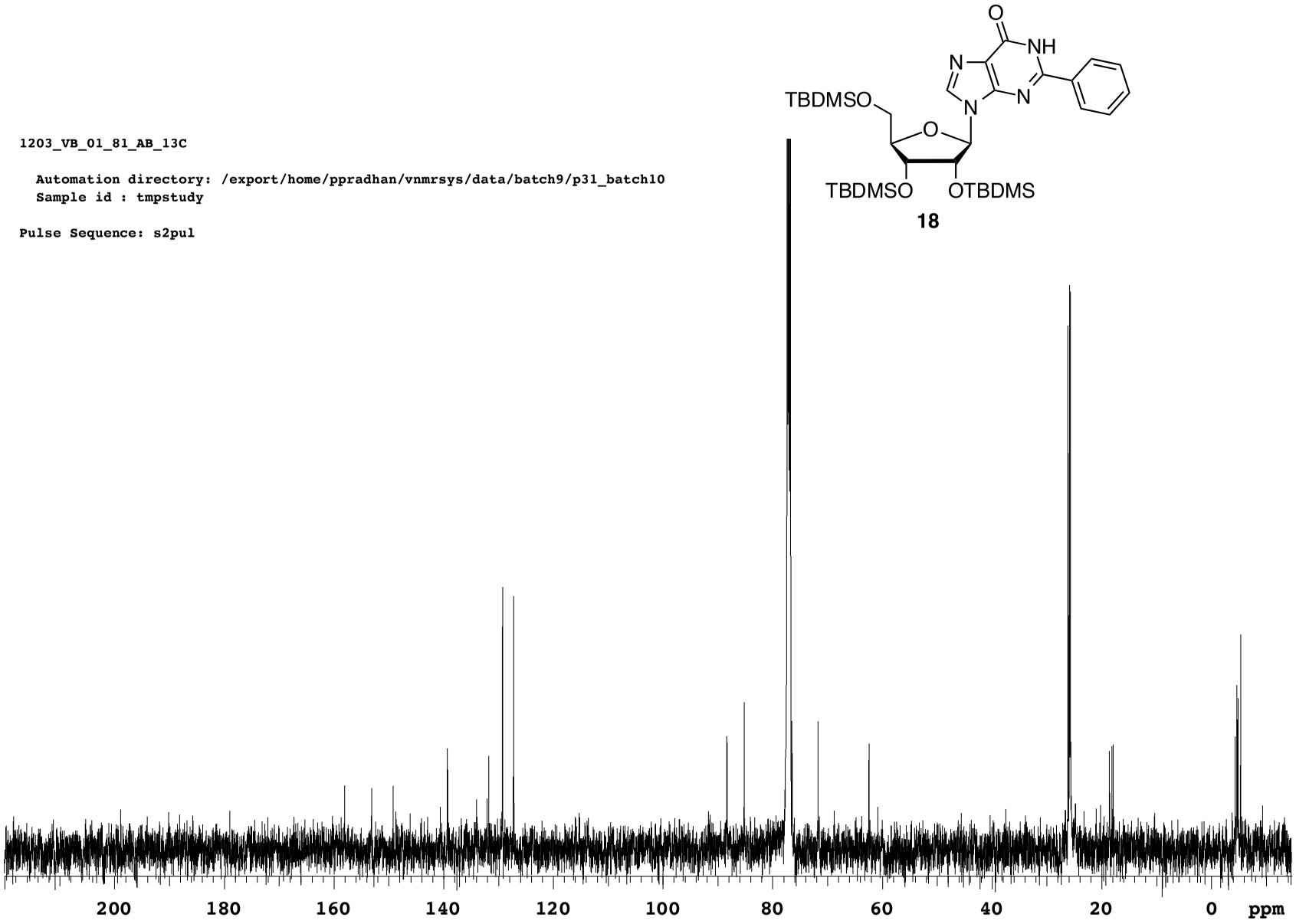

1203_VB_01_90_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
O
N
N
N
N
NH2
TBDMSO
O
TBDMSO
14
200
180
160
140
120
100
80
60
40
20
0
ppm

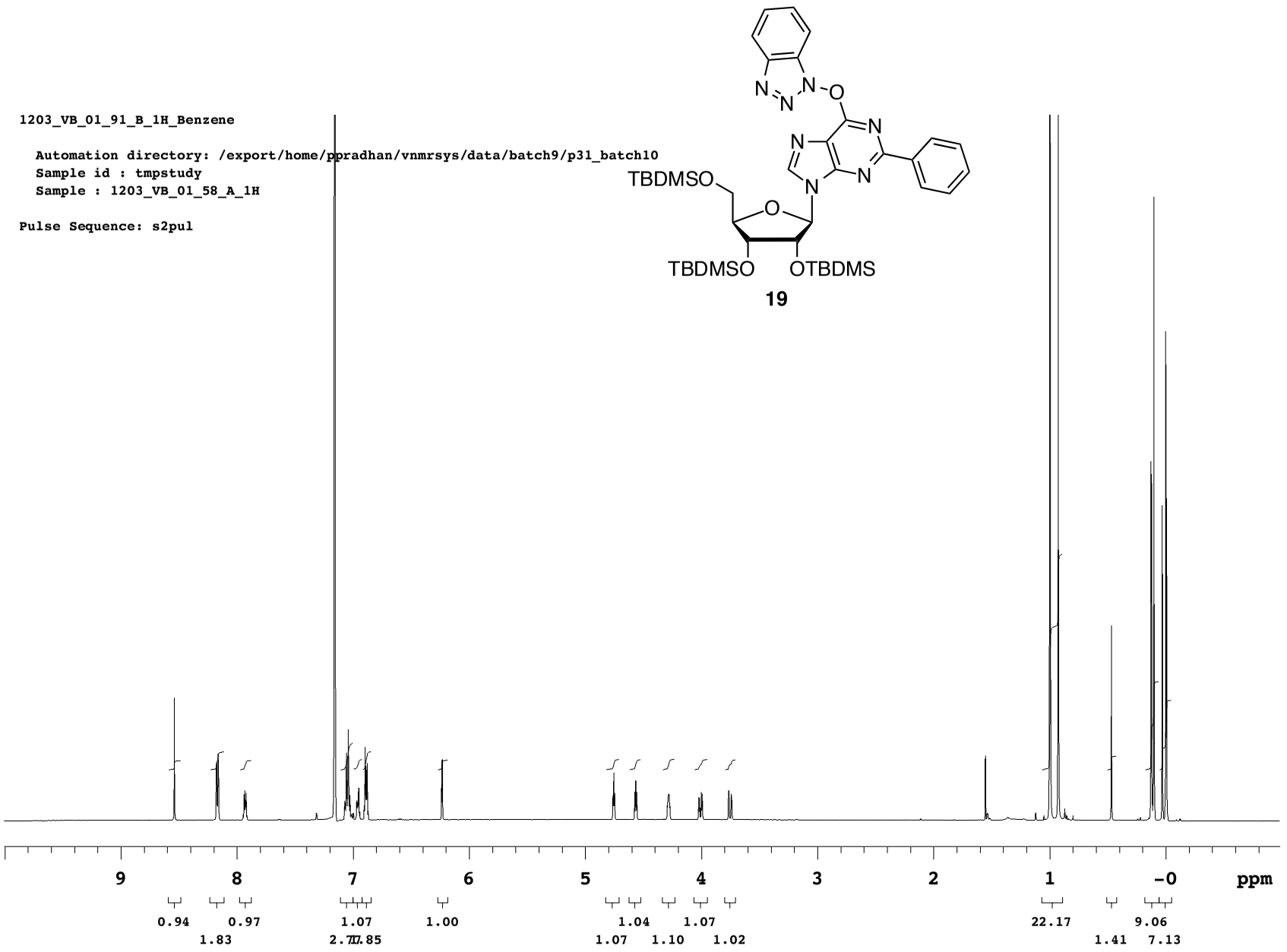

1203_VB_02_84_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
Br
16
9
8
7
6
5
4
3
2
1
-0
ppm
0.90
1.00
0.86
0.97
0.92
2.27
0.97
1.27
0.99
1.01
1.10
11.22
22.30
3.39
13.93
2.95

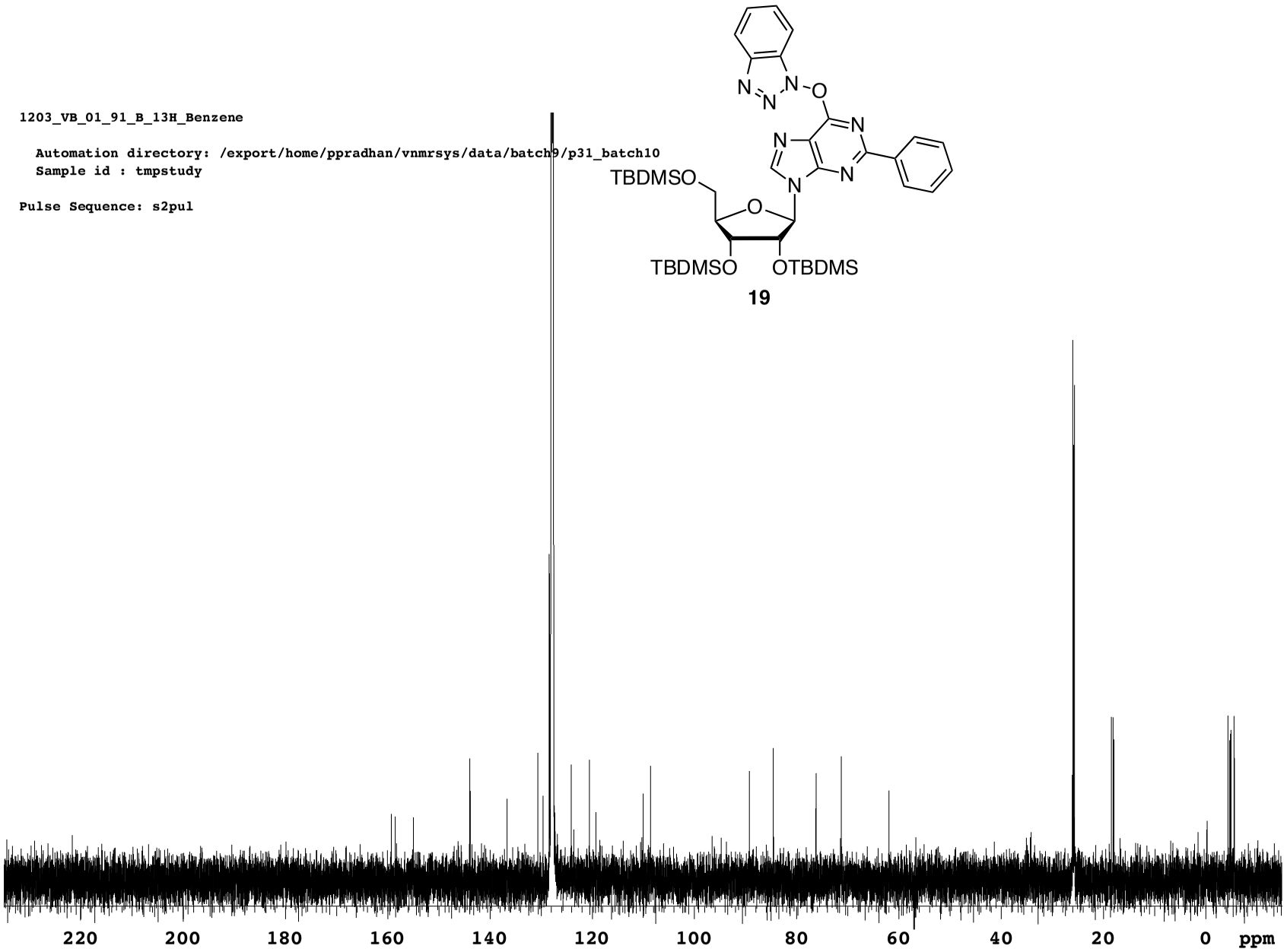

1203_VB_01_76_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : D2O
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
Br
16
220
200
180
160
140
120
100
80
60
40
20
0
ppm

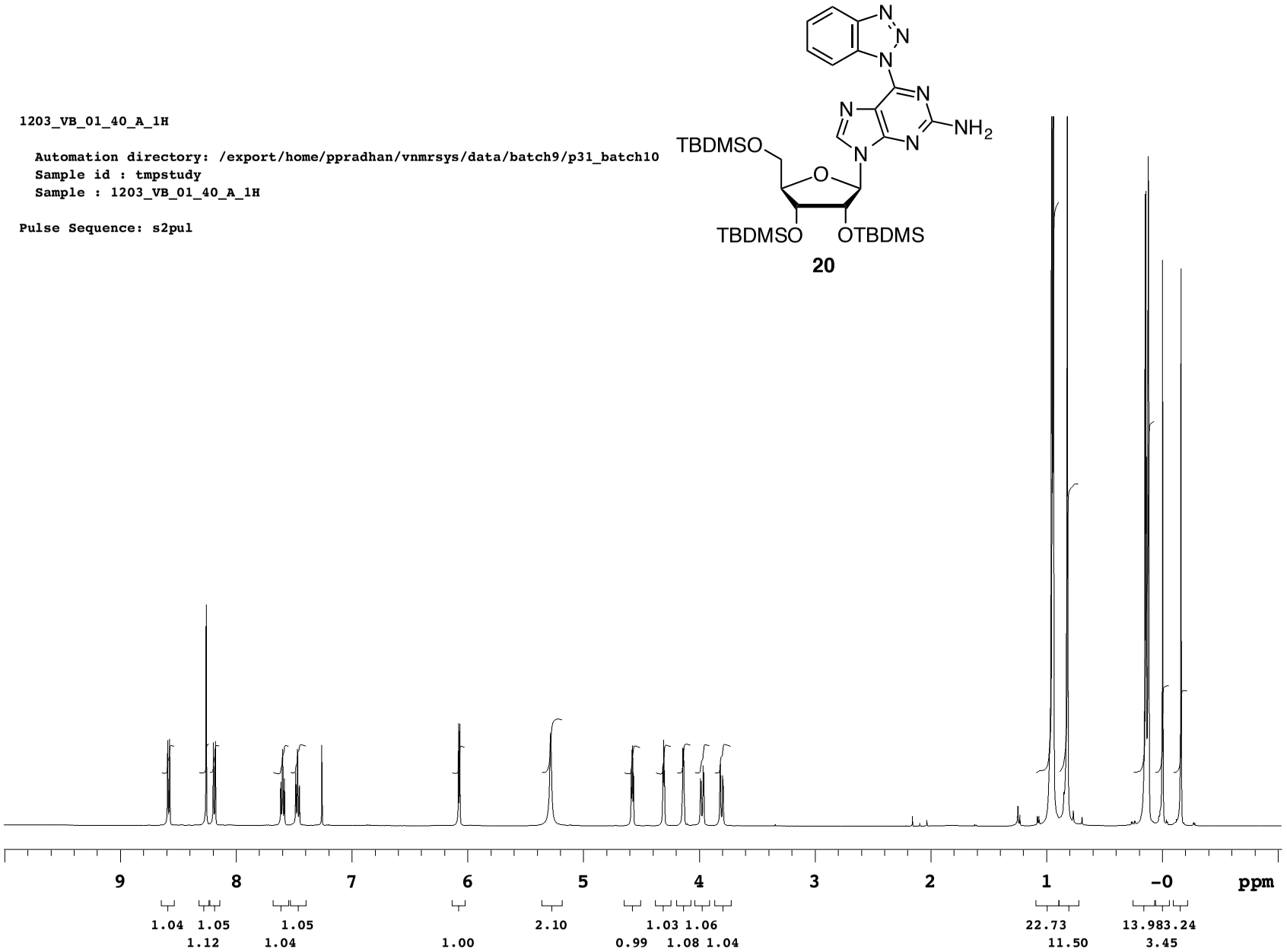

1203_VB_01_76_B_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Br
Br
O
N
N
N
N
Br
TBDMSO
O
TBDMSO
OTBDMS
17
9
8
7
6
5
4
3
2
1
-0
ppm
0.80
1.00
2.01
1.26
1.17
1.28
1.33
1.30
3.24
1.60
16.59
9.18
10.21
3.03
2.94

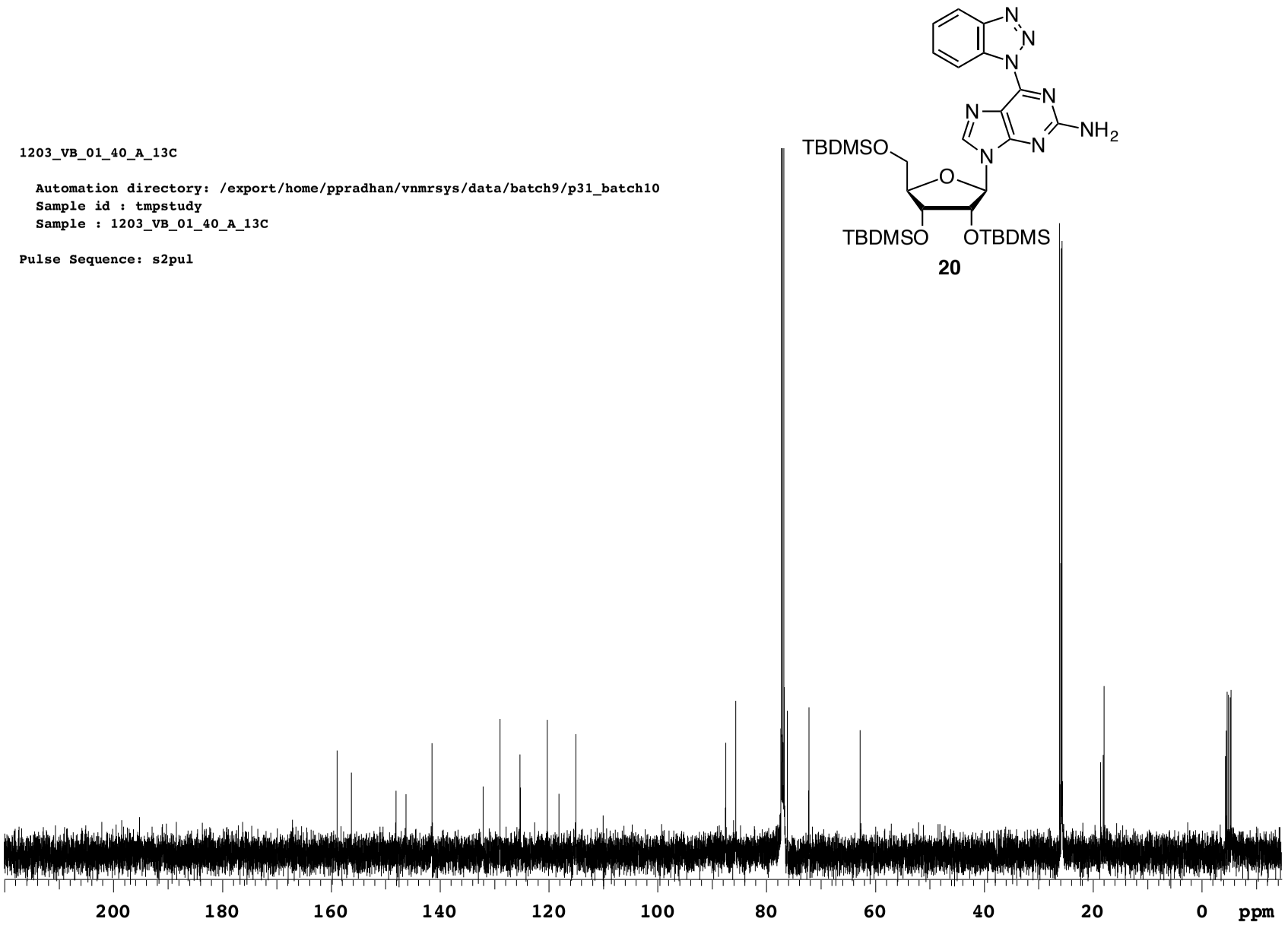

1203_VB_01_81_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
18
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.93
1.56
2.40
0.89
0.50
0.42
1.00
1.02
1.02
1.19
1.03
1.04
22.51
9.67
2.53
2.72


1203_VB_01_81_AB_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
O
NH
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
18
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_01_91_B_1H_Benzene
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_58_A_1H
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
19
9
8
7
6
5
4
3
2
1
-0
ppm
0.94
0.97
1.07
1.00
1.04
1.07
22.17
9.06
1.83
2.77
7.85
1.07
1.10
1.02
1.41
7.13


