Supporting Information for

Reaction Intermediate Analogues as Bisubstrate Inhibitors of Pantothenate Synthetase

HPLC Purity of Inhibitors. HPLC purity was determined for all final target inhibitors **1-5**. For inhibitors **1-5**, two separate reverse-phase HPLC conditions were performed. A Varian Pursuit C18 column (4. 6 × 150 mm, 5μm particle size) with detection at 254 nm and the indicated HPLC conditions (Solvent A = H_2O , Solvent B = MeCN, flow rate = 1 mL/min, Methods A: 0-20 min: gradient 10%-95% B; isocratic 20-30 min: 95% B) as described below was employed to determine the purity of inhibitors. The purity of **1-5** was above 95%.

Spectrum data

7 (colorless oil)：^{1}H NMR (400 MHz, $CDCl_3$) δ 3.90 (s, 1H), 1.02 (s, 9H). ESI-MS calcd. for $C_6H_{11}O_3$ ($[M-H]^-$) 131.1, found 131.4.

8 (colorless oil)：^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (br s, 1H), 3.83 (s, 1H), 0.97 (s, 9H), 0.93 (s, 9H), 0.08 (s, 3H), 0.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ176.6, 80.0, 35.4, 26.0, 25.8, 18.3, -5.2(2 C); MS (ESI–) calcd for $C_{12}H_{25}O_3Si$ $[M-H]^-$ 245.2, found 245.2.

9 (colorless oil)：^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (s, 1H), 2.81 (br, 4H),1.05 (s, 9H), 0.92 (s, 9H), 0.12 (s, 3H), 0.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 168.1, 78.5, 36.0, 25.7 (8 C),

18.2, -5.2, -5.5; MS (ESI–) calcd for $C_{16}H_{29}NO_5Si[M]^-$ 343.2, found 342.8.

11 (a yellow solid): MS (ESI–) calcd for $C_{25}H_{41}N_6O_8SSi$ $[M–H]^-$ 613.2, found 613.6.

1 (a white solid): ^{1}H NMR (400 MHz, CD_3OD) δ 8.57 (s, 1H), 8.33 (s, 1H), 6.38 (s, 1H), 5.05 – 5.00 (m, 1H), 4.79 – 4.77 (m, 1H), 4.74 – 4.70 (m, 1H), 4.40 – 4.37 (m, 1H), 4.14 – 4.10 (m, 1H), 3.62 (s, 1H), 0.99 (s, 9H); ^{13}C NMR (100MHz, CD_3OD) δ 179.0, 158.7, 150.3, 140.9, 140.6, 121.2, 95.3, 85.2, 80.3, 77.2, 71.7, 59.7, 36.1, 26.5; MS (ESI–) calcd for $C_{16}H_{23}N_6O_8S$ $[M–H]^-$ 459.1, found 459.2. HRMS (ESI–) calcd for $C_{16}H_{23}N_6O_8S$ $[M–H]^-$ 459.1304, found 459.1310.

13 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.03 (s, 1H), 6.48 (d, J = 3.6 Hz, 1H), 5.59 (s, 2H), 4.34 – 4.32 (m, 1H), 4.19 – 4.16 (m, 1H), 4.03 – 3.98 (m, 1H), 3.88 – 3.84 (m, 2H), 0.94 (s, 9H), 0.92 (s, 9H), 0.72 (s, 9H), 0.15 (s, 6H), 0.09 (s, 3H), 0.08 (s, 3H), -0.08 (s, 3H), -0.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.5, 153.0, 149.6, 140.8, 119.3, 86.5, 85.9, 78.3, 77.6, 63.0, 26.1, 25.9, 25.7, 18.5, 18.1, 17.9, -4.4, -5.2, -5.5; MS (ESI+) calcd for $C_{28}H_{56}N_5O_4Si_3[M+H]^+$ 610.4, found 610.0.

14 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.05 (s, 1H), 6.44 (d, J = 4.0 Hz, 1H), 5.83 (s, 2H), 4.38 – 4.34 (m, 1H), 4.31 – 4.27 (m, 1H), 4.13 (s, 1H), 4.08 – 4.04 (m, 1H), 3.92 – 3.88 (m, 2H), 0.94 (s, 9H), 0.67 (s, 9H), 0.16 (s, 6H), -0.06 (s, 3H), -0.41 (s, 3H); ^{13}C NMR (75 MHz, CD_3OD) δ 156.8, 153.6, 149.7, 141.9, 119.5, 88.0, 87.1, 79.1, 78.4, 62.6, 26.2, 26.0, 18.6, 18.3, -4.2, -4.4, -4.8, -5.4; MS (ESI+) calcd for $C_{22}H_{42}N_5O_4Si_2$ $[M+H]^+$ 496.3, found 496.0.

15 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 2H), 6.48 (d, J = 3.2 Hz, 1H), 4.48 (dd, J = 10.4, 7.2 Hz, 1H), 4.40 – 4.24 (m, 4H), 0.98 (s, 9H), 0.72 (s, 9H), 0.22 (s, 6H), -0.02 (s, 3H), -0.43 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 155.9, 152.7, 149.1, 139.8, 118.3, 84.2, 81.9, 77.3, 76.5, 68.1, 25.7, 25.4, 17.6, 17.3, -4.6, -4.7, -5.4, -5.8; MS (ESI+) calcd for $C_{22}H_{43}N_6O_6SSi_2$ $[M+H]^+$ 575.2, found 574.8.

16(a yellow solid): ESI-MS calcd. for $C_{34}H_{65}N_6O_8SSi_3$ ($[M-H]^-$) 801.4, found 801.5.