1203_VB_01_91_B_13H_Benzene
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
19
220
200
180
160
140
120
100
80
60
40
20
0
ppm

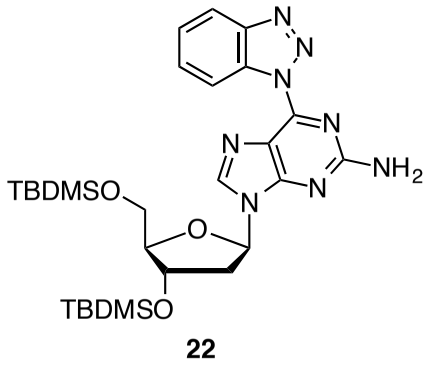

1203_VB_01_40_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_40_A_1H
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
NH2
20
9
8
7
6
5
4
3
2
1
-0
ppm
1.04 1.05 1.05 2.10 1.03 1.06 22.73 13.983.24
1.12 1.04 1.00 0.99 1.08 1.04 11.50 3.45


1203_VB_01_40_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_40_A_13C
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
NH2
20
200
180
160
140
120
100
80
60
40
20
0
ppm

1203_VB_01_41_A_1H

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_41_A_1H

Pulse Sequence: s2pul



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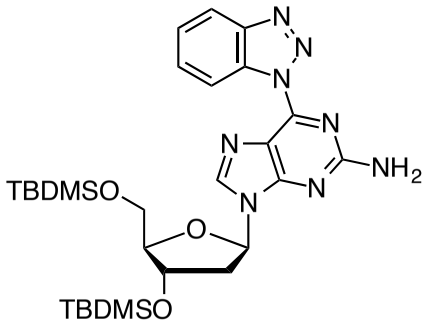
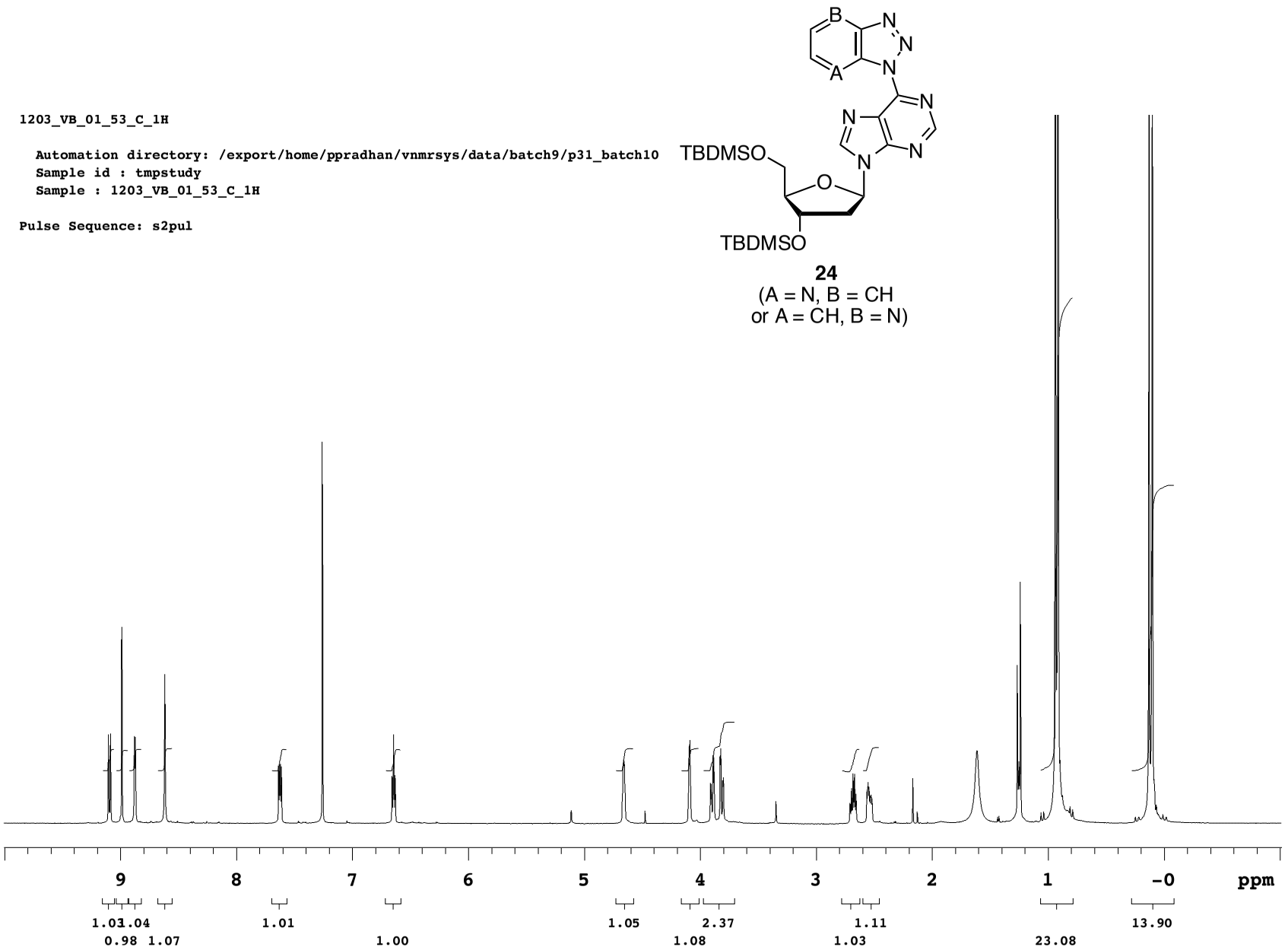
1203_VB_01_41_A_13C

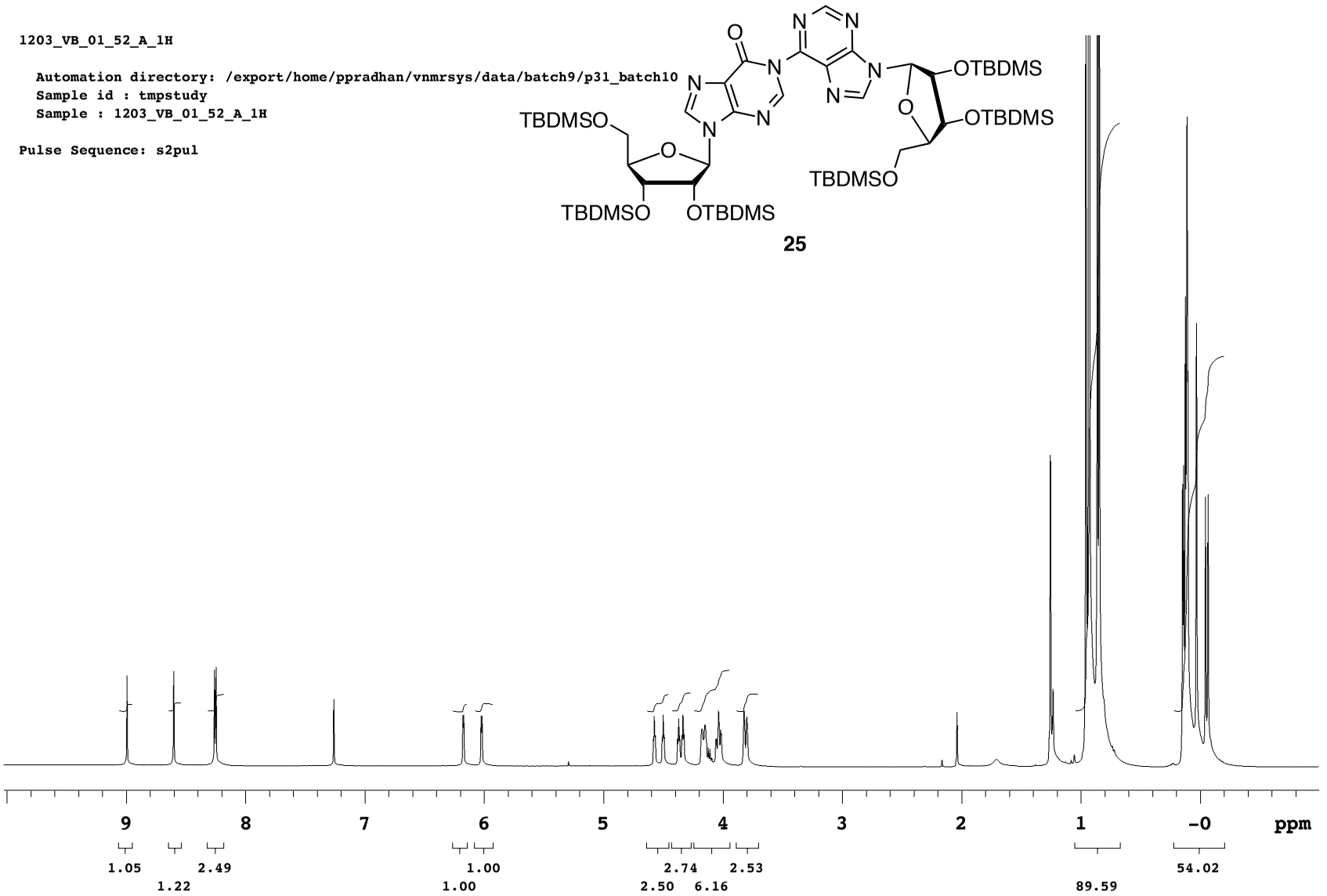
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_41_A_13C

Pulse Sequence: s2pul

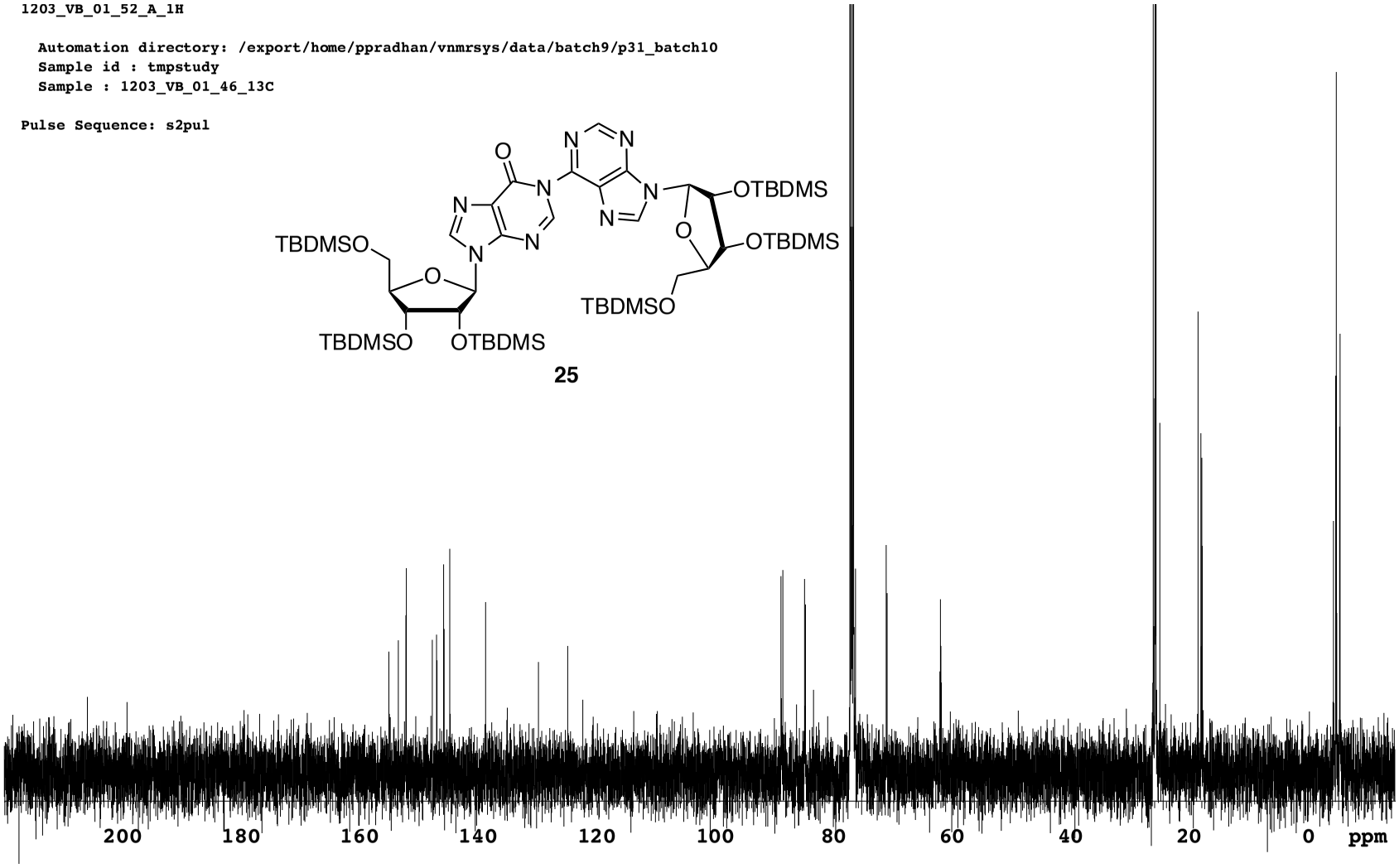


22


1203_VB_01_53_C_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_53_C_1H
Pulse Sequence: s2pul
TBDMSO
TBDMSO
24
(A = N, B = CH
or A = CH, B = N)
9
8
7
6
5
4
3
2
1
-0
ppm
1.03
1.04
0.98
1.07
1.01
1.00
1.05
2.37
1.08
1.11
1.03
23.08
13.90


1203_VB_01_52_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_52_A_1H
Pulse Sequence: s2pul
TBDMSO
OTBDMS
TBDMSO
OTBDMS
TBDMSO
OTBDMS
9
8
7
6
5
4
3
2
1
-0
ppm
1.05
1.22
2.49
1.00
1.00
2.74
2.50
6.16
2.53
89.59
54.02

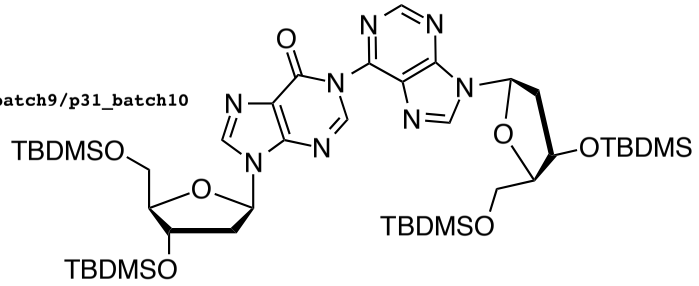
25


1203_VB_01_52_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_46_13C
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
OTBDMS
TBDMSO
OTBDMS
25
200
180
160
140
120
100
80
60
40
20
0
ppm

1203_VB_01_53_B_1H

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_53_B_1H

Pulse Sequence: s2pul



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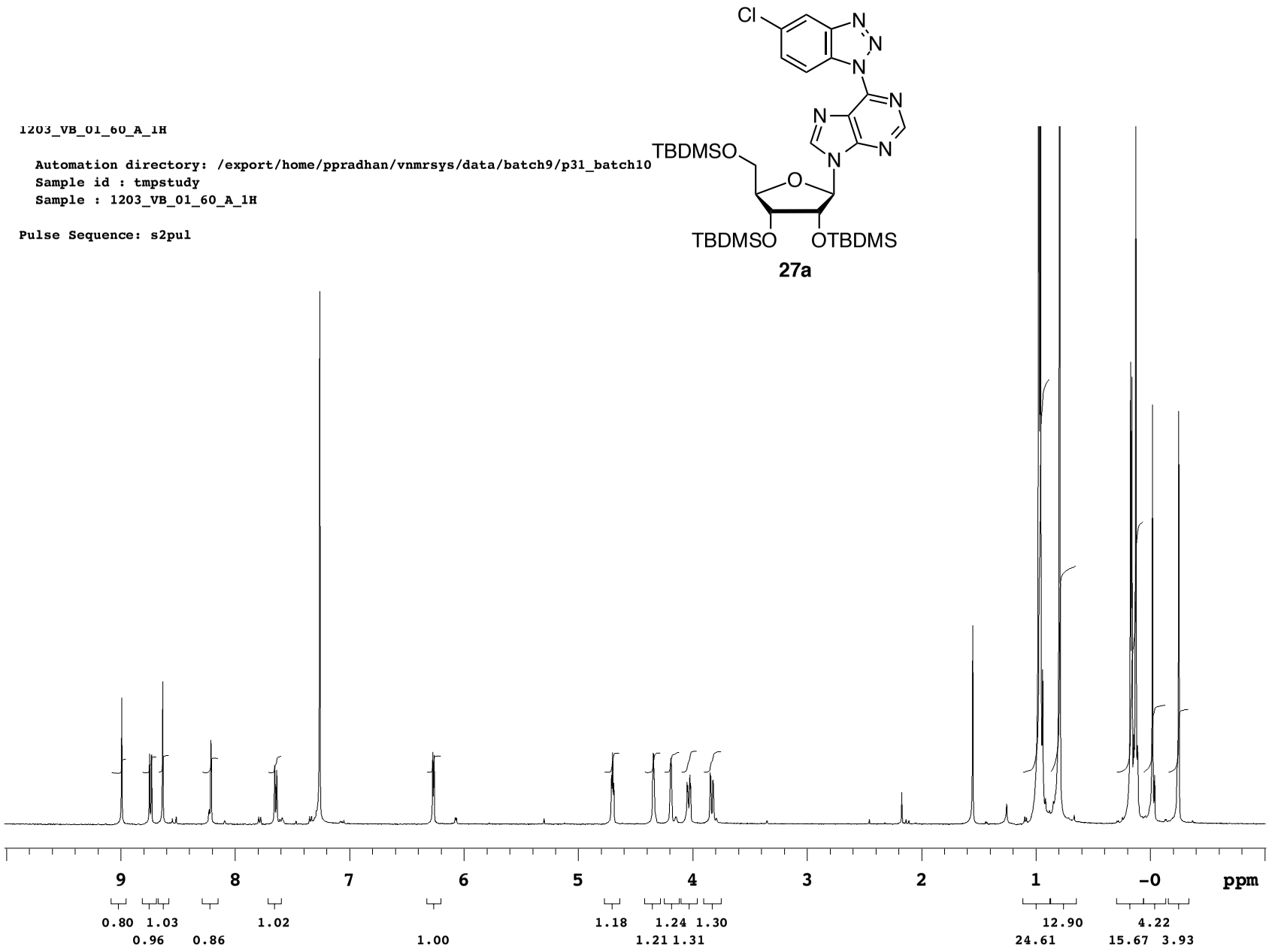
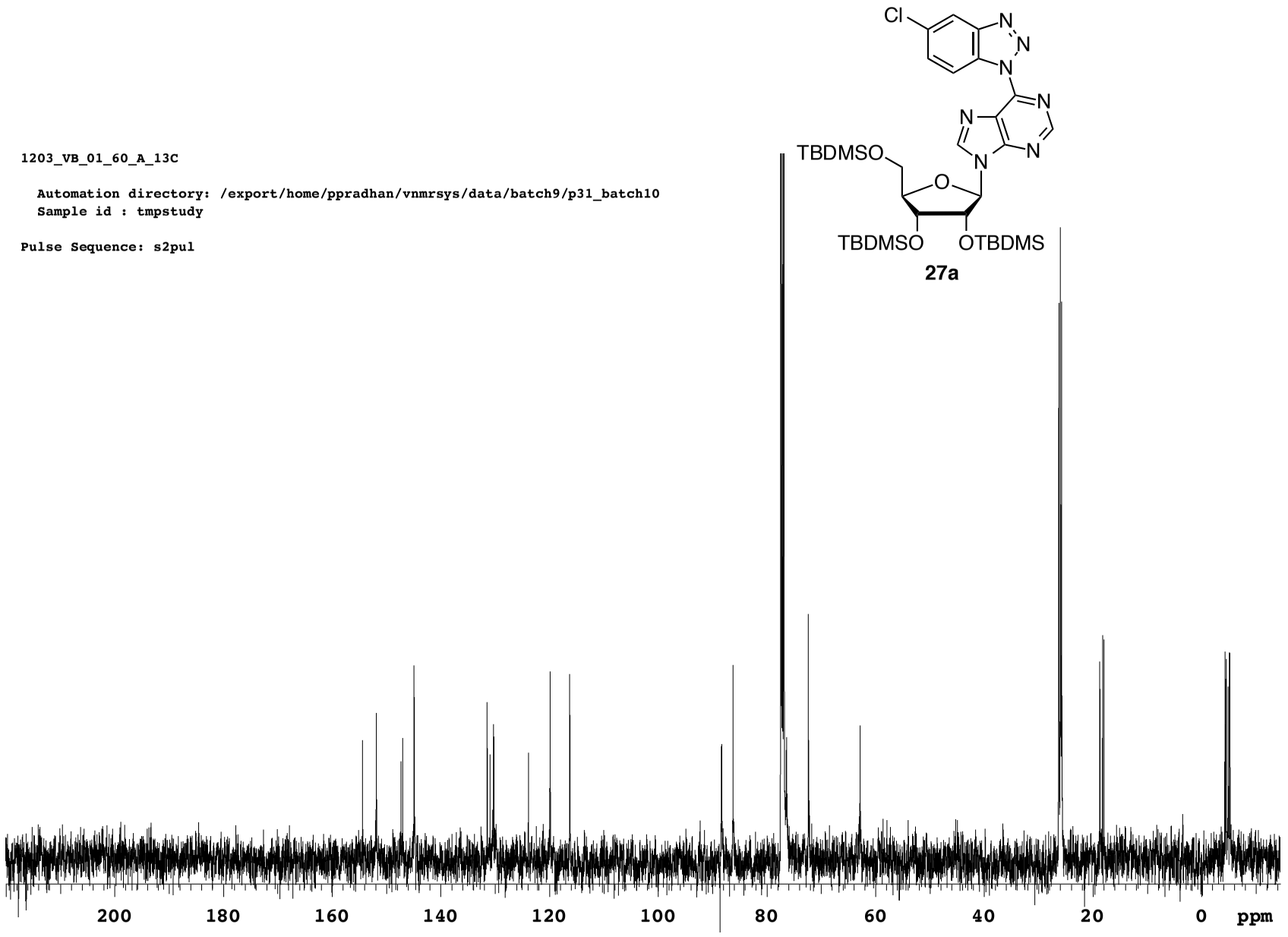
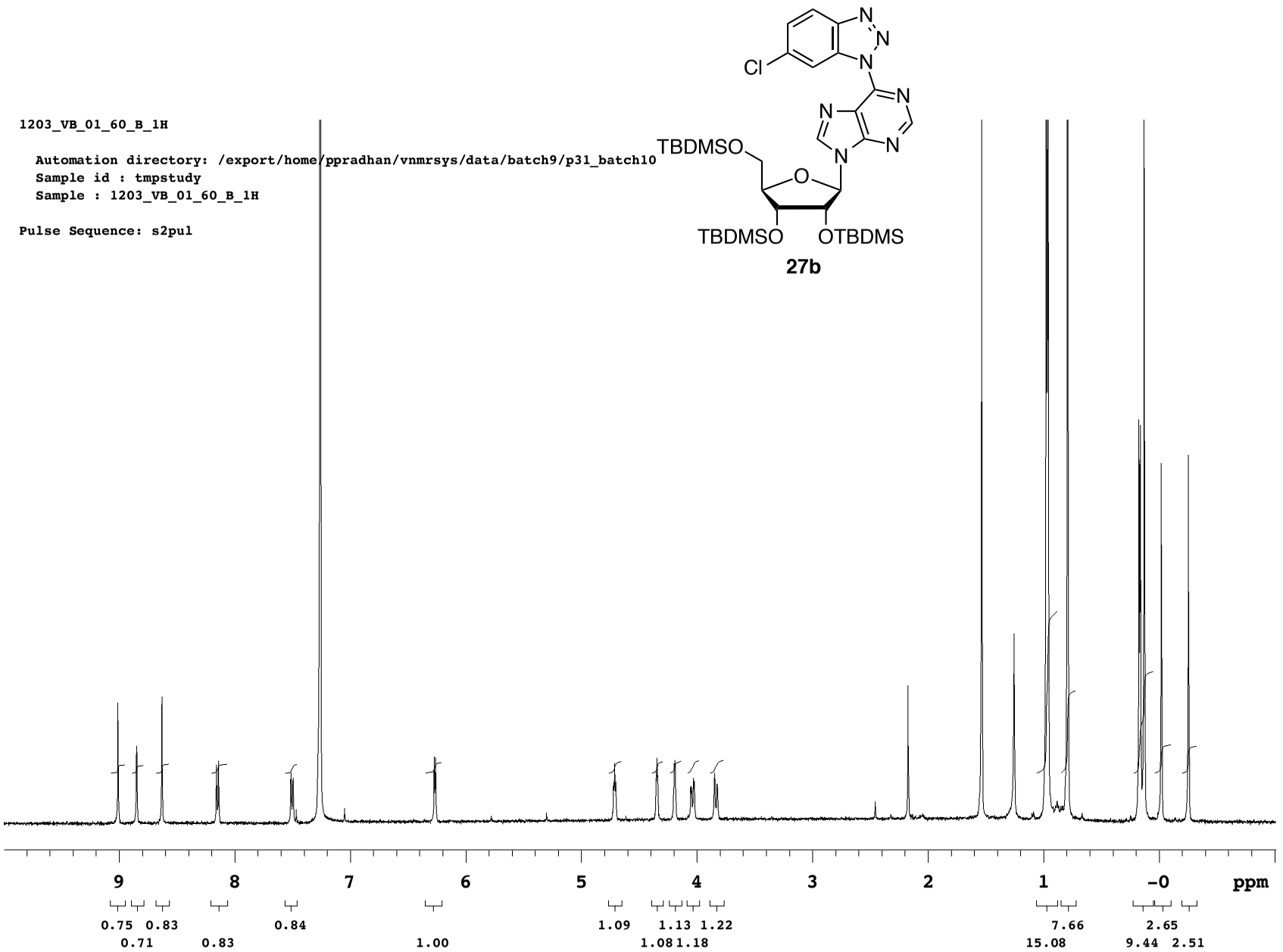
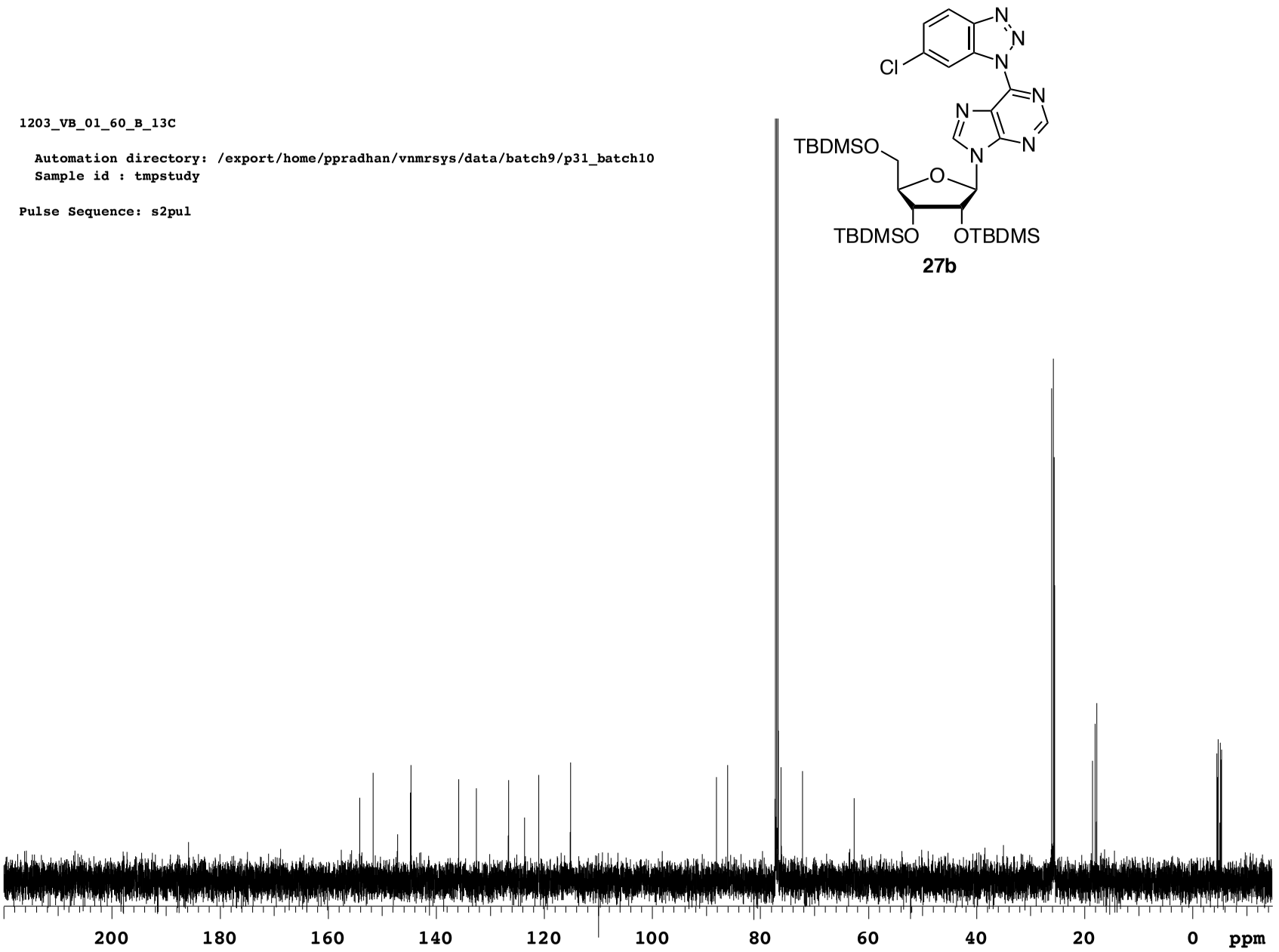
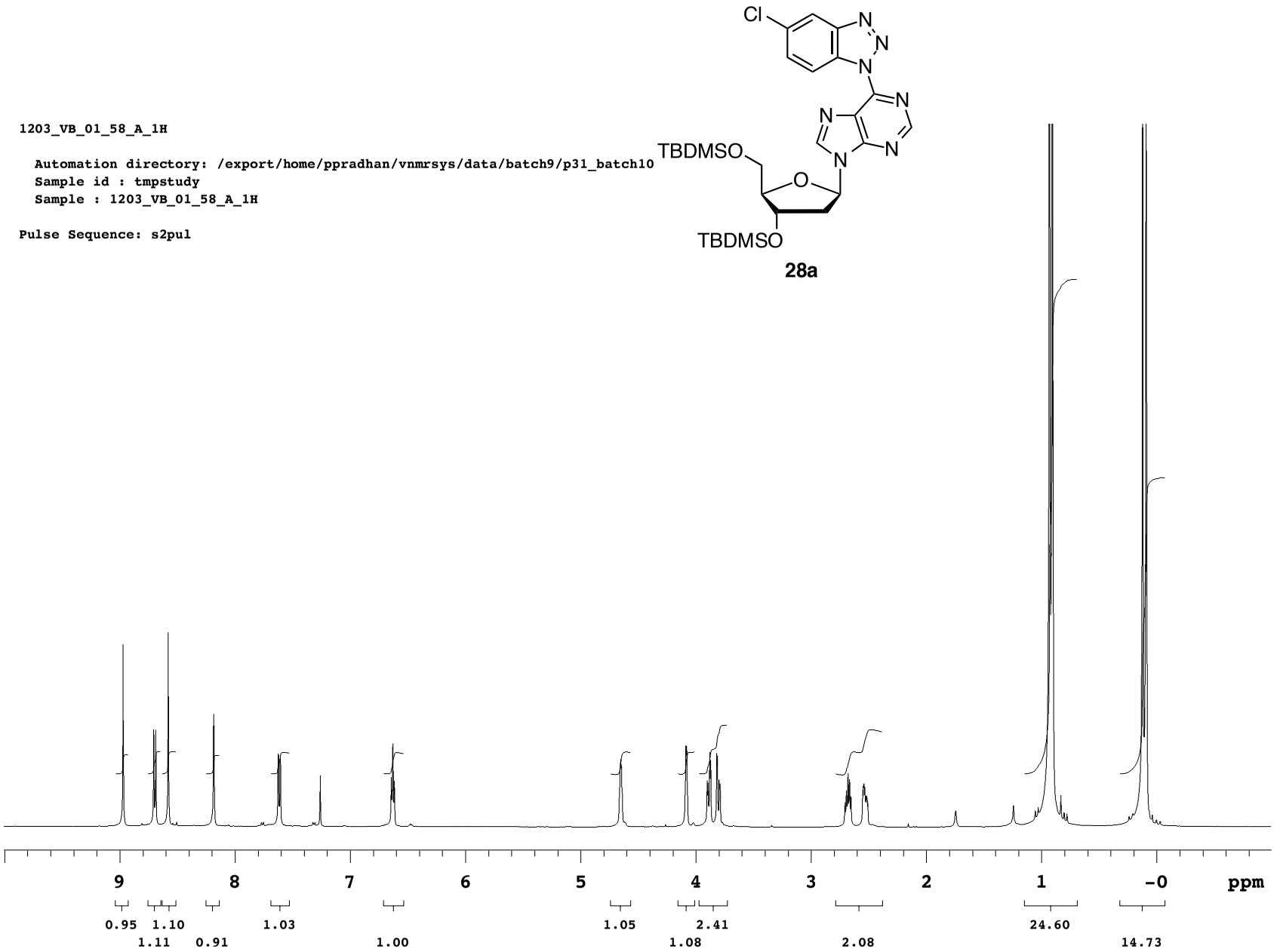
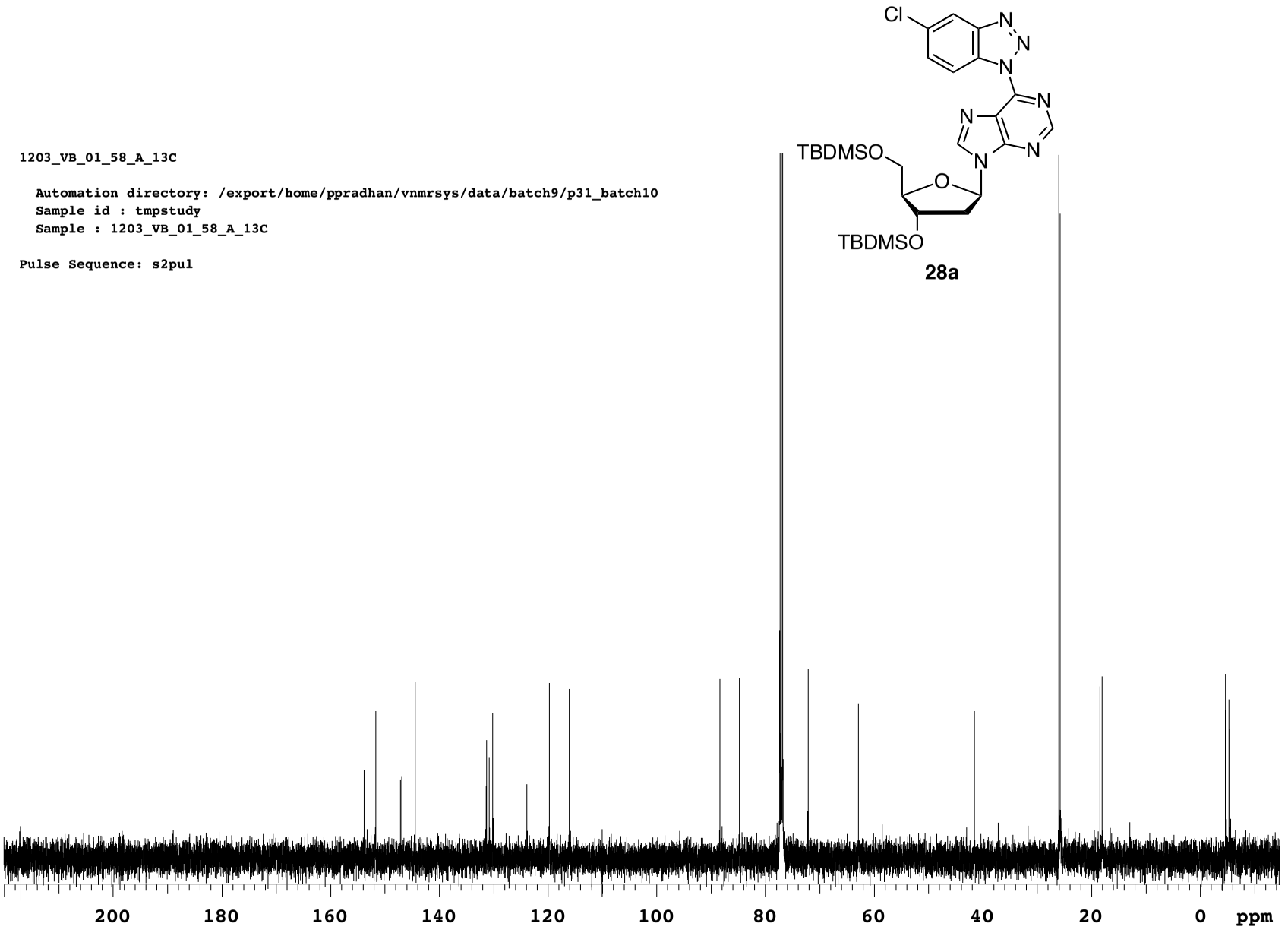

1203_VB_01_60_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_60_A_1H
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
27a
9
8
7
6
5
4
3
2
1
-0
ppm
0.80 1.03
0.96 0.86
1.02
1.00
1.18
1.24 1.30
1.21 1.31
12.90
24.61
4.22
15.67 3.93


1203_VB_01_60_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
27a
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_01_60_B_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_60_B_1H
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
27b
9
8
7
6
5
4
3
2
1
-0
ppm
0.75 0.83
0.71
0.83
0.84
1.00
1.09
1.13 1.22
1.08 1.18
7.66
15.08
2.65
9.44 2.51


1203_VB_01_60_B_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
27b
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_01_58_A_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_58_A_1H
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
28a
9
8
7
6
5
4
3
2
1
-0
ppm
0.95
1.10
1.11
0.91
1.03
1.00
1.05
1.08
2.41
2.08
24.60
14.73

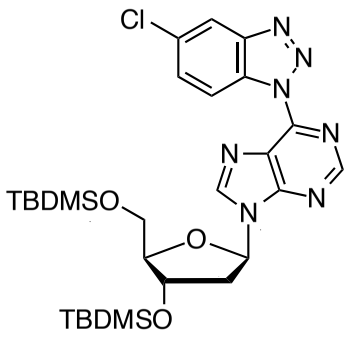

1203_VB_01_58_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_58_A_13C
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
28a
200
180
160
140
120
100
80
60
40
20
0
ppm

1203_VB_01_58_A_NOESY_3

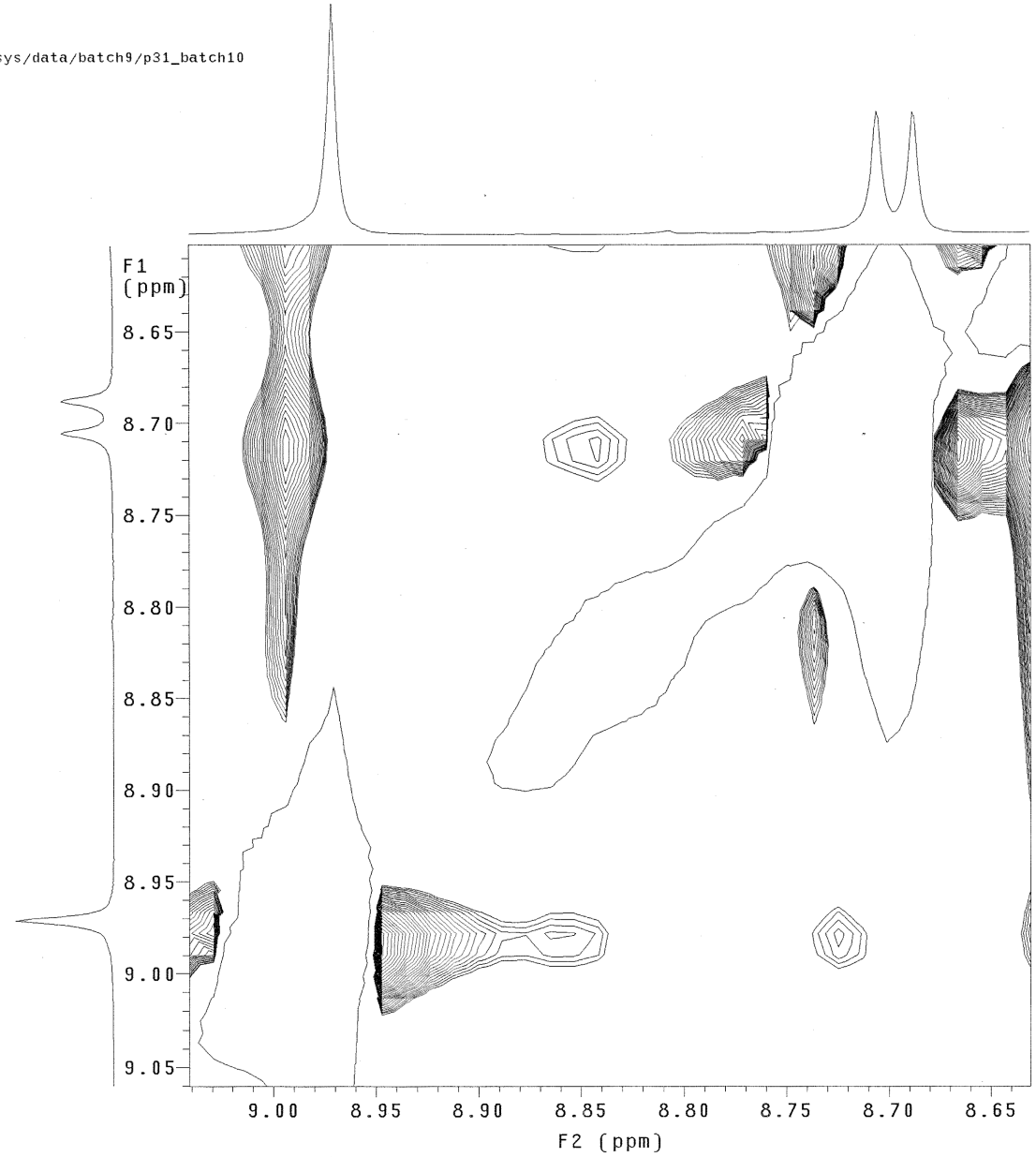
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