2 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.19 (s, 1H), 6.38 (d, *J* = 5.2 Hz, 1H), 5.01 (d, *J* = 13.6 Hz, 1H), 4.74 (d, *J* = 2.4 Hz, 1H), 4.68 (dd, *J* = 16.0, 2.4 Hz, 1H), 4.52 (t, *J* = 5.2 Hz, 1H), 3.95 (t, *J* = 5.2 Hz, 1H), 3.64 (s, 1H), 1.00 (s, 9H); ^{13}C NMR (100 MHz, CD_3OD) δ 179.6, 158.7, 150.1, 142.2, 141.5, 121.3, 91.8, 85.7, 81.3, 80.2, 76.9, 59.8, 36.2, 26.5;MS (ESI–) calcd for $C_{16}H_{23}N_6O_8S$ $[M–H]^-$ 459.1, found 459.2. HRMS (ESI–) calcd for $C_{16}H_{23}N_6O_8S$ $[M–H]^-$ 459.1304, found 459.1318.

17 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.27 (s, 1H), 6.33 (d, *J* = 2.4 Hz, 1H), 5.65 (s, 2H), 4.88 (d, *J* = 10.0 Hz, 1H), 4.37 – 4.34 (m, 1H), 4.14 (d, *J* = 10.0 Hz, 1H), 4.07 (s, 1H), 3.96 (d, *J* = 11.2 Hz, 1H), 3.81 (d, *J* = 11.2 Hz, 1H), 0.93 (s, 9H), 0.93 (s, 9H), 0.15 (s, 6H), 0.14 (s, 6H); MS (ESI+) calcd for $C_{22}H_{42}N_5O_4Si_2$ $[M+H]^+$ 496.3, found 496.4.

18 (a white solid): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.16 (s, 1H), 6.25 (dd, *J* = 15.6, 1.6 Hz, 1H), 6.05 (s, 2H), 5.32 (dd, *J* = 52.8, 1.6 Hz, 1H), 4.73 – 4.64 (m, 1H), 4.16 – 4.12 (m, 1H), 4.02 (dd, *J* = 12.0, 2.4 Hz, 1H), 3.79 (dd, *J* = 12.0, 2.4 Hz, 1H), 0.93 (s, 9H), 0.89 (s, 9H), 0.14 (s, 3H), 0.13 (s, 3H), 0.08 (s, 3H), 0.06 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.8, 153.3, 149.4, 139.3, 120.1, 93.0 (d, *J* = 191.3 Hz), 87.0 (d, *J* = 33.0 Hz), 84.0, 69.4 (d, *J* = 15.8 Hz), 61.3, 26.0, 25.8, 18.5, 18.2, -4.6, -4.9, -5.3, -5.4; MS (ESI+) calcd for $C_{22}H_{41}FN_5O_3Si_2$ $[M+H]^+$ 498.3, found 498.3.

19 (a white solid): ^{1}H NMR (400 MHz, CD_3OD) δ 8.37 (s, 1H), 8.19 (s, 1H), 6.27 (dd, *J* = 15.2, 4.0 Hz, 1H), 5.51 (dt, *J* = 52.8, 4.0 Hz, 1H), 4.79 – 4.72 (m, 1H), 4.15 (d, *J* = 2.0 Hz, 1H), 3.90 (d, *J* = 12.4 Hz, 1H), 3.71 (dd, *J* = 12.8, 2.4 Hz, 1H), 0.96 (s, 9H), 0.18 (s, 3H), 0.17 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 156.2, 152.6, 148.8, 139.6, 119.2, 92.3 (d, *J* = 189.0 Hz), 85.7 (d, *J* = 32.3 Hz), 84.7, 70.0 (d, *J* = 15.0 Hz), 60.3, 25.6, 17.9, -4.9, -5.1;MS (ESI+) calcd for $C_{16}H_{27}FN_5O_3Si[M+H]^+$ 384.2, found 384.2.

20 (a white solid): ^{1}H NMR (300 MHz, CD_3OD) ^{1}H NMR (300 MHz, CD_3OD) δ 8.26 (s, 1H), 8.21 (s, 1H), 6.31 (dd, *J* = 17.1, 2.7 Hz, 1H), 5.53 (ddd, *J* = 52.5, 4.5, 2.7 Hz, 1H), 4.94 – 4.91 (m,

1H), 4.46 – 4.40 (m, 1H), 4.32 – 4.26 (m, 2H), 0.97 (s, 9H), 0.21 (s, 1H), 0.19 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 156.2, 152.8, 148.8, 139.7 , 119.1, 92.2 (d, J = 187.5 Hz), 86.1 (d, J = 33.8 Hz), 80.3, 70.2 (d, J = 15.0 Hz), 67.7, 25.6, 17.8, -4.9, -5.1; MS (ESI+) calcd for $C_{16}H_{28}FN_6O_5SSi[M+H]^+$ 463.2, found 463.2.

21 (a yellow solid): ESI-MS calcd. for $C_{28}H_{50}FN_6O_7SSi_2$ ([M-H]$^-$) 689.3, found 689.3.

3 (a white solid): ^{1}H NMR (400 MHz, CD_3OD) δ 8.56 (s, 1H), 8.30 (s, 1H), 6.68 (d, J = 6.8 Hz, 1H), 4.97 (dd, J = 51.6, 4.4 Hz, 1H), 4.86 – 4.82 (m, 2H), 4.76 (dd, J = 14.0, 2.8 Hz, 1H), 4.50 (dt, J = 18.8, 4.4 Hz, 1H), 3.63 (s, 1H), 0.98 (s, 9H)); ^{13}C NMR (100 MHz, CD_3OD) δ 179.1, 158.7, 150.4, 141.0, 140.5, 121.3, 94.3 (d, J = 192.0 Hz), 92.4 (d, J = 31.0 Hz), 84.8, 80.2 (d, J = 7.0 Hz), 71.5 (d, J = 16.0 Hz), 59.5, 36.2, 26.5; HRMS (ESI–) calcd for $C_{16}H_{22}FN_6O_7S[M–H]^-$ 461.1260, found 461.1280 (error 4.3 ppm).

23 (a yellow solid): MS (ESI–) calcd for $C_{26}H_{43}N_6O_7SSi[M–H]^-$ 611.3, found 611.8.

4 (a white solid): ^{1}H NMR (400 MHz, CD_3OD) δ 8.56 (s, 1H), 8.27 (s, 1H), 5.04 (d, J = 4.8 Hz, 1H), 4.93 (dd, J = 13.6, 3.6 Hz, 1H), 4.55 (dd, J = 13.6, 2.8 Hz, 1H), 4.11 – 4.07 (m, 1H), 4.02 (d, J = 4.8 Hz, 1H), 3.69 (s, 1H), 3.05 – 2.96 (m, 1H), 2.80 (d, J = 10.0 Hz, 1H), 2.04 (d, J = 14.4 Hz, 1H), 1.00 (s, 9H); ^{13}C NMR (100 MHz, CD_3OD) δ 179.1, 158.6, 150.5, 143.5, 141.2, 121.7, 80.3, 77.5, 74.4, 67.4, 60.6, 44.0, 36.1, 33.5, 26.5; MS (ESI–) calcd for $C_{17}H_{25}N_6O_7S[M–H]^-$ 457.2, found 457.3. HRMS (ESI–) calcd for $C_{17}H_{25}N_6O_7S$ $[M–H]^-$ 457.1511, found 457.1510.

26 (a white solid)：^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 6.8 Hz, 2H), 7.43–7.33 (m, 3H), 5.51 (s, 1H), 3.69–3.60(m, 5H), 1.14 (s, 3H), 0.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 129.2, 128.4, 126.4, 102.2, 86.0, 79.0, 61.6, 31.7, 21.5, 19.3. MS (ESI+) calcd for $C_{13}H_{19}O_3$ $[M+H]^+$ 223.1, found 223.0.

27 (a white solid)：^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 2H), 7.48 – 7.34 (m, 5H), 7.27 (d, J = 8.0 Hz, 2H), 5.43 (s, 1H), 4.28 (dd, J = 10.8, 2.0 Hz, 1H), 4.11 – 4.03 (m, 1H), 3.91 –

3.85 (m, 1H), 3.65 (dd, *J* = 30.0, 11.2 Hz, 2H), 2.43 (s, 3H), 1.10 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 138.0, 132.9, 129.8, 129.0, 128.2, 128.0, 126.2, 101.6, 82.5, 78.5, 69.5, 31.8, 21.7, 21.4, 18.8; MS (ESI+) calcd for $C_{20}H_{24}O_5SNa$ $[M+Na]^+$ 399.1, found 399.0.

28 (a white solid)：^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 6.8 Hz, 2H), 7.43 – 7.32 (m, 3H), 5.58 (s, 1H), 3.81 (d, *J* = 9.2 Hz, 1H), 3.74 (d, *J* = 11.2 Hz, 1H), 3.65 (d, *J* = 11.2 Hz, 1H), 3.46 (dd, *J* = 12.8, 9.2 Hz, 1H), 3.20 (d, *J* = 13.2 Hz, 1H), 1.16 (s, 3H), 0.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 128.9, 128.3, 126.1, 101.7, 84.7, 78.8, 50.7, 32.3, 21.5, 18.9; MS (ESI+) calcd for $C_{13}H_{17}N_3O_2Na$ $[M+Na]^+$ 270.1, found 270.0.

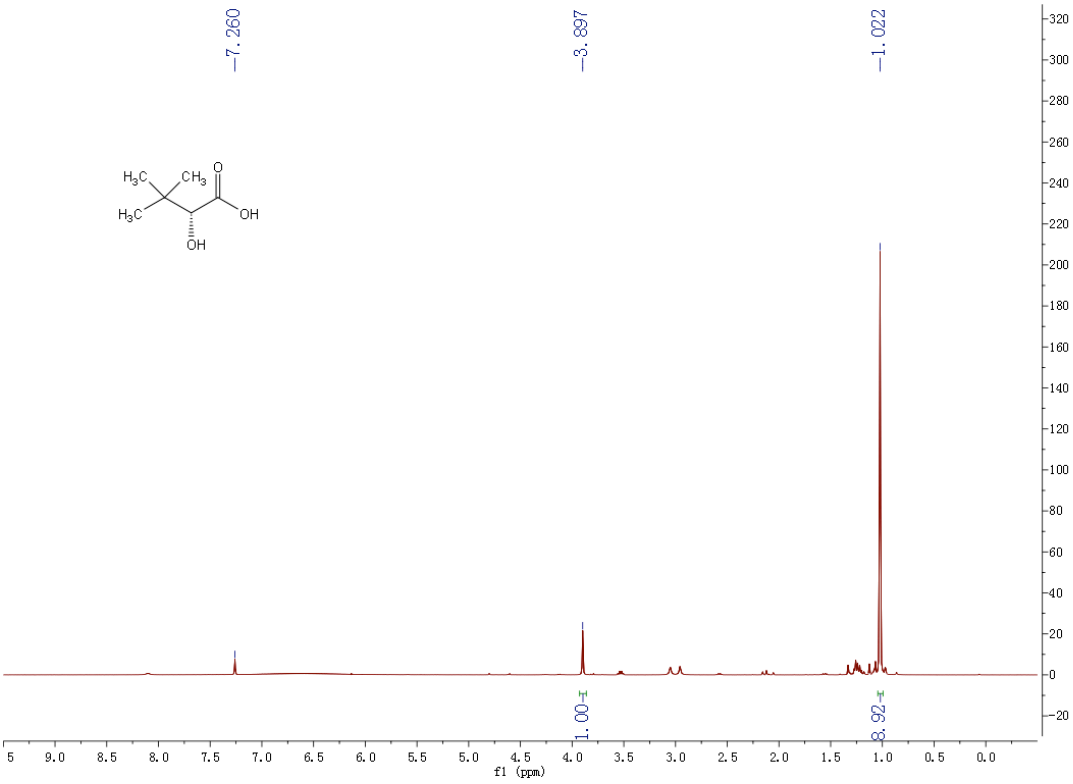
29 (a white solid)：^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 – 7.28(m, 5H), 5.47 (s, 1H), 3.89 (br, 2H), 3.60 – 3.52 (m, 3H), 2.88 – 2.67 (m, 2H), 1.08 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ138.6, 128.8, 128.2, 126.1, 101.9, 87.5, 78.8, 41.4, 32.0, 21.4, 19.0; MS (ESI+) calcd for $C_{13}H_{20}NO_2$ $[M+H]^+$ 222.1, found 222.2.