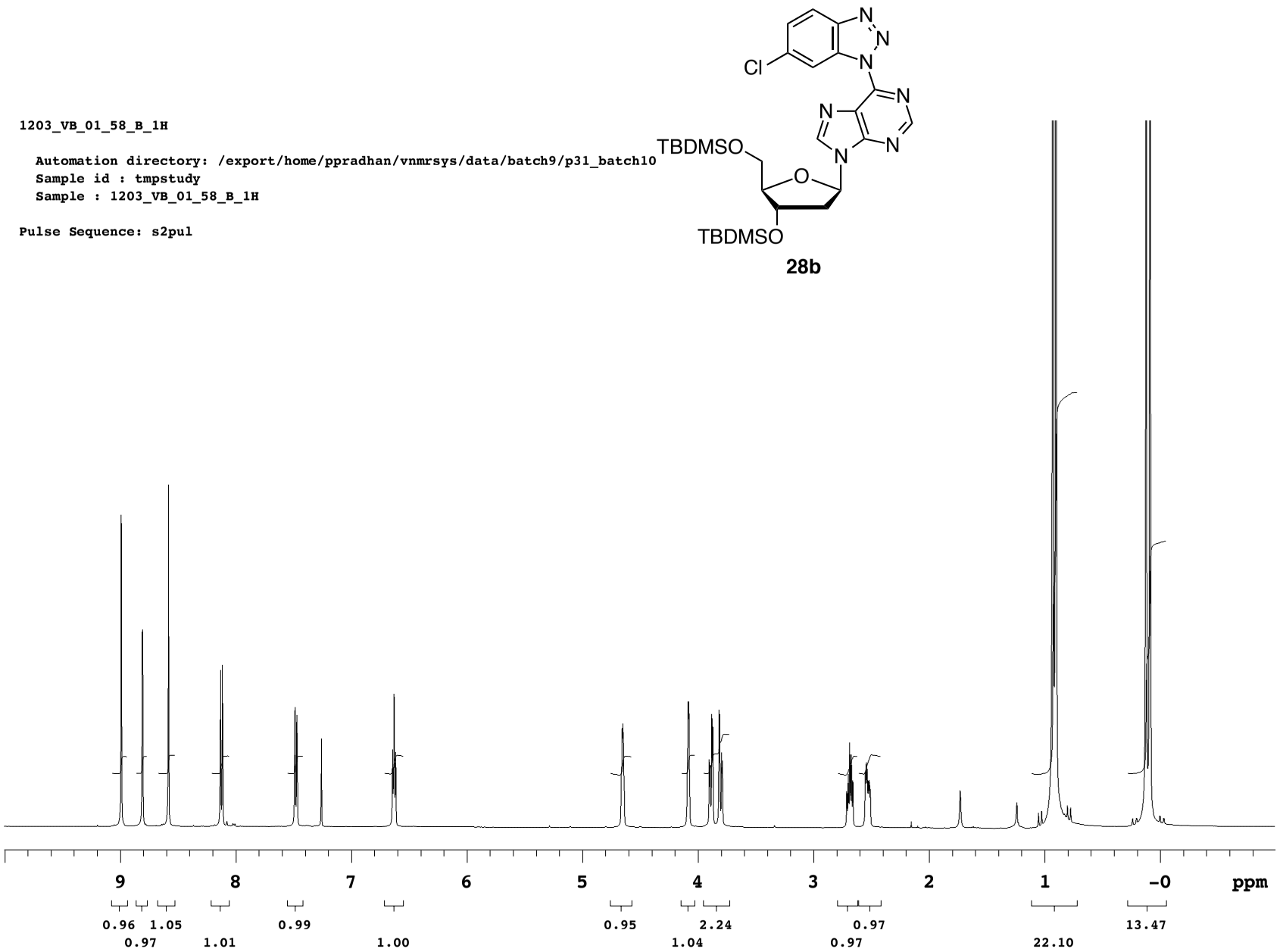
Pulse Sequence: NOESY
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: mklpd
File: 1203_VB_01_58_A_NOESY_3
INOVA-500 "riga"

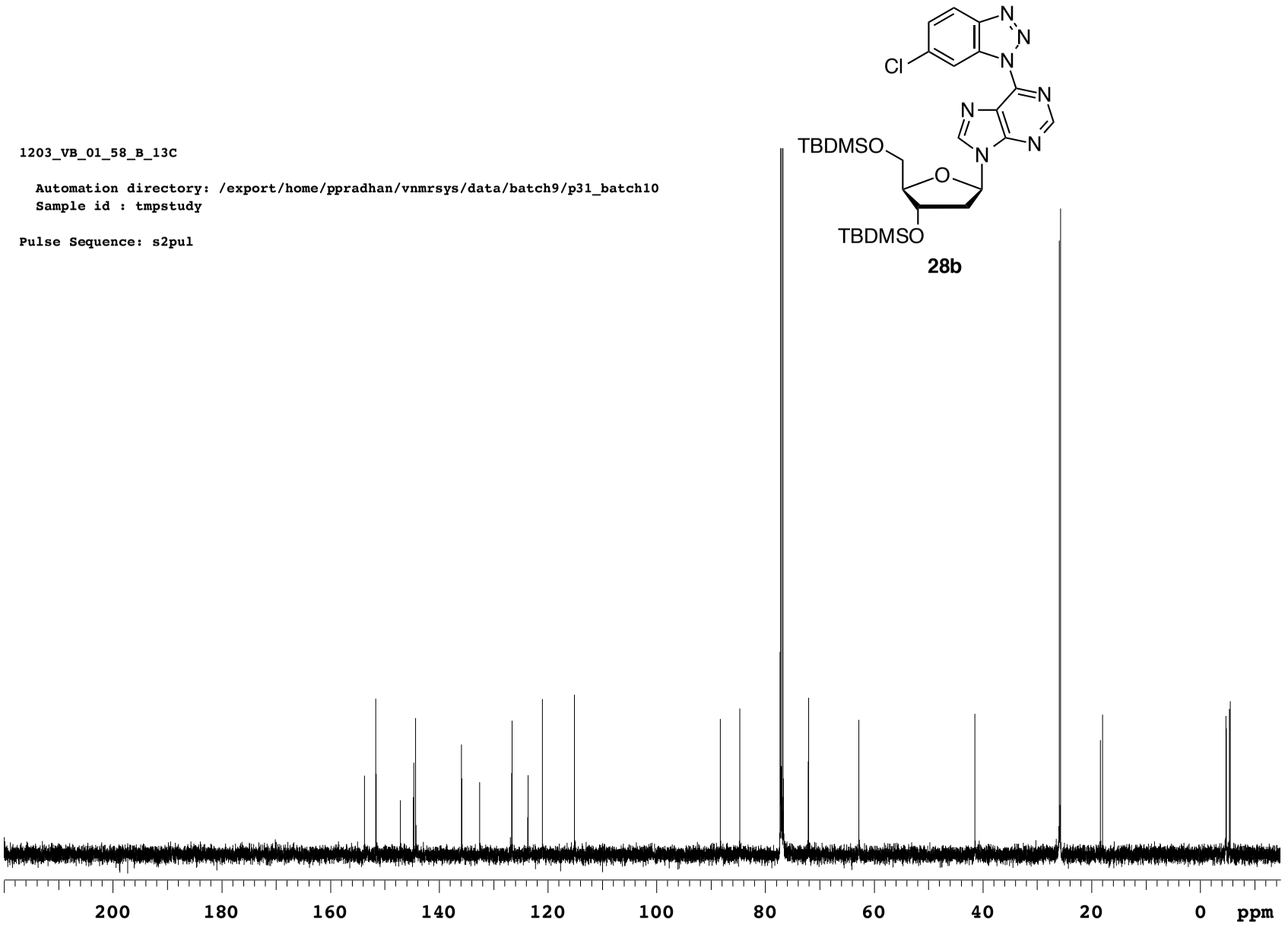
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 6000.2 Hz
2D Width 6000.2 Hz
64 repetitions
2 x 256 increments
OBSERVE H1, 499.7707234 MHz
DATA PROCESSING
Resol. enhancement 3.4 Hz
Gauss apodization 0.037 sec
F1 DATA PROCESSING
Resol. enhancement 0.0 Hz
Gauss apodization 0.021 sec
FT size 2048 x 2048
Total time 10 hr, 49 min, 53 sec

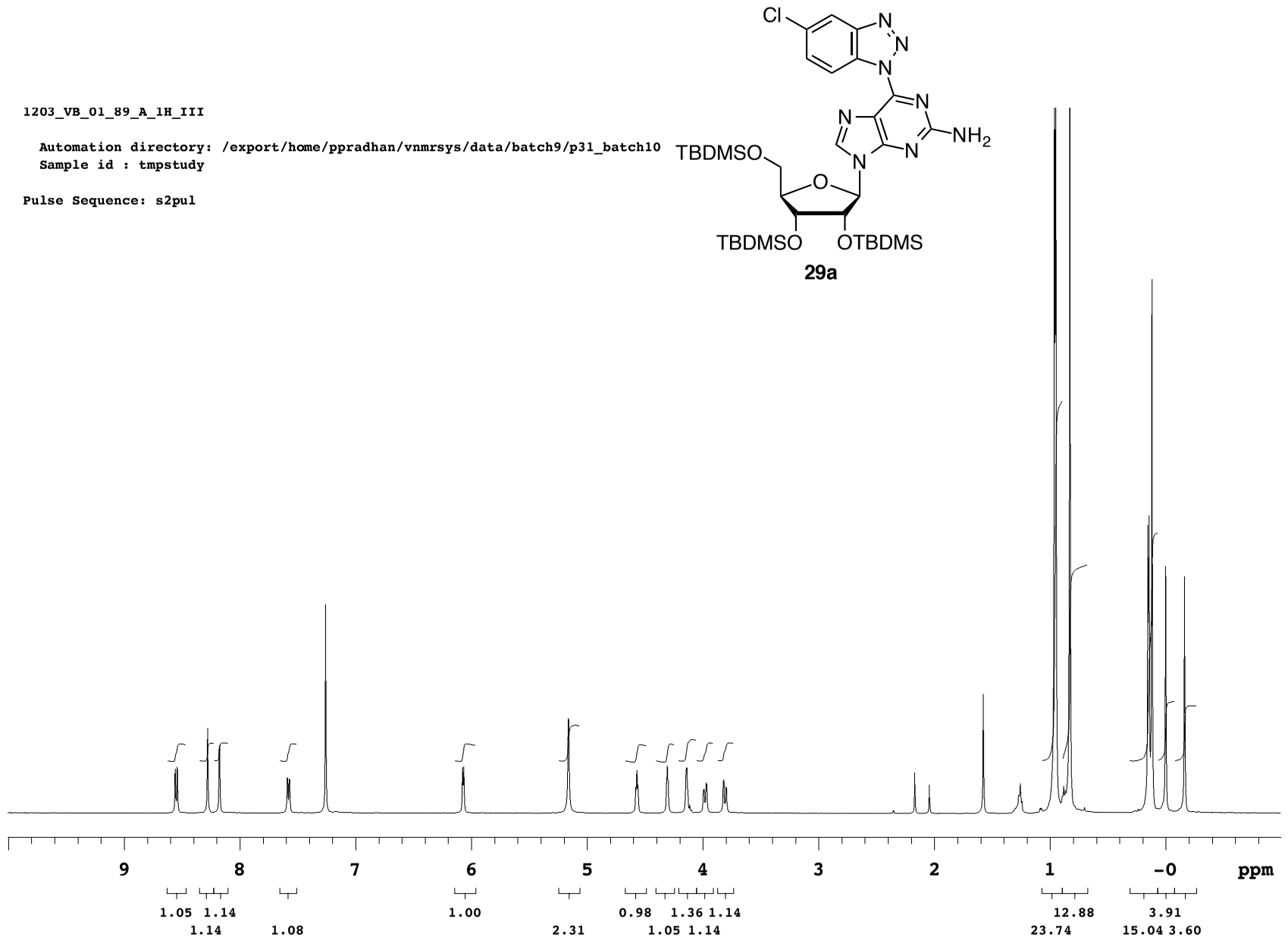


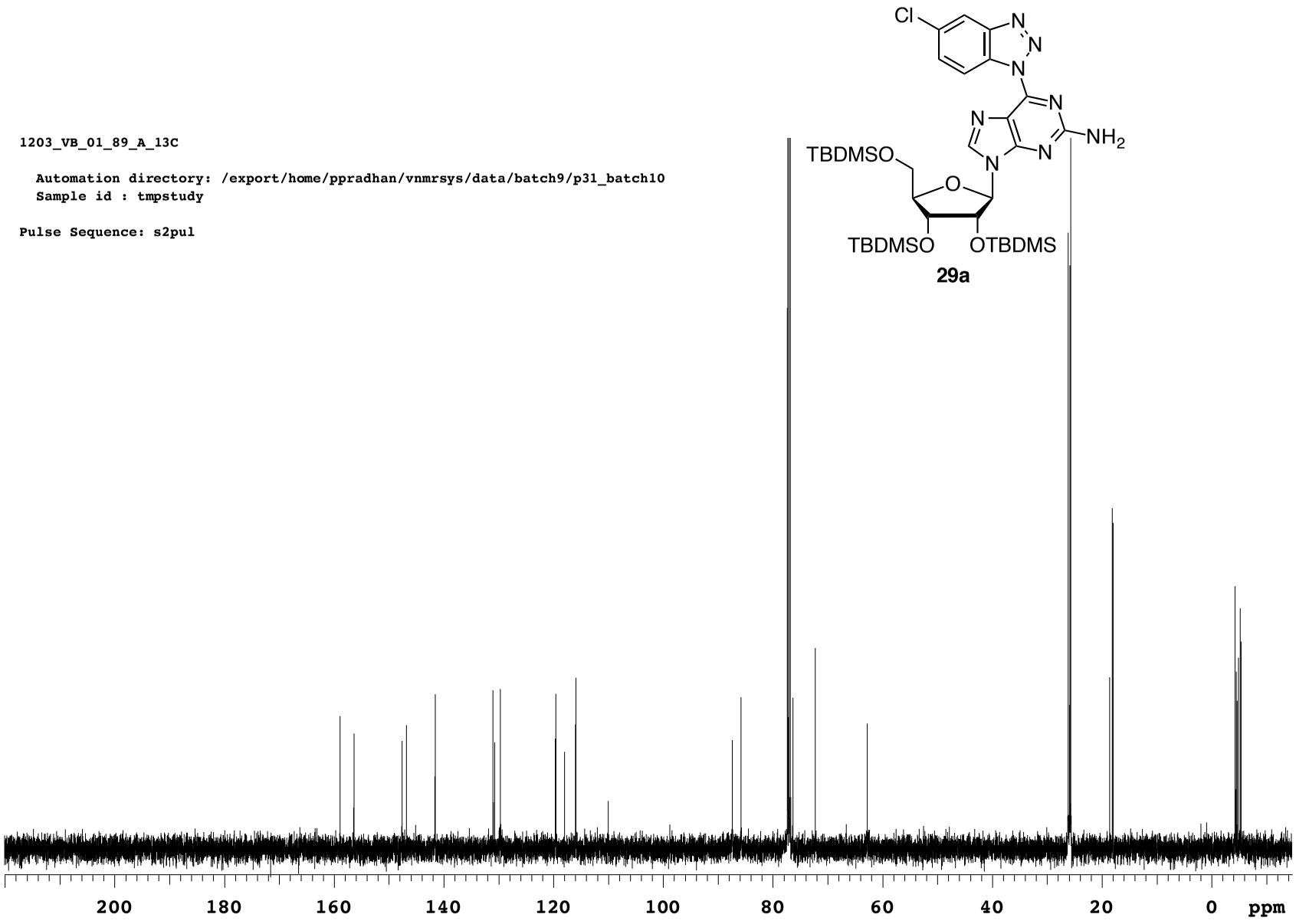
28a




1203_VB_01_58_B_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Sample : 1203_VB_01_58_B_1H
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
28b
9
8
7
6
5
4
3
2
1
-0
ppm
0.96
1.05
0.99
0.95
2.24
0.97
13.47
0.97
1.01
1.00
1.04
0.97
22.10


1203_VB_01_58_B_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
N
O
TBDMSO
TBDMSO
28b
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_01_89_A_1H_III
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
OTBDMS
29a
9
8
7
6
5
4
3
2
1
-0
ppm
1.05 1.14
1.14
1.08
1.00
2.31
0.98
1.36 1.14
1.05 1.14
12.88
23.74
3.91
15.04 3.60


1203_VB_01_89_A_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
OTBDMS
29a
200
180
160
140
120
100
80
60
40
20
0
ppm