30 (a white solid)：^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.2 Hz, 2H), 7.50 – 7.33 (m, 7H), 5.45 (s, 1H), 3.80 – 3.70 (m, 2H), 3.61 (d, *J* = 11.2 Hz, 1H), 3.57 – 3.49 (m, 1H), 3.32 – 3.21 (m, 1H), 1.20 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 145.8, 137.7, 129.5, 128.4, 126.4, 125.4, 122.6, 102.1, 82.8, 78.3, 44.1, 31.9, 21.1, 18.7; MS (ESI+) calcd for $C_{19}H_{22}N_2O_7SNa$ $[M+Na]^+$ 445.1, found 444.8.

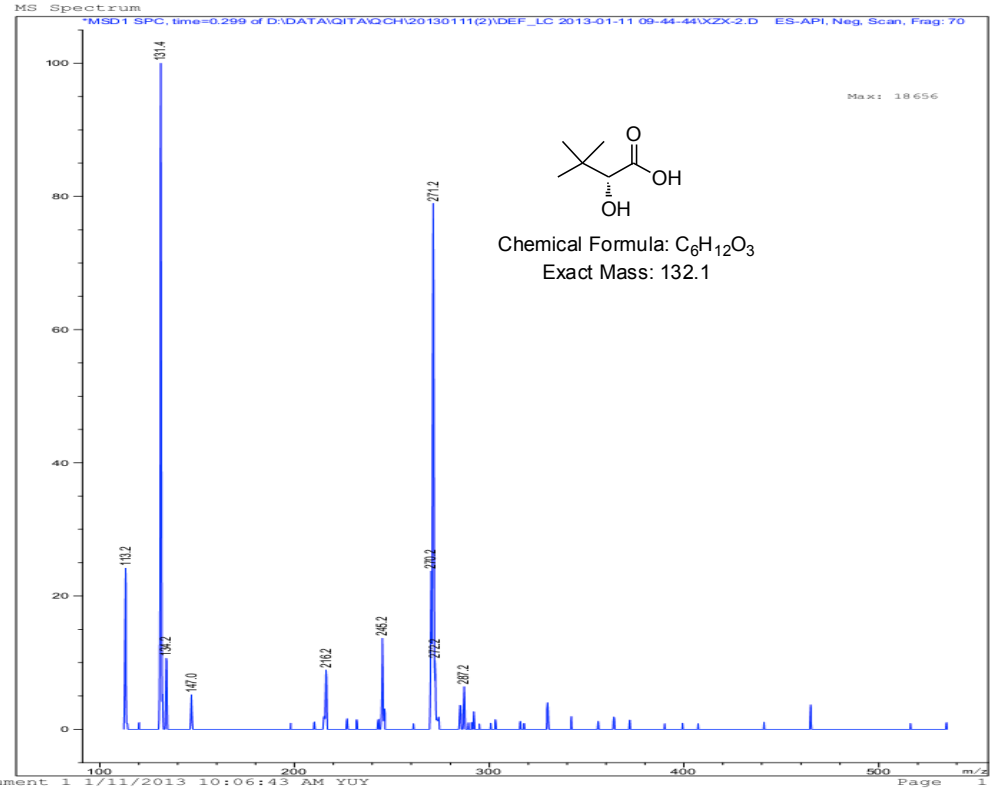
32 (a white solid)： MS (ESI+) calcd for $C_{26}H_{35}N_7O_7SNa$ $[M+Na]^+$ 612.2, found 611.8.

5 (a white solid): ^{1}H NMR (400 MHz, CD_3OD) δ 8.28 (s, 1H), 8.23 (s, 1H), 5.90 (d, *J* = 6.8 Hz, 1H), 4.91 – 4.89 (m, 1H), 4.36 (dd, *J* = 5.2, 2.0 Hz, 1H), 4.32 – 4.28 (m, 1H), 3.64 – 3.55 (m, 2H), 3.40 – 3.34 (m, 3H), 3.16 (dd, *J* = 12.4, 2.0 Hz, 1H), 2.85 (dd, *J* = 12.8, 10.0 Hz, 1H), 0.81 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 157.6, 153.9, 150.0, 142.5, 121.2, 91.6, 85.9, 76.3, 74.3,73.0, 70.2, 46.1, 45.8, 39.6, 21.8, 20.1;HRMS (ESI–) calcd for $C_{16}H_{26}N_7O_7S$ $[M–H]^-$ 460.1620, found 460.1635.

化合物 **7**(^{1}H NMR MS)



Print of window 80: MS Spectrum



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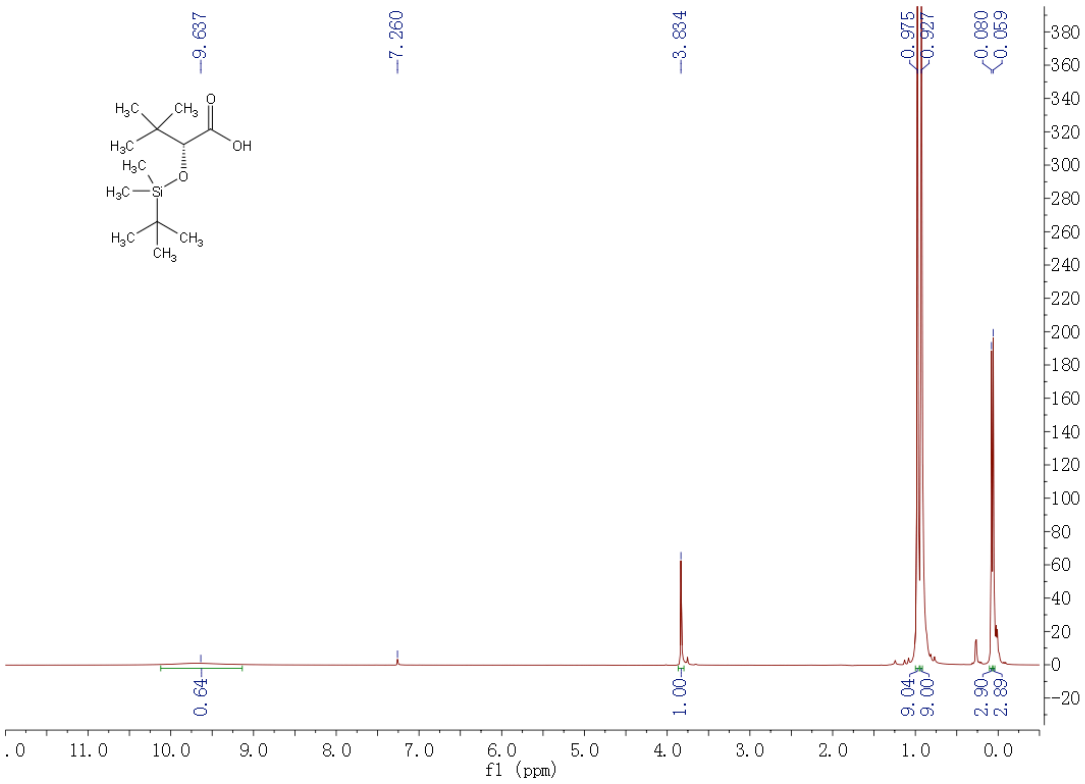