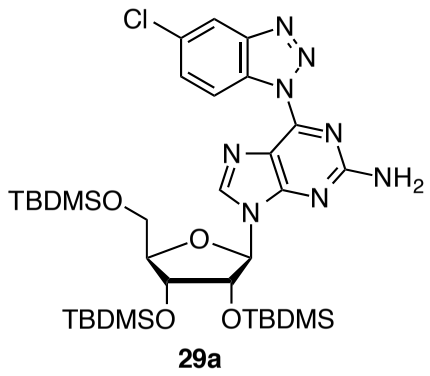
1203_VB_01_89_A_NOESY_III

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

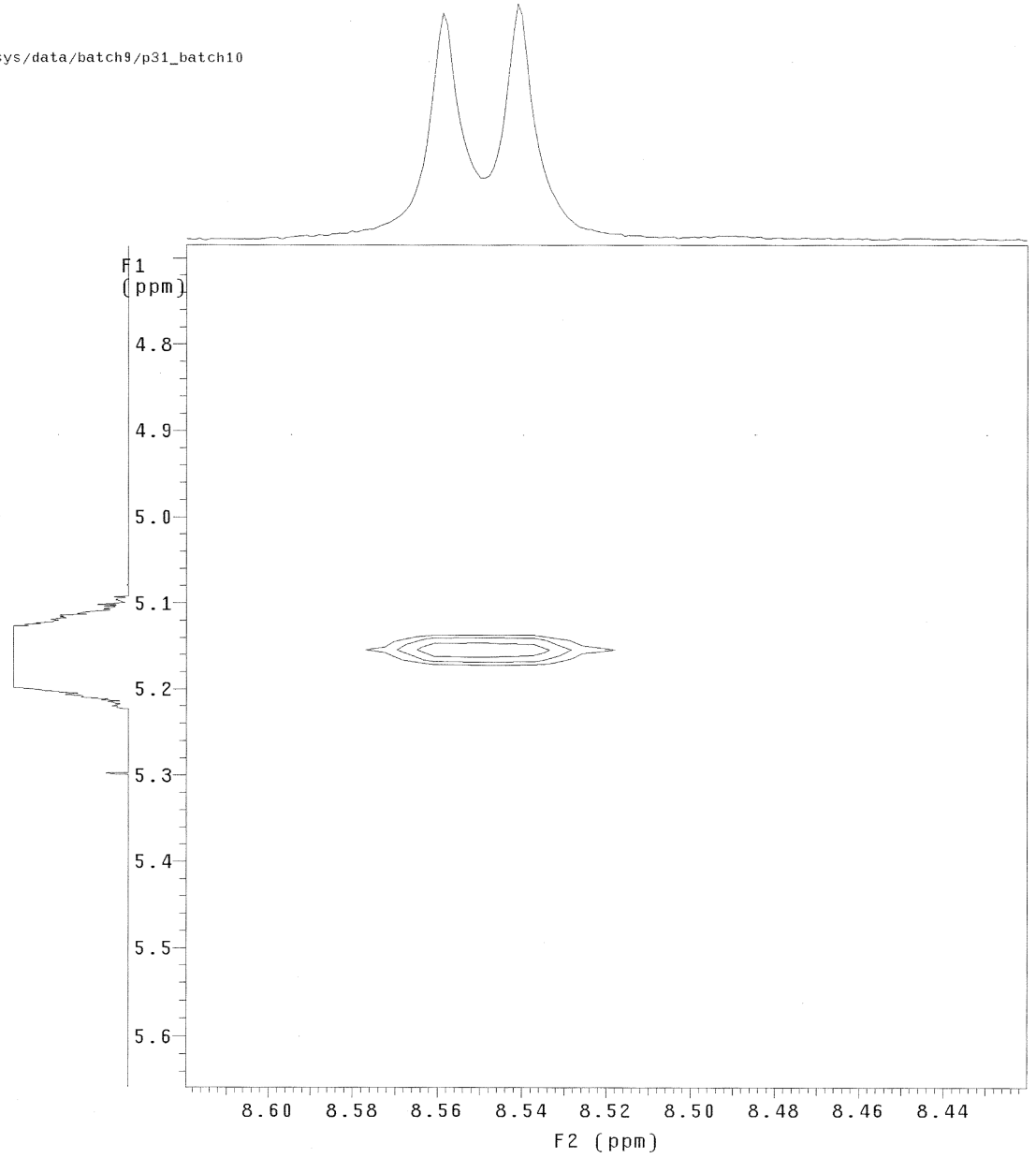
Pulse Sequence: NOESY

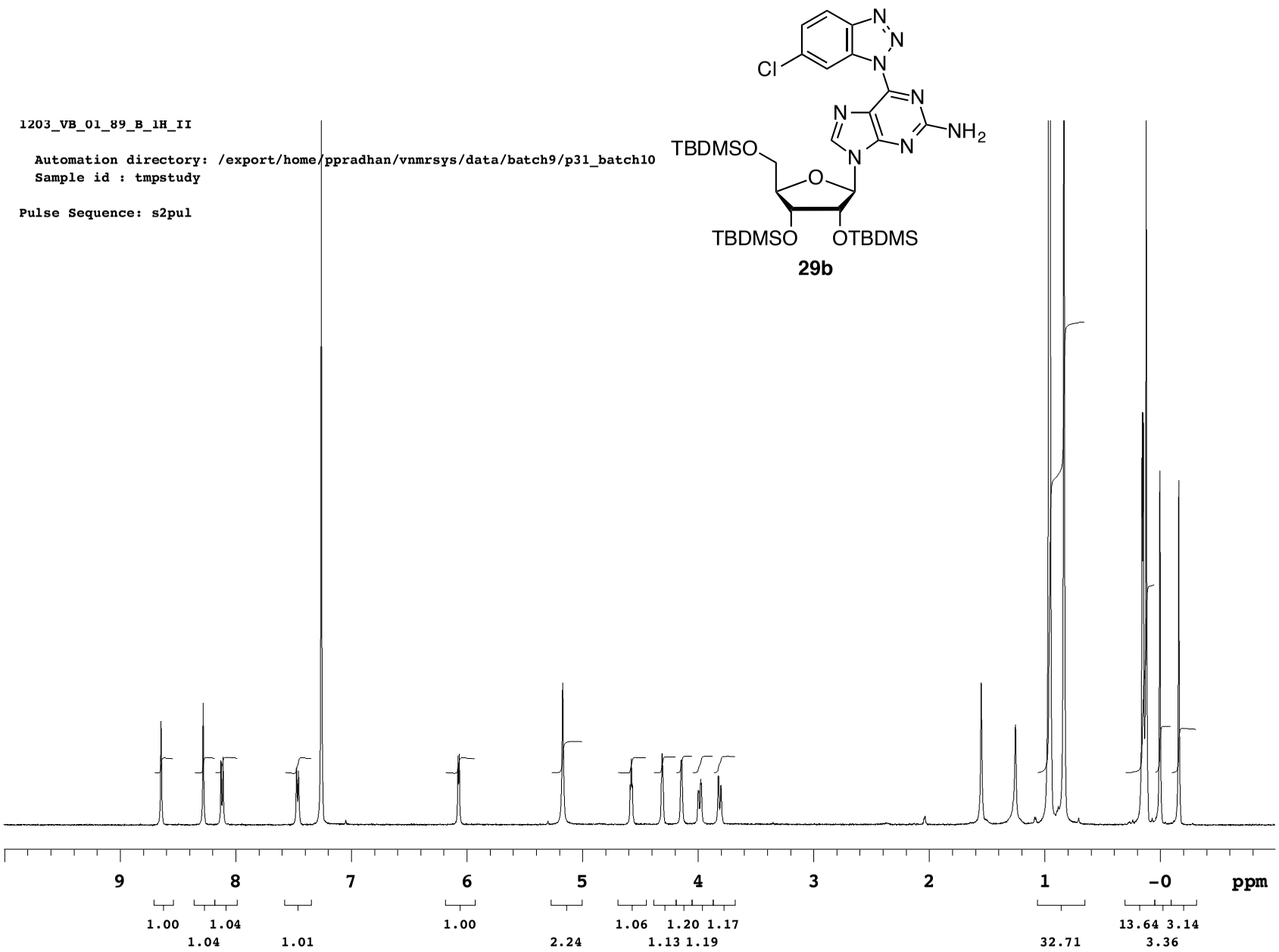
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: mklpd
File: 1203_VB_01_89_A_NOESY_III
INOVA-500 "riga"

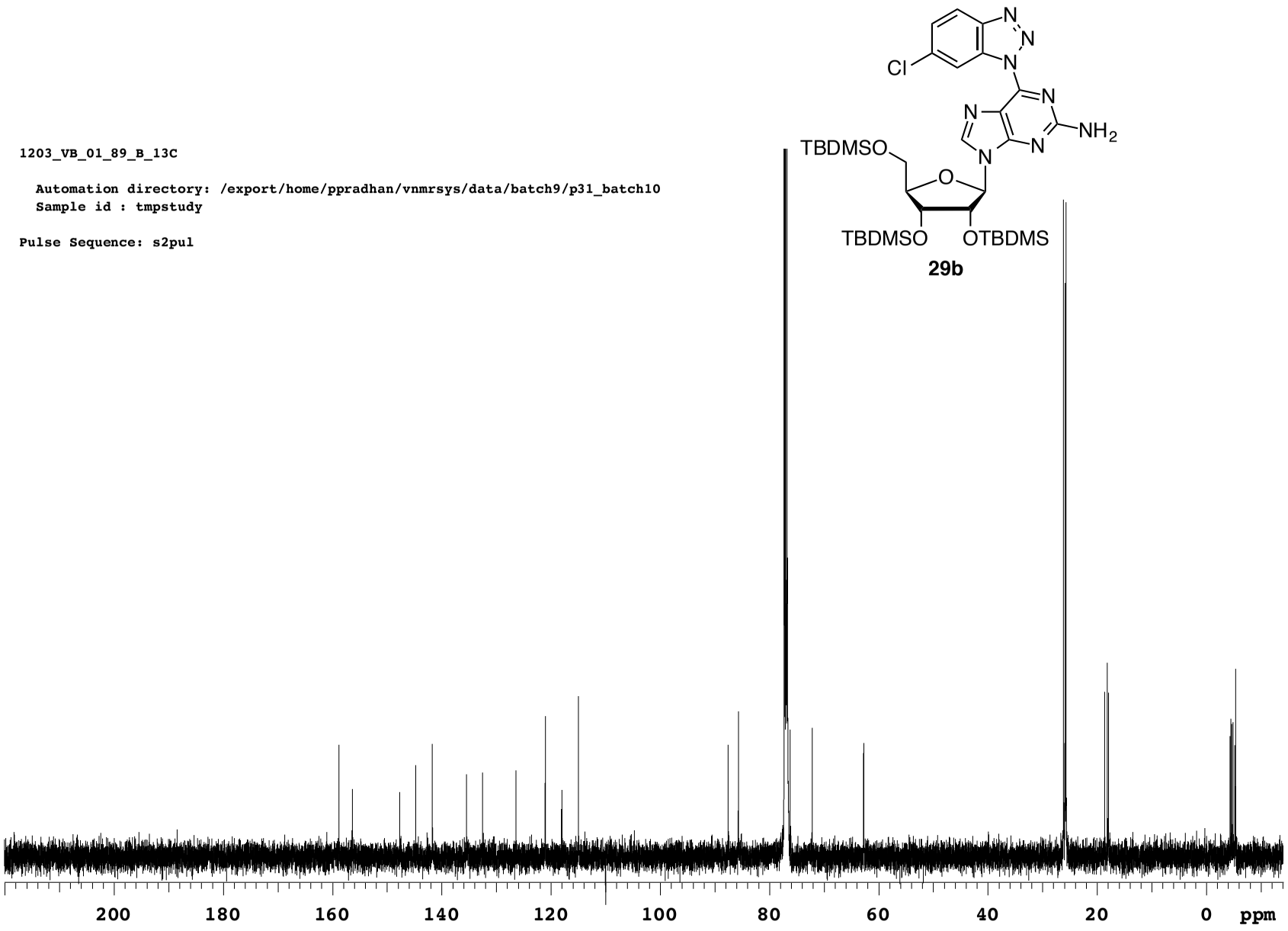
Relax. delay 1.000 sec
Acq. time 0.150 sec
Width 5997.5 Hz
2D Width 5997.5 Hz
64 repetitions
2 x 256 increments
OBSERVE H1, 499.7707221 MHz
DATA PROCESSING
Gauss apodization 0.069 sec
F1 DATA PROCESSING
Gauss apodization 0.031 sec
FT size 2048 x 2048
Total time 10 hr, 49 min, 55 sec