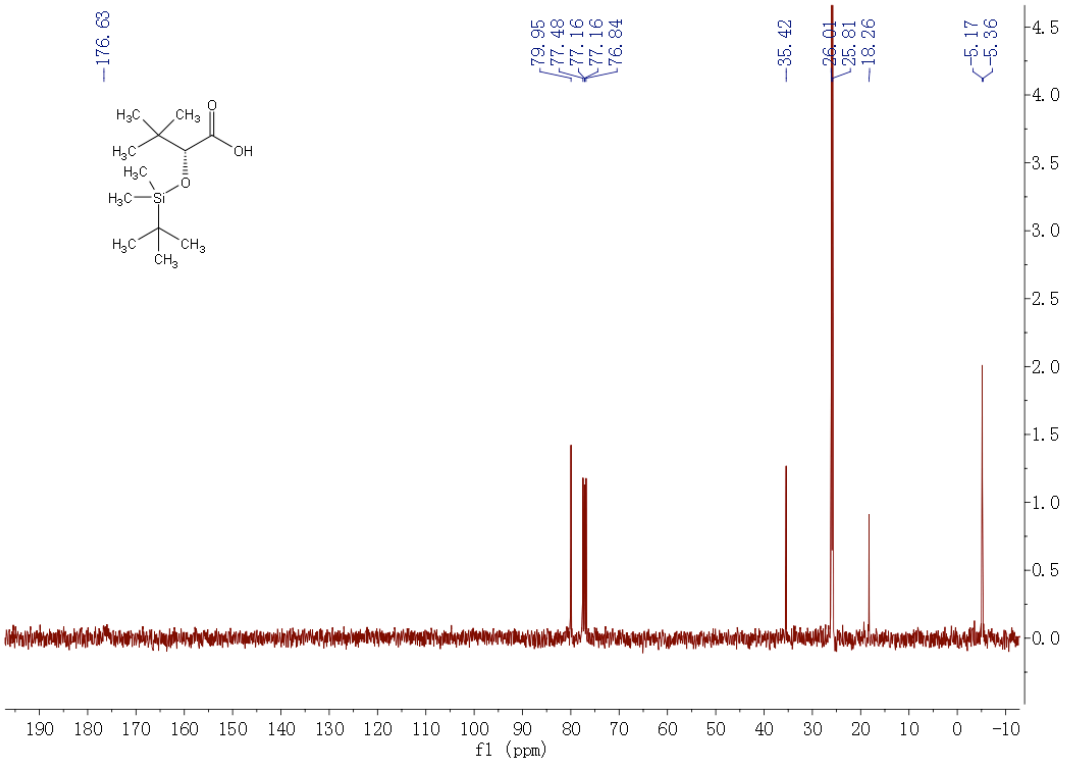
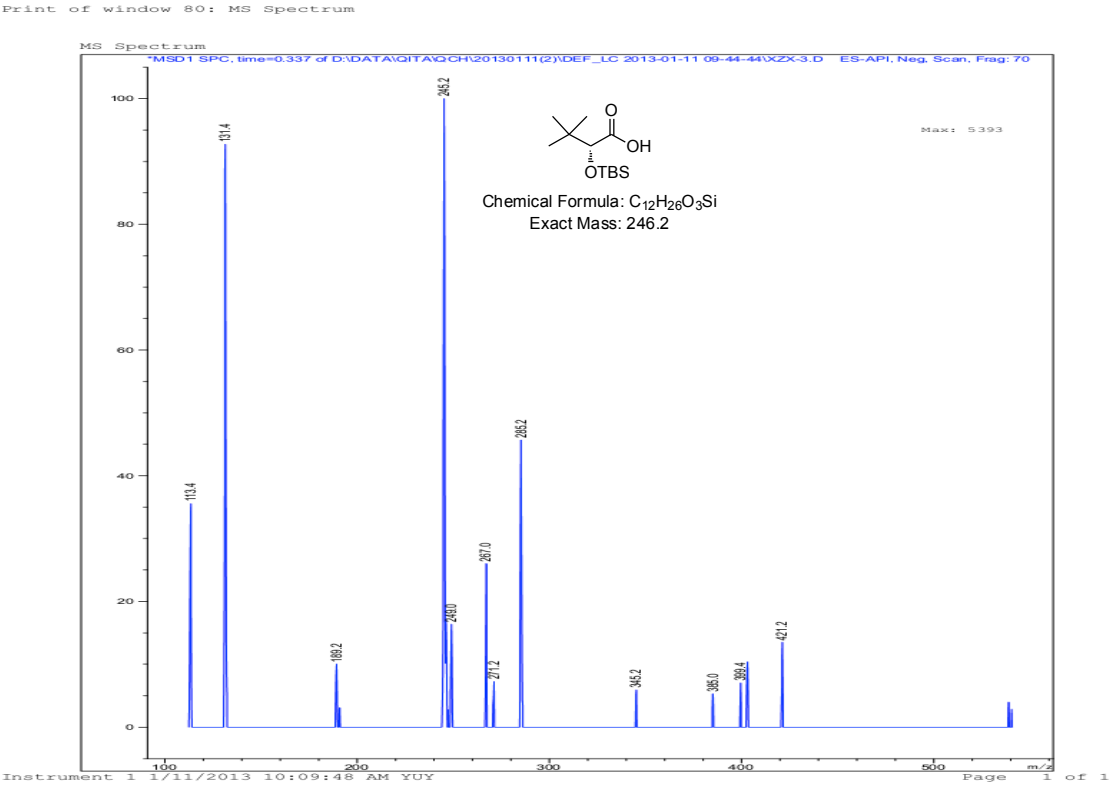
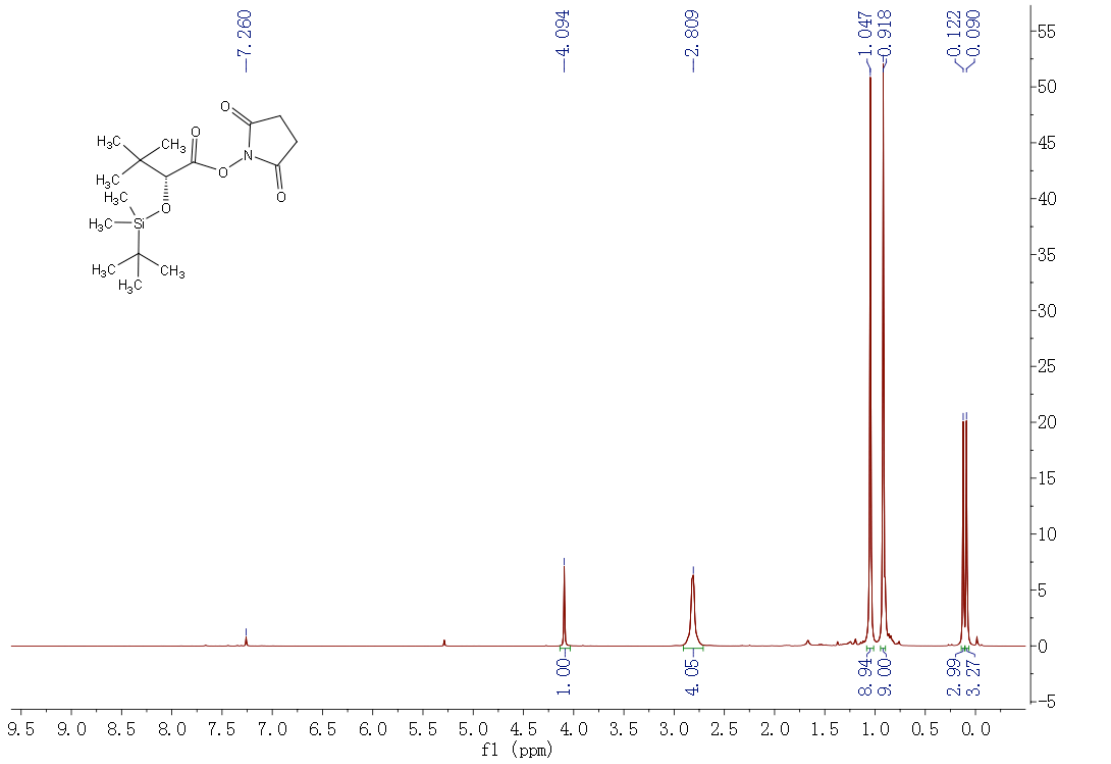
化合物 **8**(^{1}H NMR ^{13}C NMR MS)

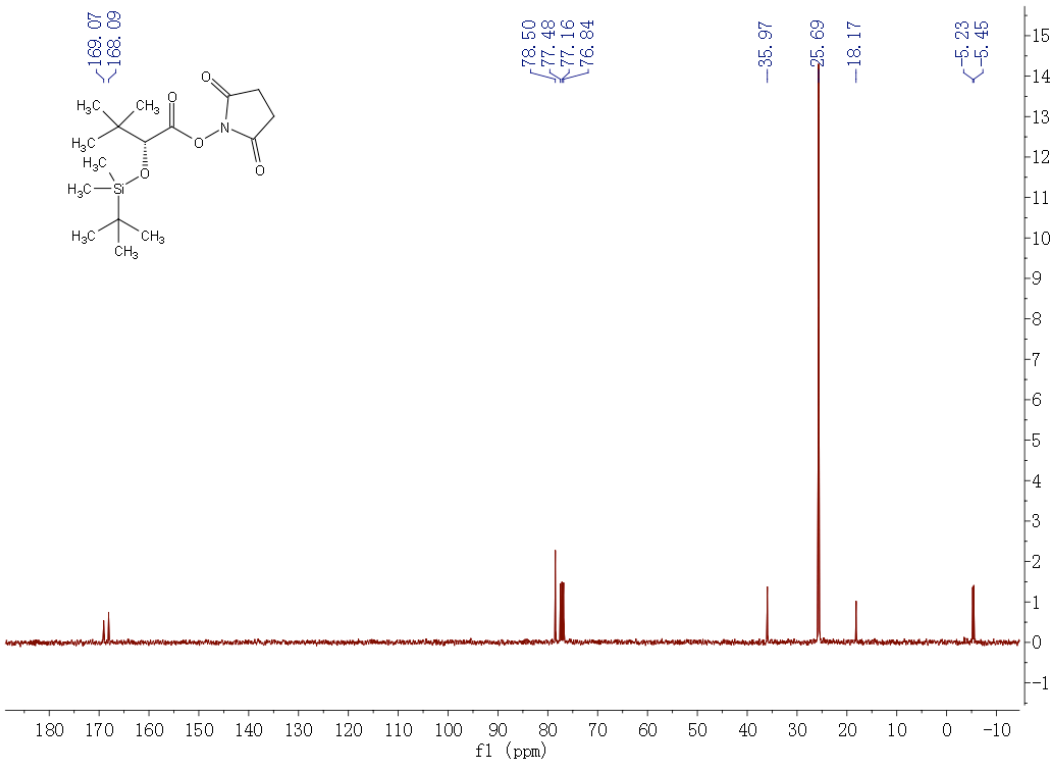




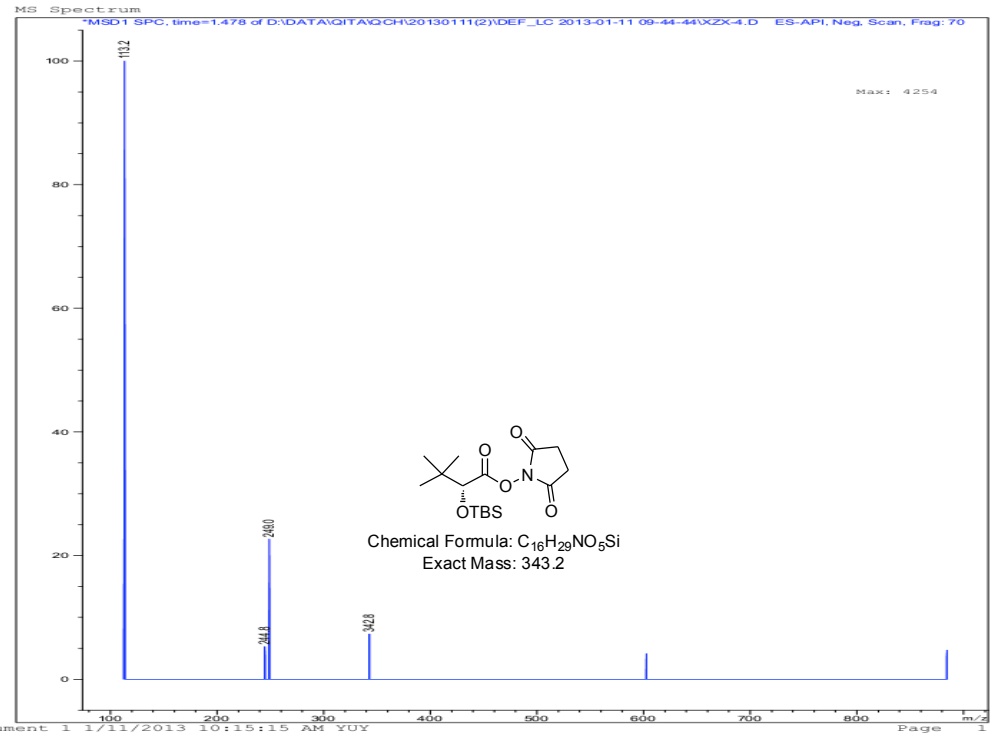


化合物 **9**(^{1}H NMR ^{13}C NMR MS)