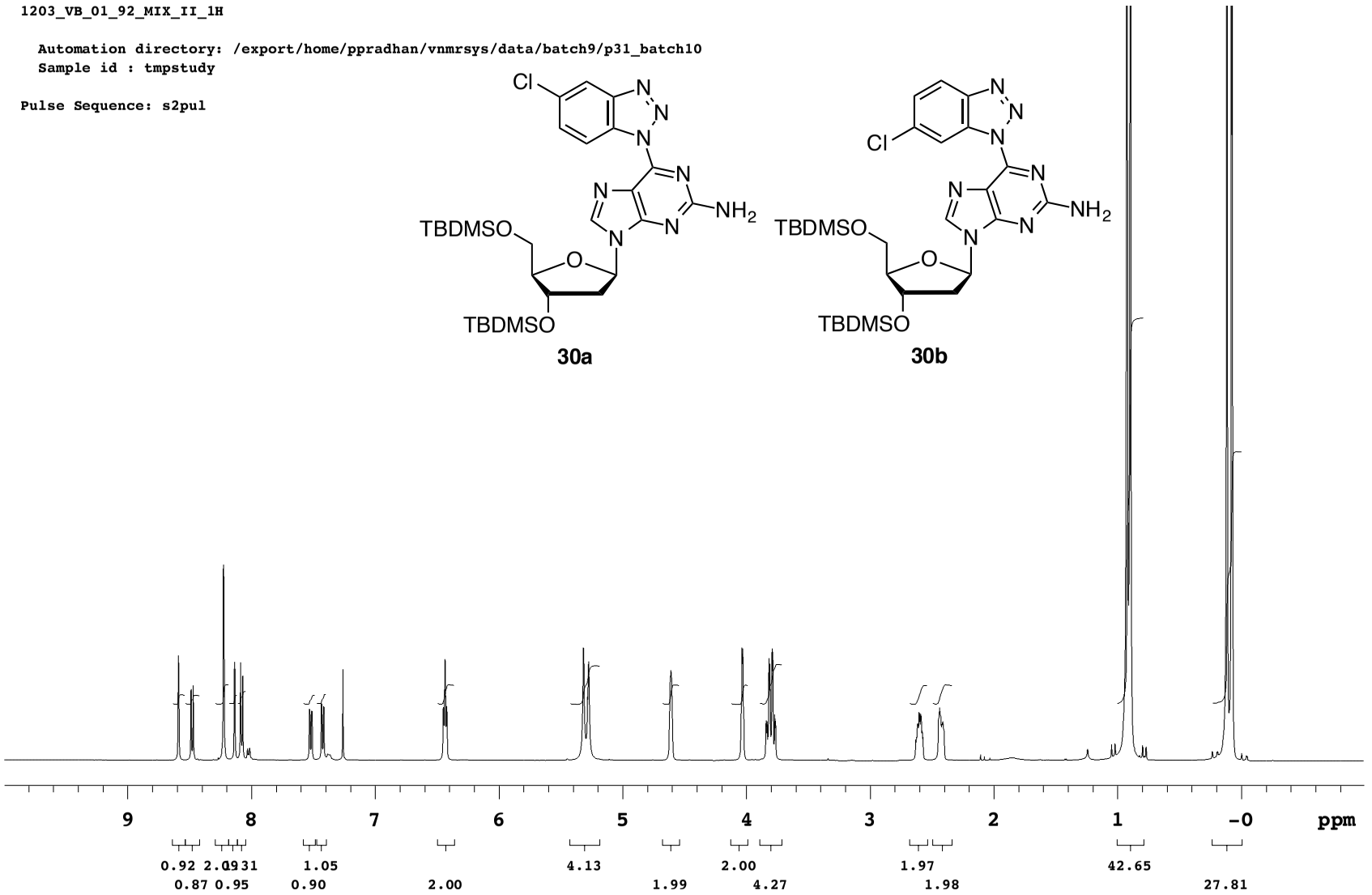


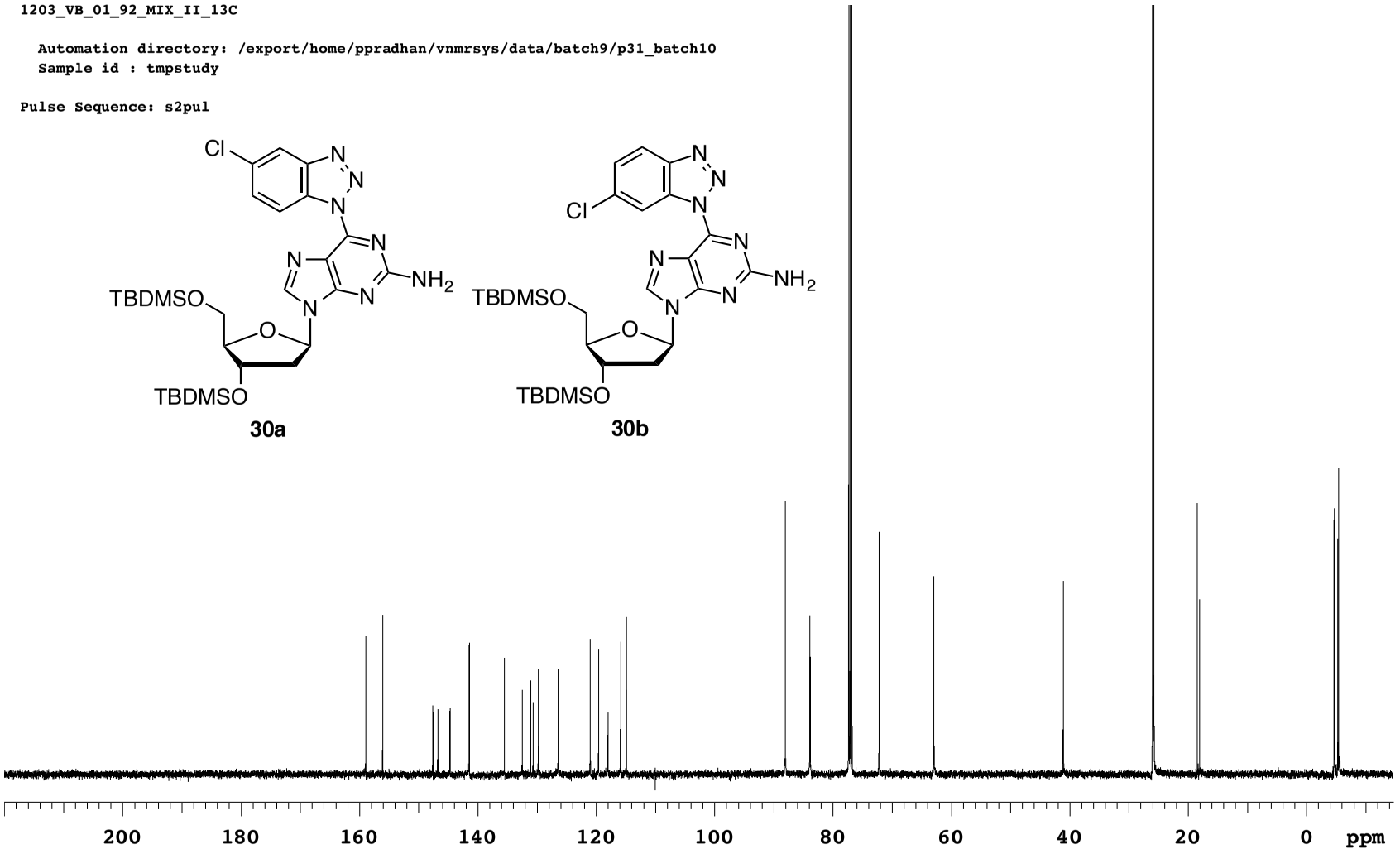
29a

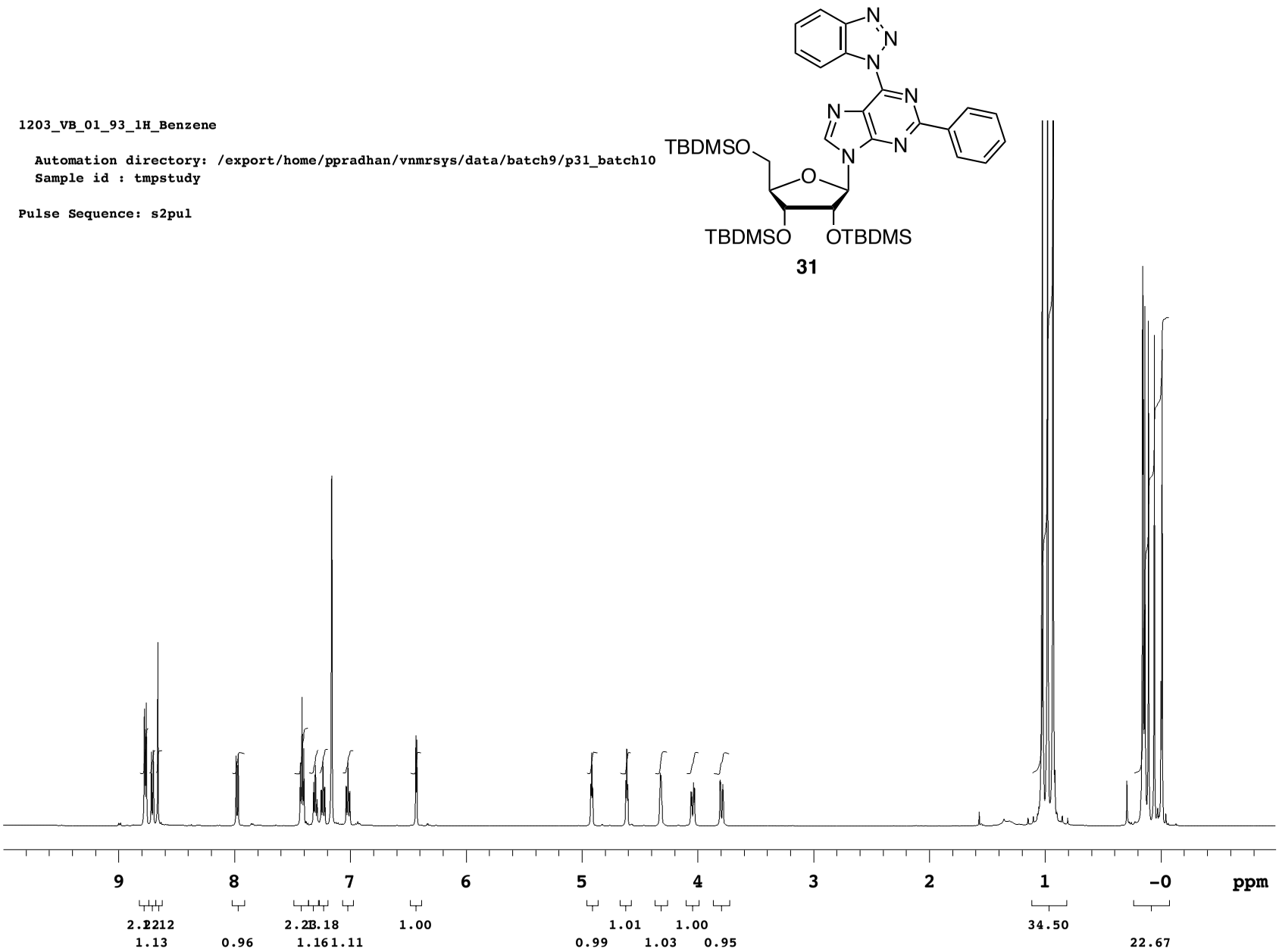


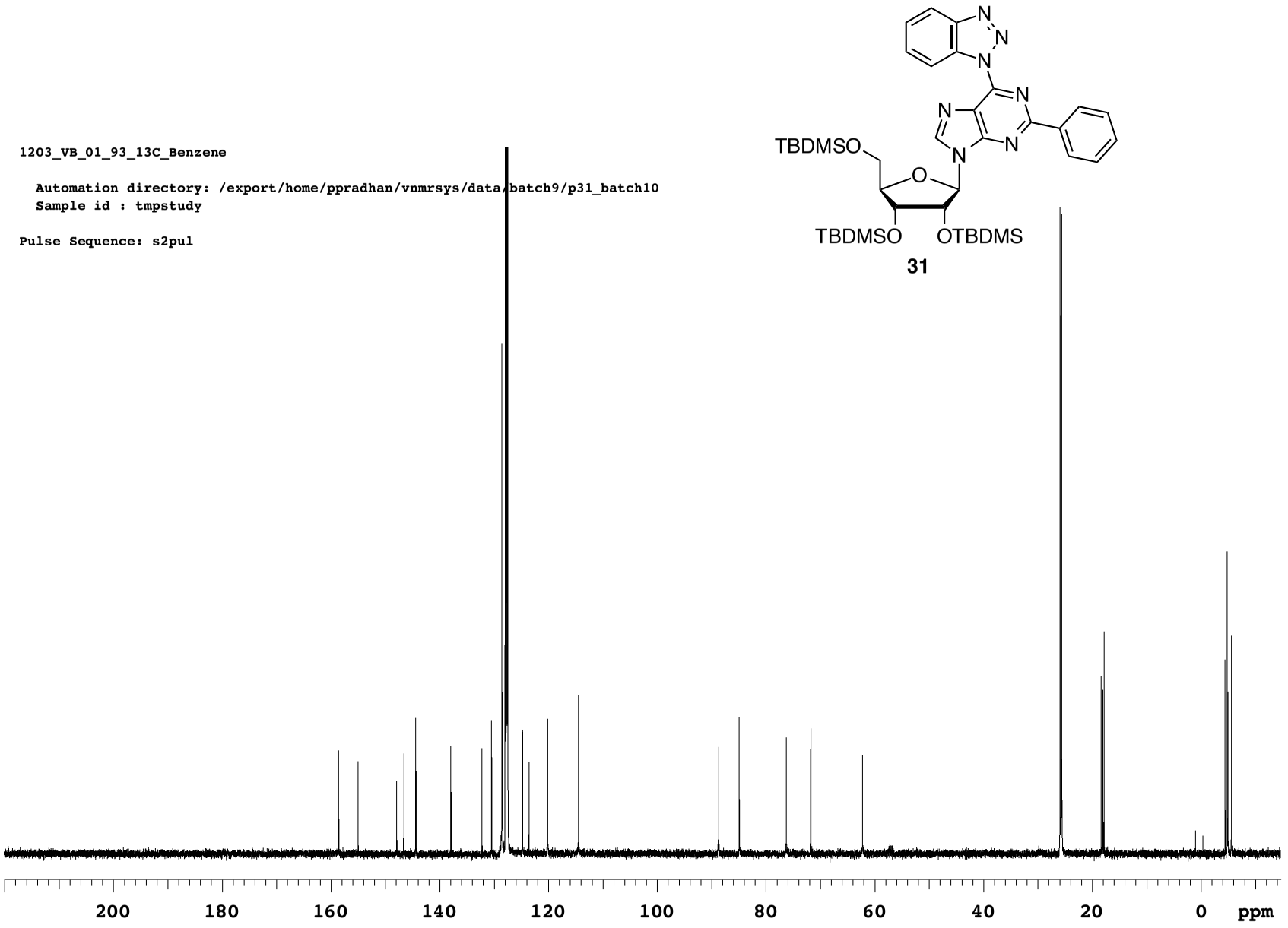

1203_VB_01_89_B_1H_II
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
29b
9
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.04
1.04
1.01
1.00
2.24
1.06
1.20
1.17
1.13
1.19
32.71
13.64
3.14
3.36

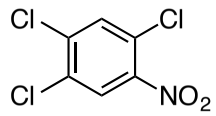

1203_VB_01_89_B_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
OTBDMS
29b
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_01_92_MIX_II_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
30a
30b
9
8
7
6
5
4
3
2
1
-0
ppm
0.92
2.00
0.87
0.95
1.31
0.90
1.05
2.00
4.13
1.99
2.00
4.27
1.97
1.98
42.65
27.81

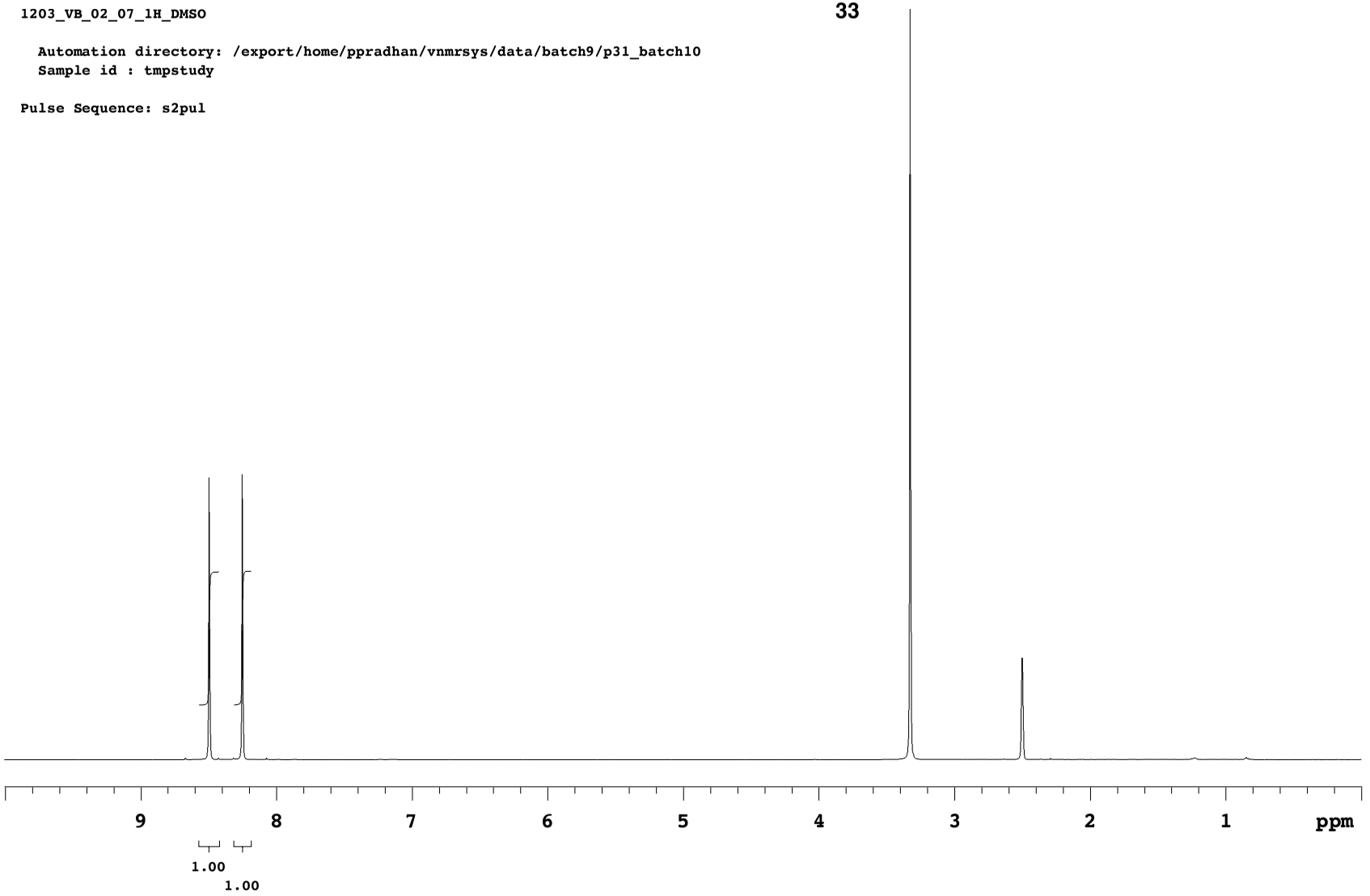

1203_VB_01_92_MIX_II_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
30a
Cl
N
N
N
N
N
N
N
NH2
TBDMSO
O
TBDMSO
30b
200
180
160
140
120
100
80
60
40
20
0
ppm

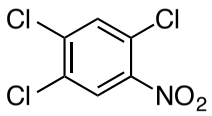

1203_VB_01_93_1H_Benzene
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
31
9
8
7
6
5
4
3
2
1
-0
ppm
2.12
1.13
0.96
2.23
3.18
1.16
1.11
1.00
0.99
1.01
1.03
1.00
0.95
34.50
22.67


1203_VB_01_93_13C_Benzene
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
TBDMSO
TBDMSO
OTBDMS
31
200
180
160
140
120
100
80
60
40
20
0
ppm

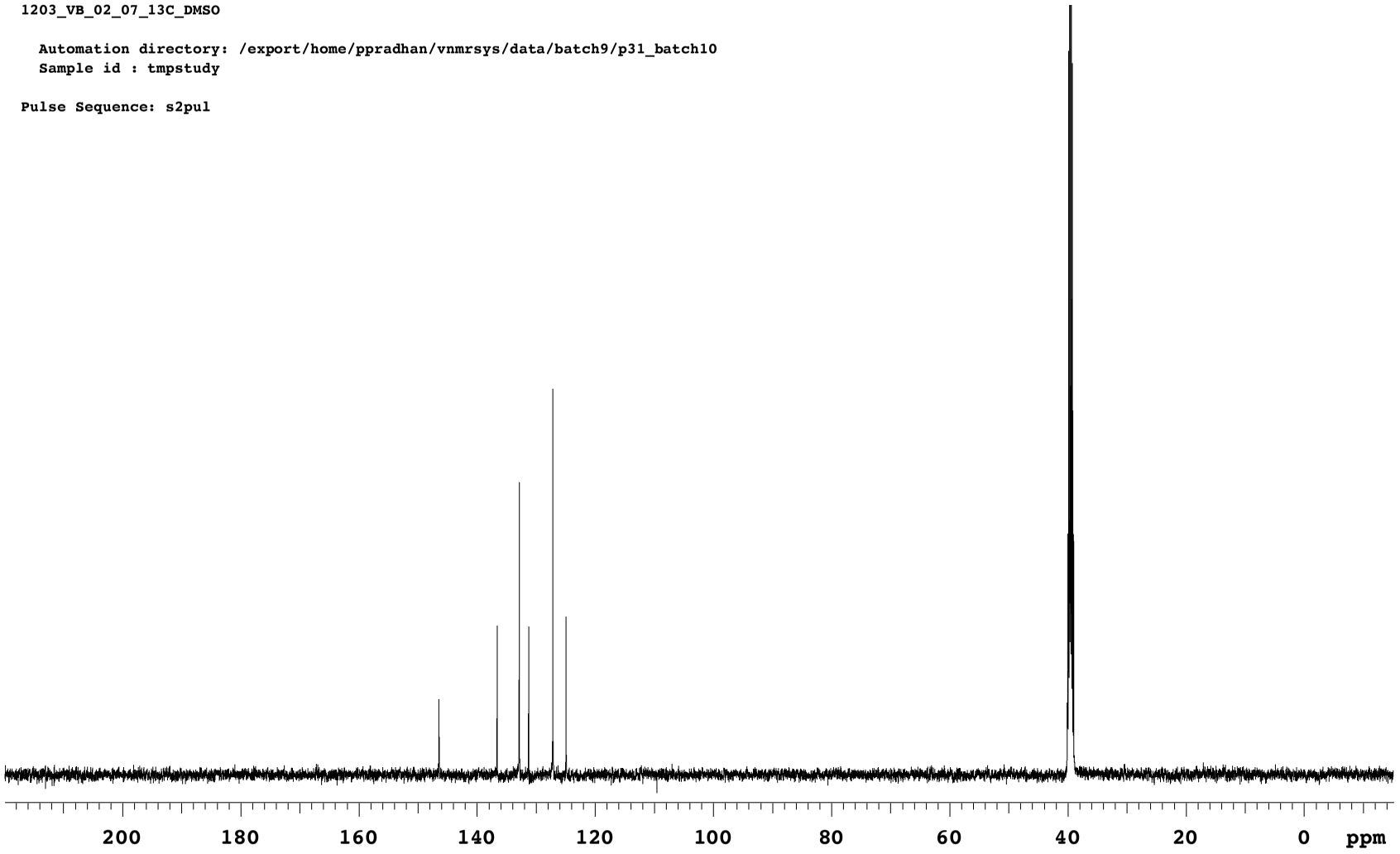

Cl
Cl
Cl
NO2

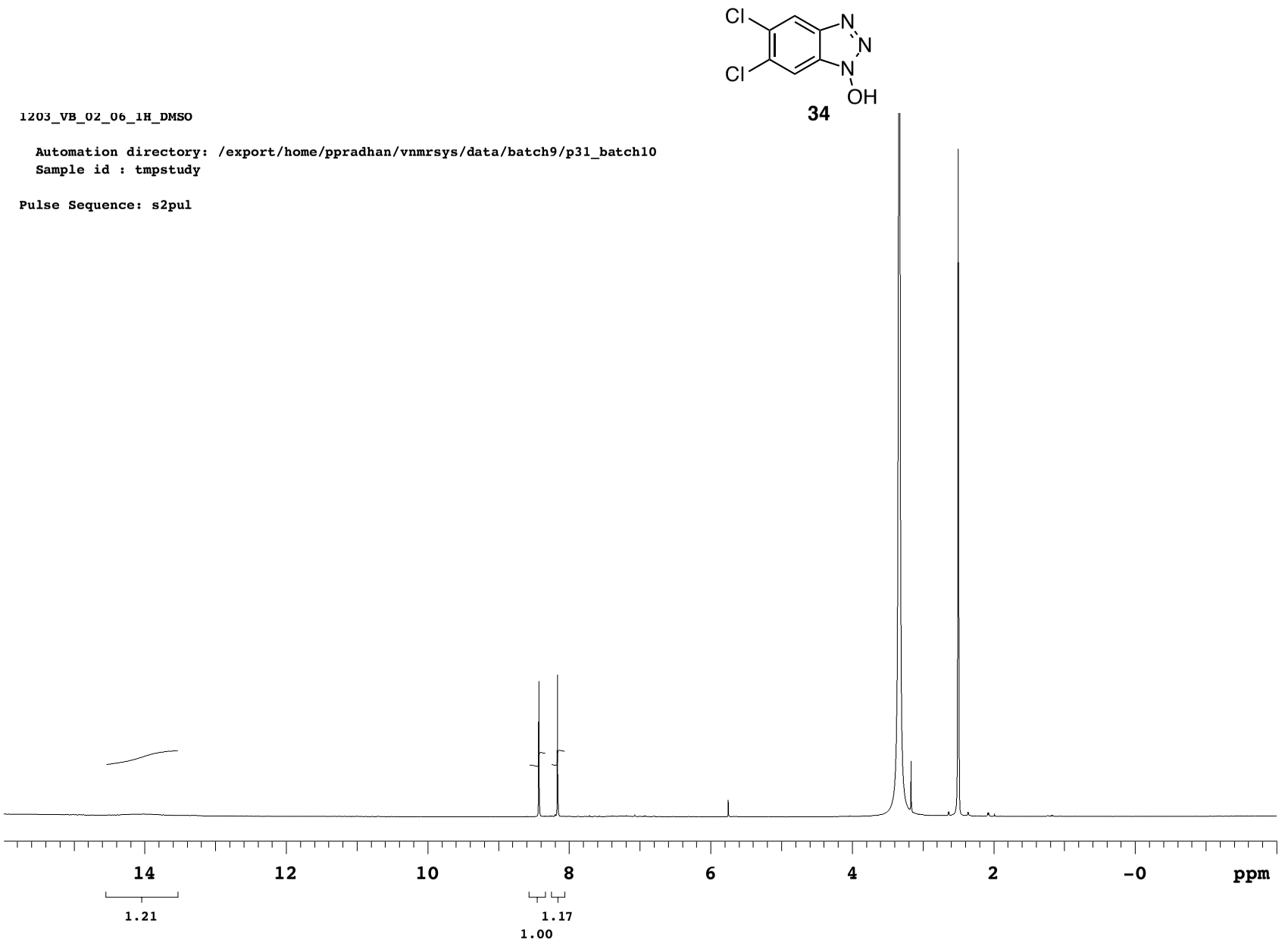
33

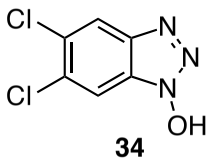

1203_VB_02_07_1H_DMSO
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00


Cl
Cl
Cl
NO2

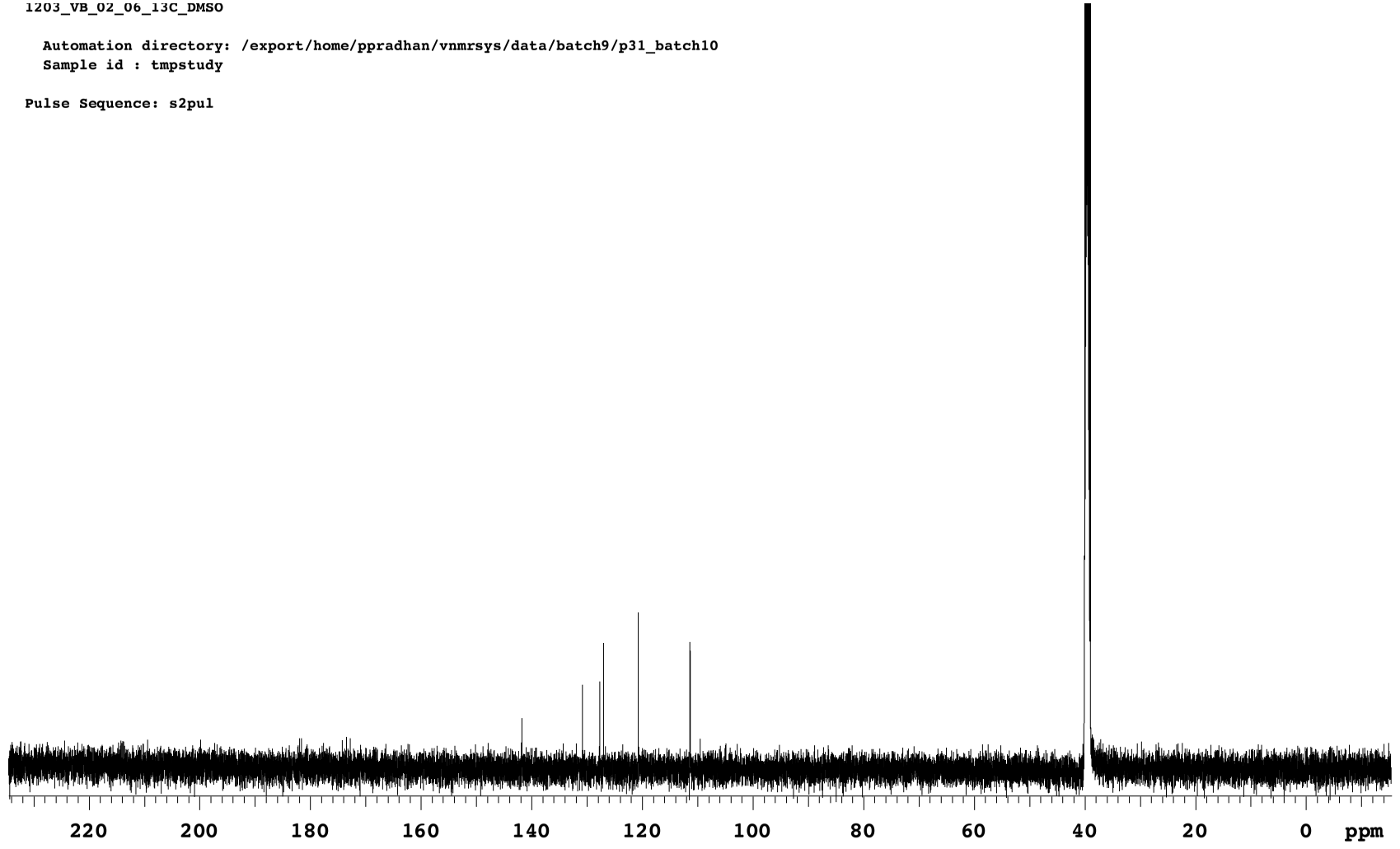
33

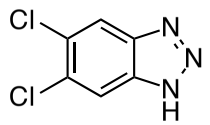

1203_VB_02_07_13C_DMSO
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
200
180
160
140
120
100
80
60
40
20
0
ppm


Cl
Cl
N
N
N
OH
34
1203_VB_02_06_1H_DMSO
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
14
12
10
8
6
4
2
-0
ppm
1.21
1.17
1.00

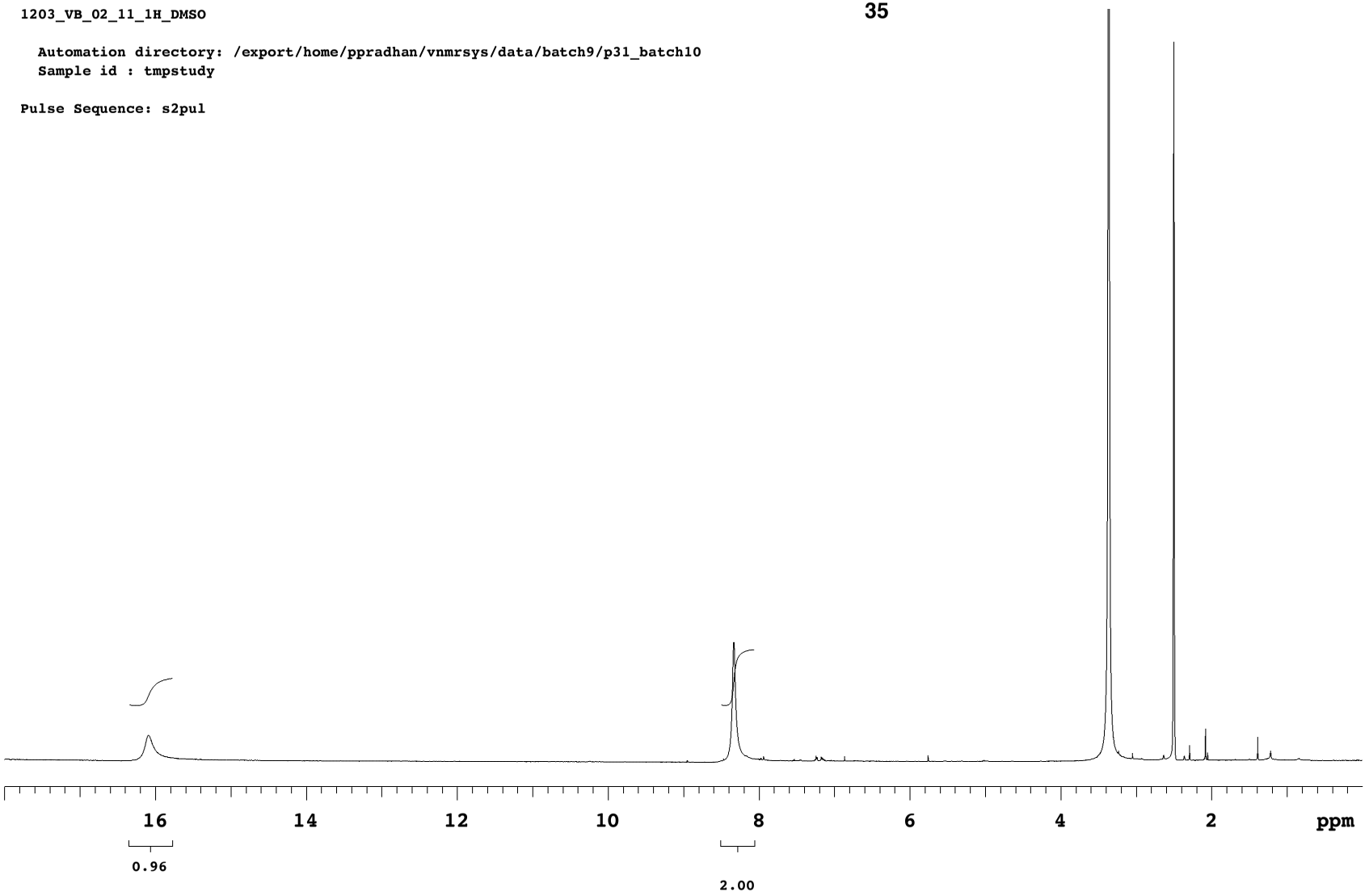

Cl
Cl
N
N
N
OH

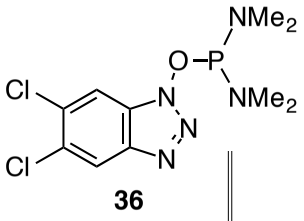
34


1203_VB_02_06_13C_DMSO
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
220
200
180
160
140
120
100
80
60
40
20
0
ppm


Cl
Cl
N
N
N
H

35


1203_VB_02_11_1H_DMSO
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
16
14
12
10
8
6
4
2
ppm
0.96
2.00

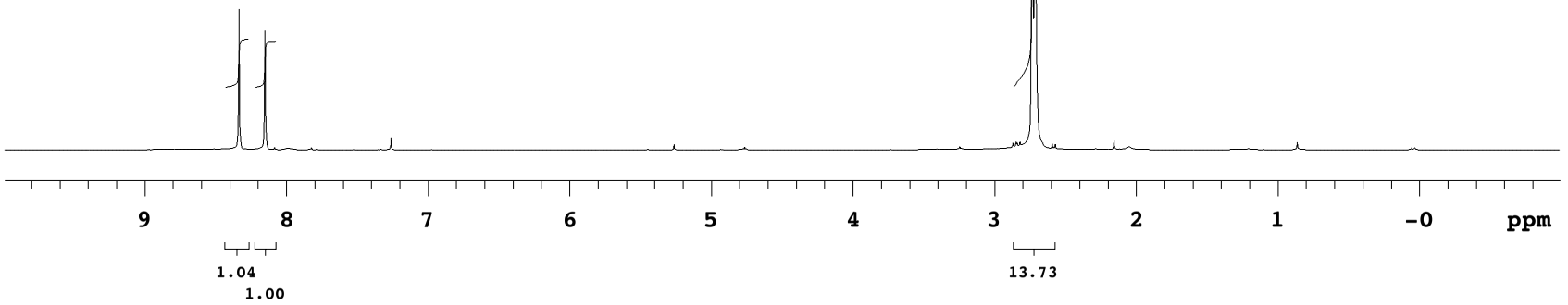


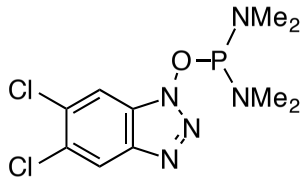
36

1203_VB_02_16_1H

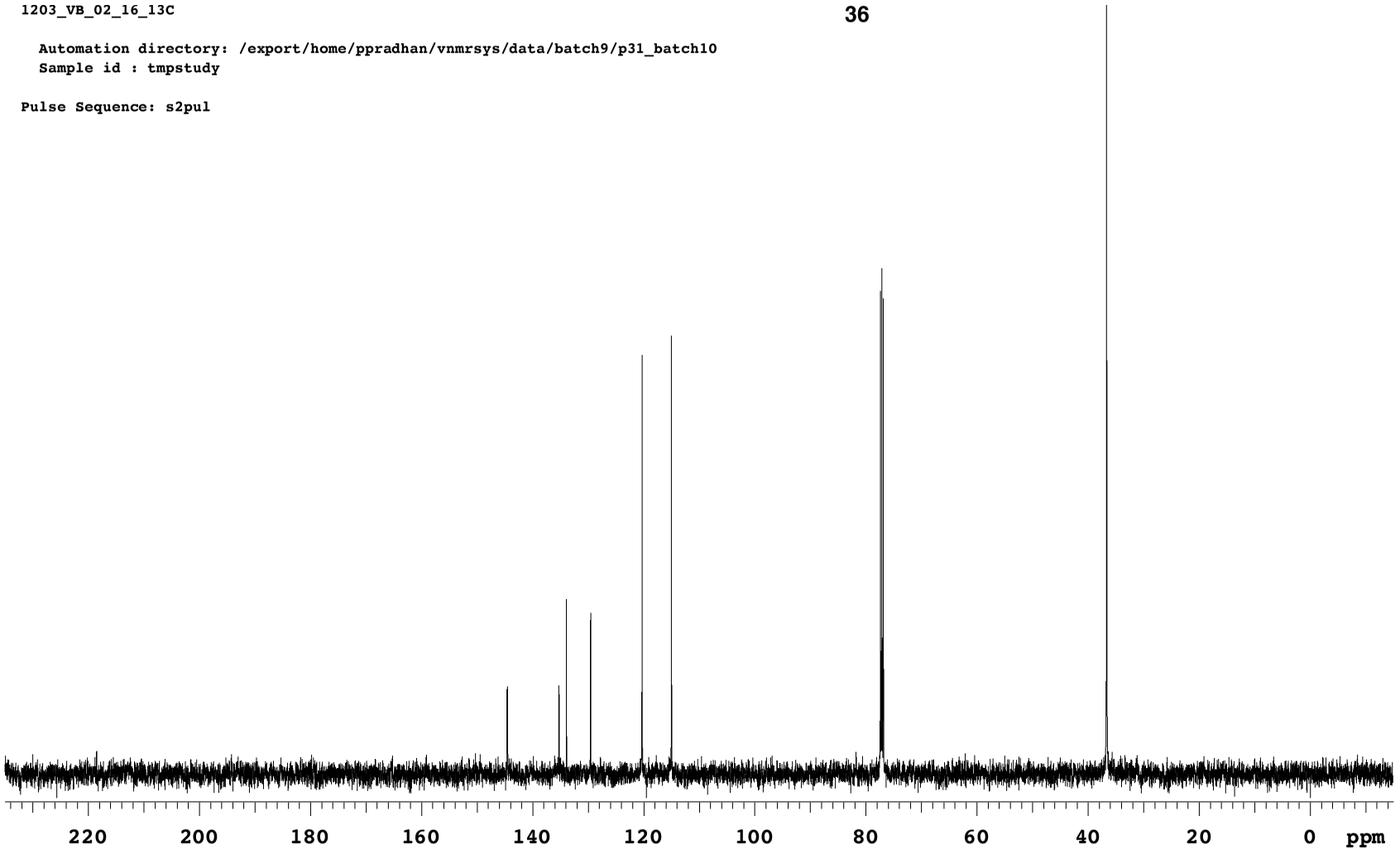
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

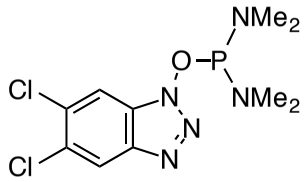
Pulse Sequence: s2pul




NMe2
O
P
NMe2
Cl
N
N
N
Cl

36


1203_VB_02_16_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
220
200
180
160
140
120
100
80
60
40
20
0
ppm

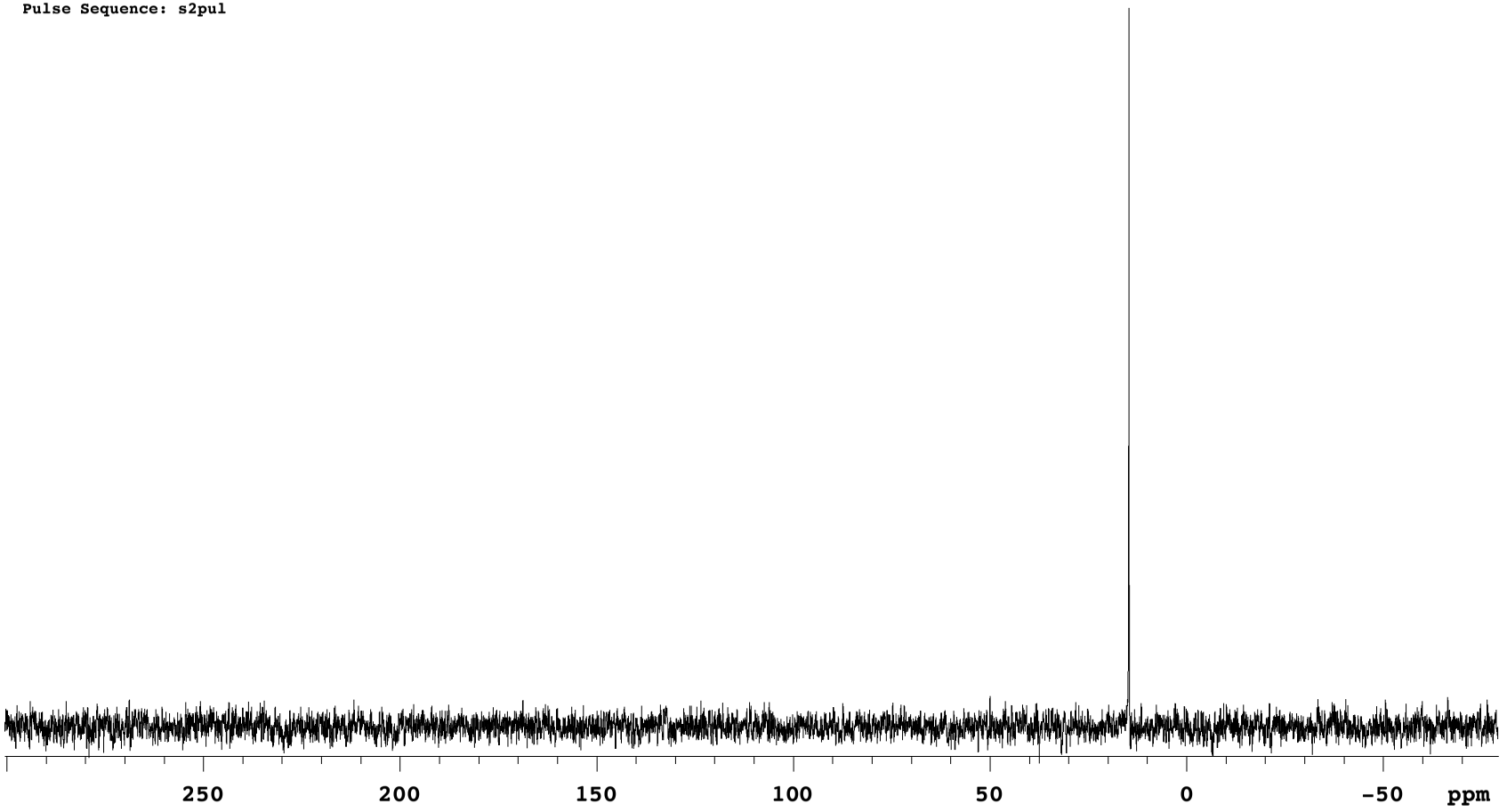


36

1203_VB_02_16_31P

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

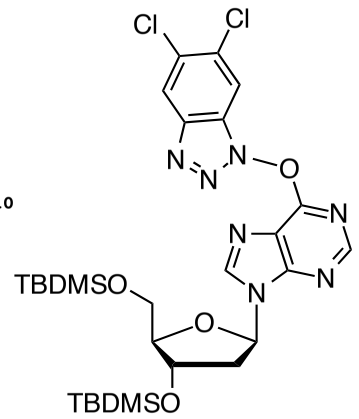
Pulse Sequence: s2pul



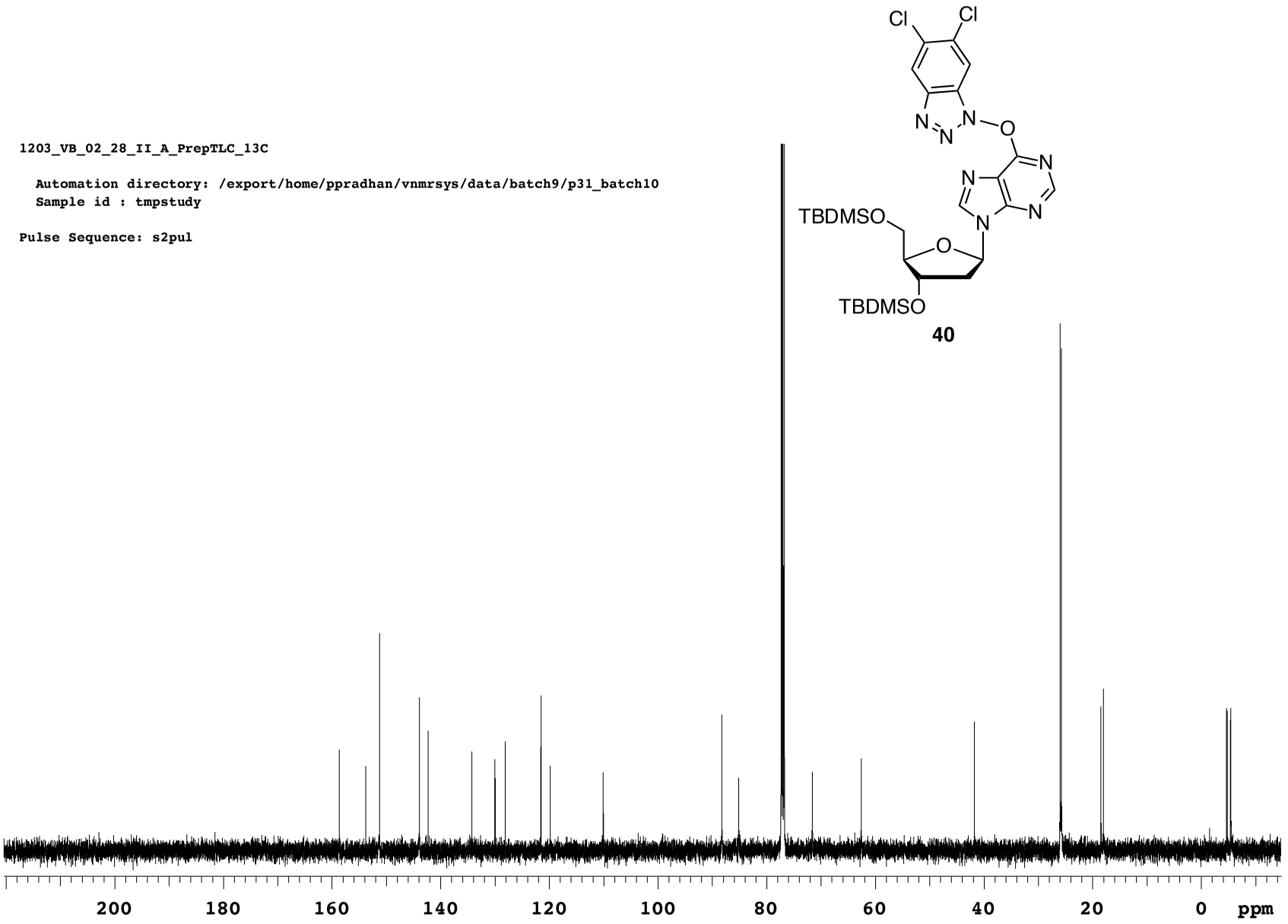
1203_VB_02_28_II_A_PrepTLC_1H

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

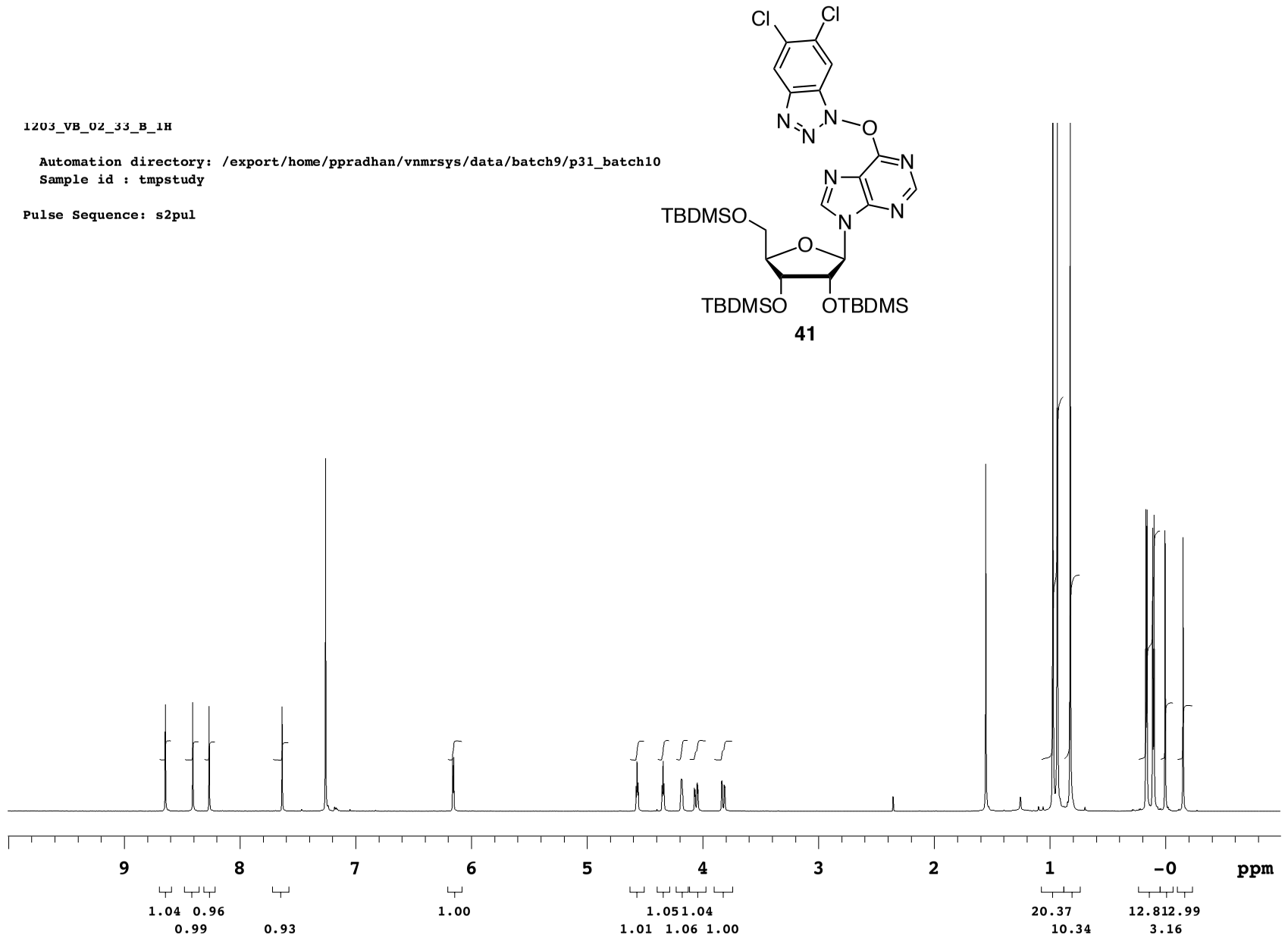
Pulse Sequence: s2pul

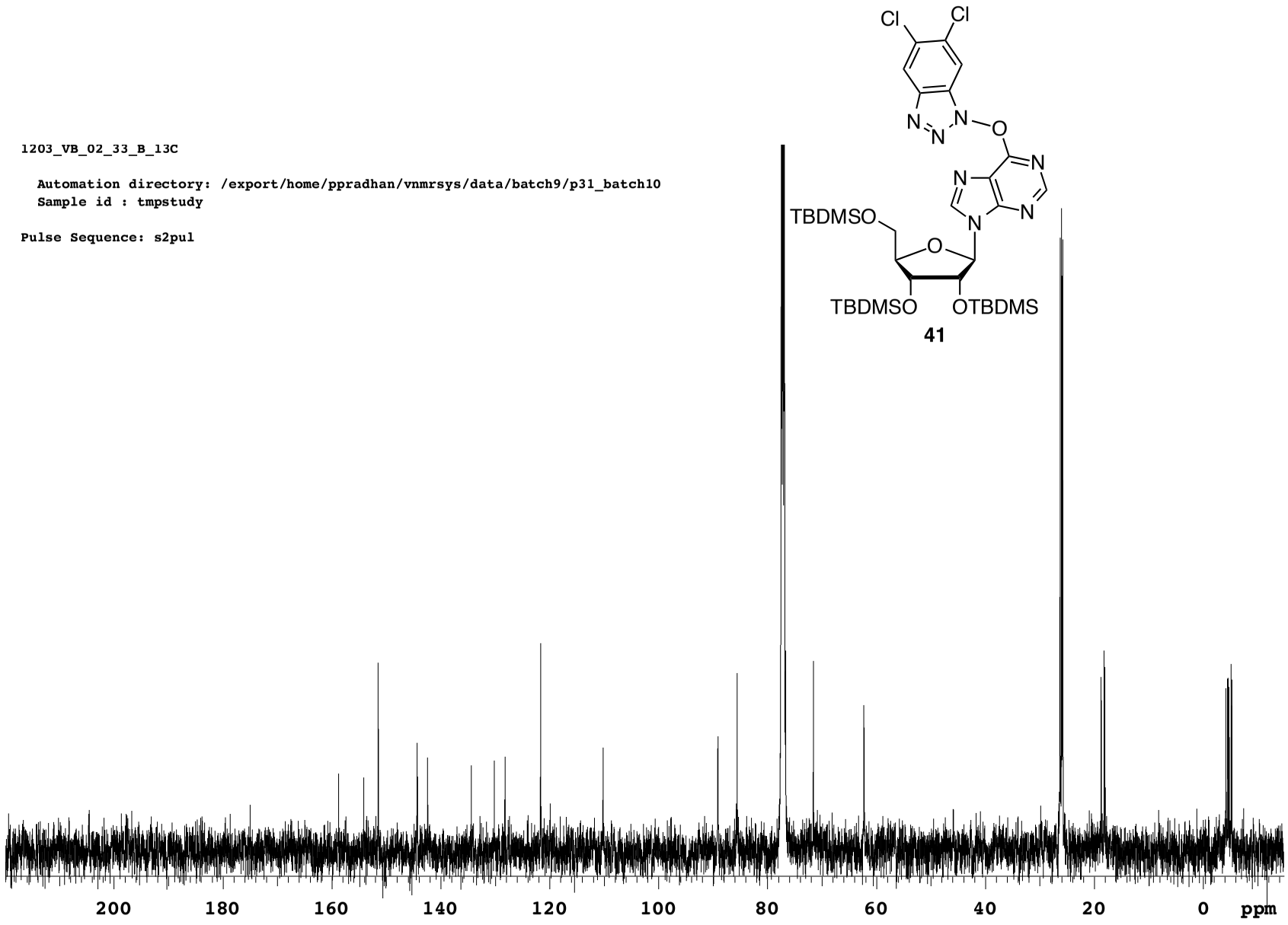


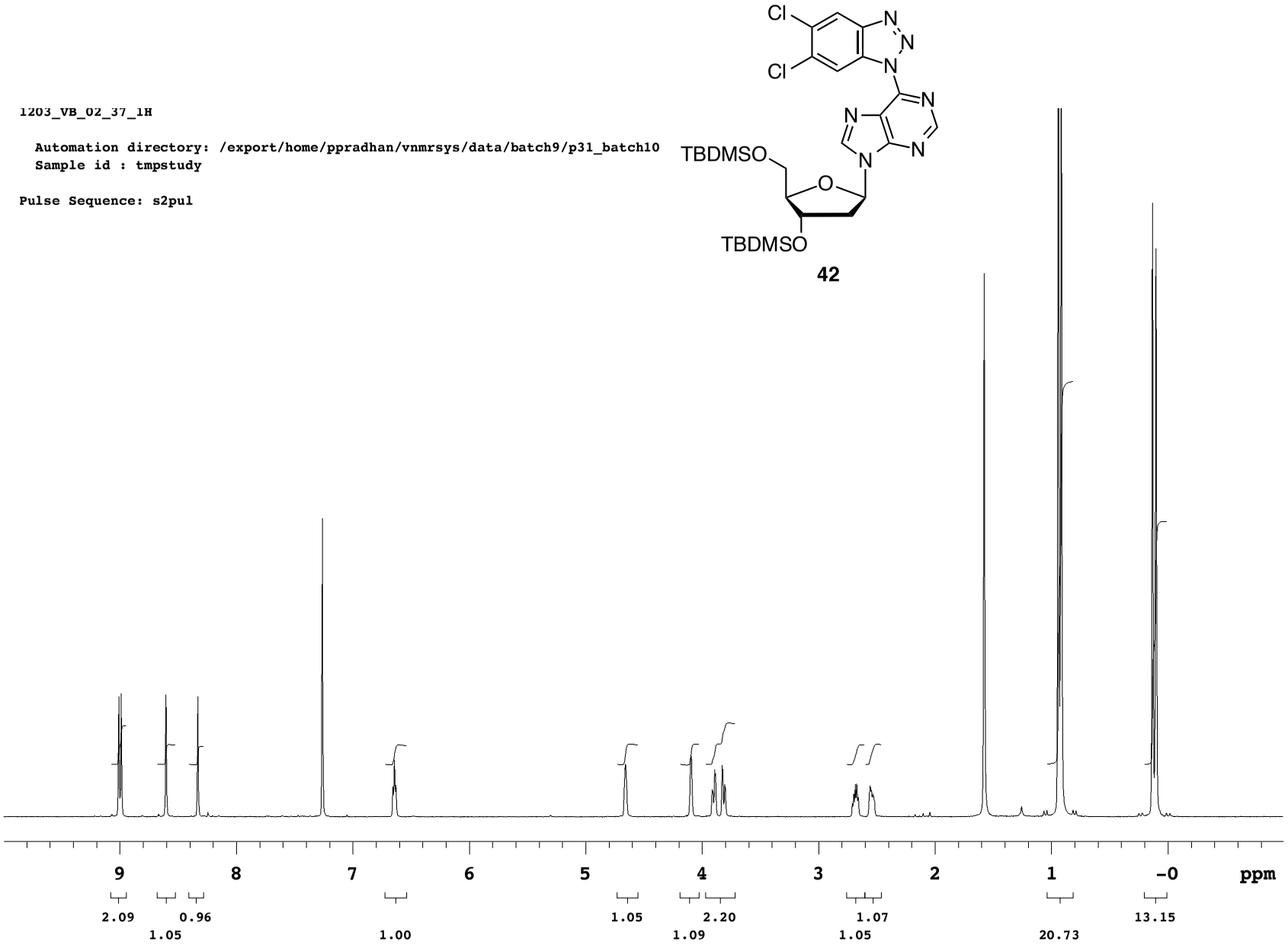
40


1203_VB_02_28_II_A_PrepTLC_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
O
N
N
N
N
N
TBDMSO
O
TBDMSO
200
180
160
140
120
100
80
60
40
20
0
ppm

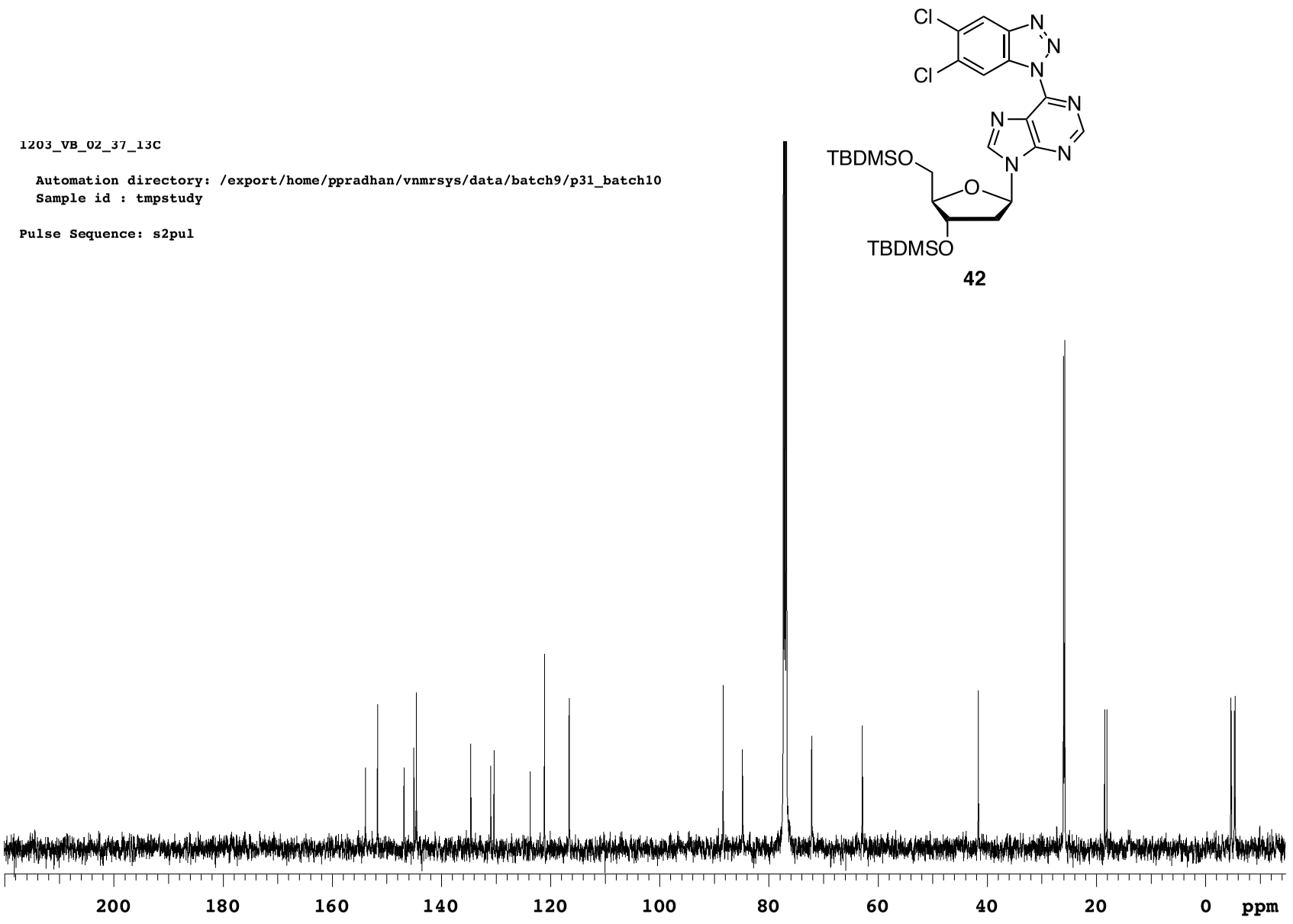
40


1203_VB_02_33_B_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
O
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
41
9
8
7
6
5
4
3
2
1
-0
ppm
1.04 0.96
0.99
0.93
1.00
1.01 1.06 1.00
1.05 1.04
20.37
10.34
12.81 2.99
3.16


1203_VB_02_33_B_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
O
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
41
200
180
160
140
120
100
80
60
40
20
0
ppm


1203_VB_02_37_1H
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
9
8
7
6
5
4
3
2
1
-0
ppm
2.09
0.96
1.05
1.00
1.05
2.20
1.09
1.07
1.05
20.73
13.15

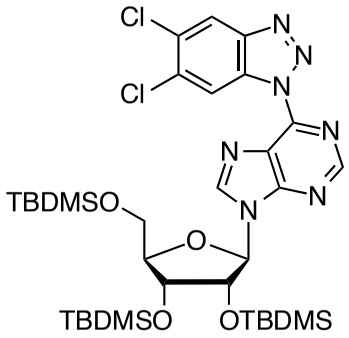
42


1203_VB_02_37_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
42
200
180
160
140
120
100
80
60
40
20
0
ppm

1203_VB_02_39_1H

Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy

Pulse Sequence: s2pul



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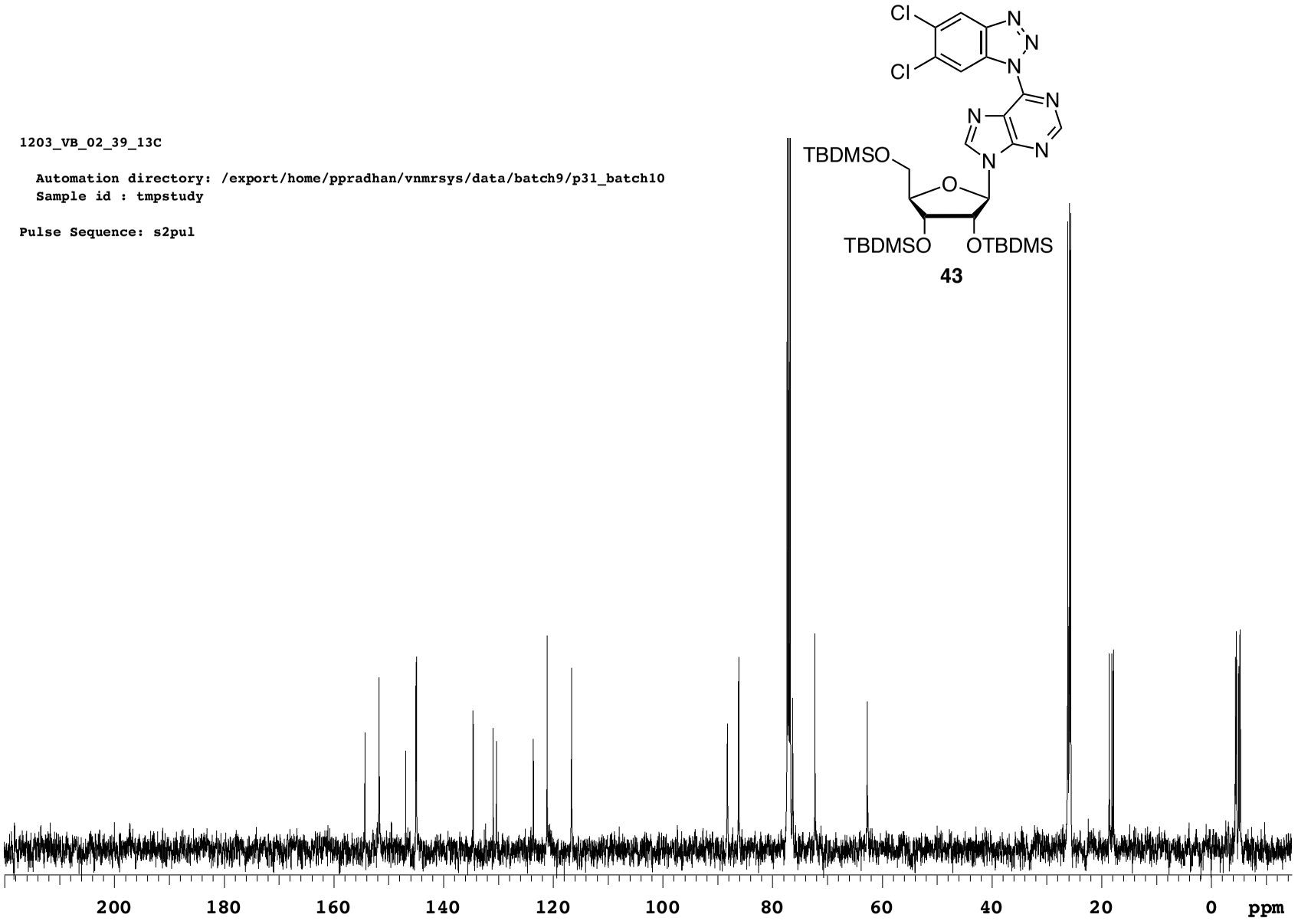
1203_VB_02_39_13C
Automation directory: /export/home/ppradhan/vnmrsys/data/batch9/p31_batch10
Sample id : tmpstudy
Pulse Sequence: s2pul
Cl
Cl
N
N
N
N
N
N
N
TBDMSO
O
TBDMSO
OTBDMS
43
200
180
160
140
120
100
80
60
40
20
0
ppm