Print of window 80: MS Spectrum



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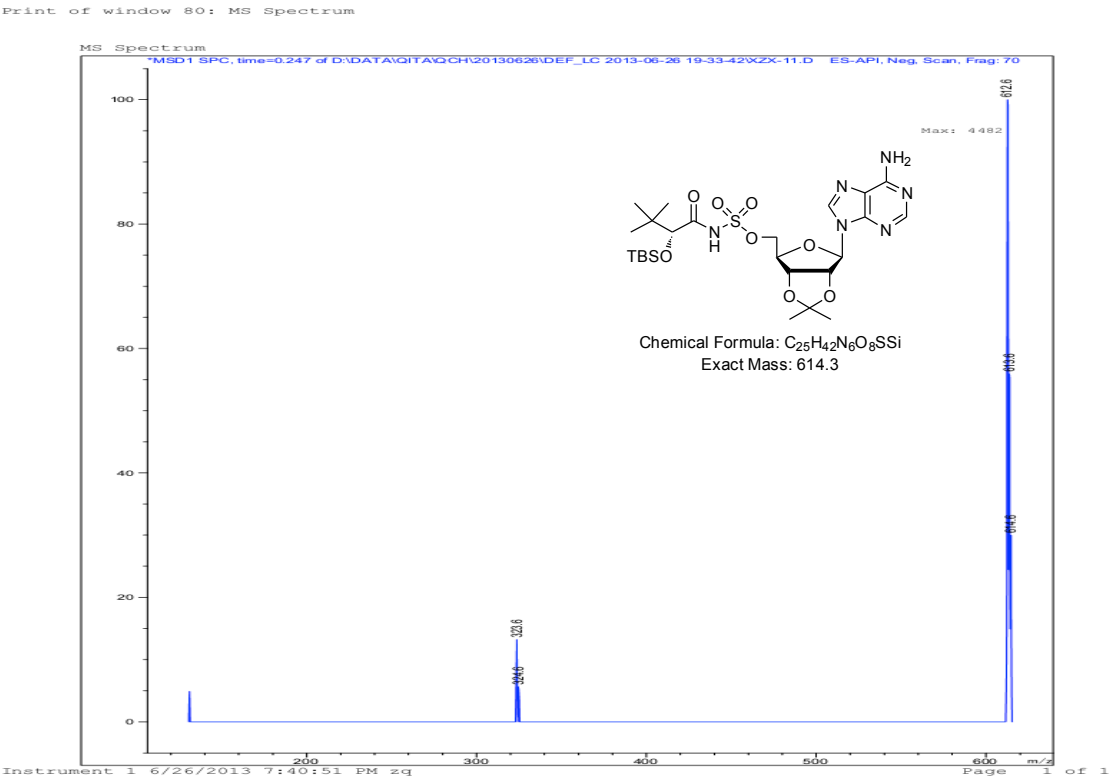
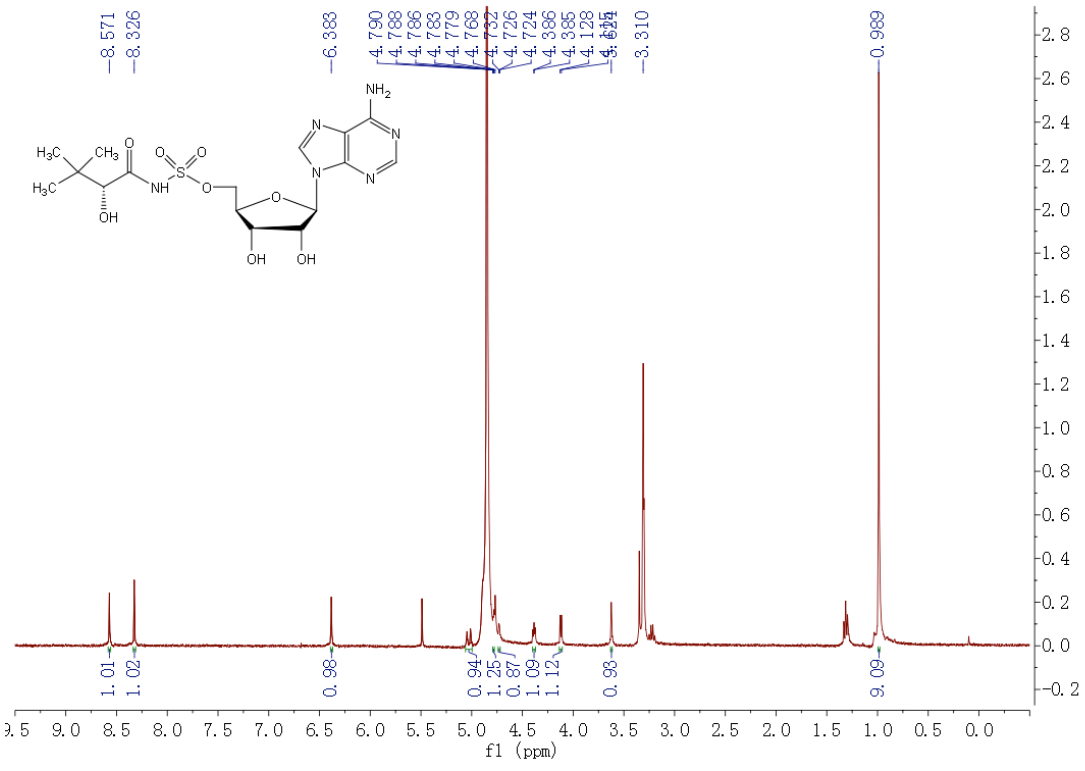
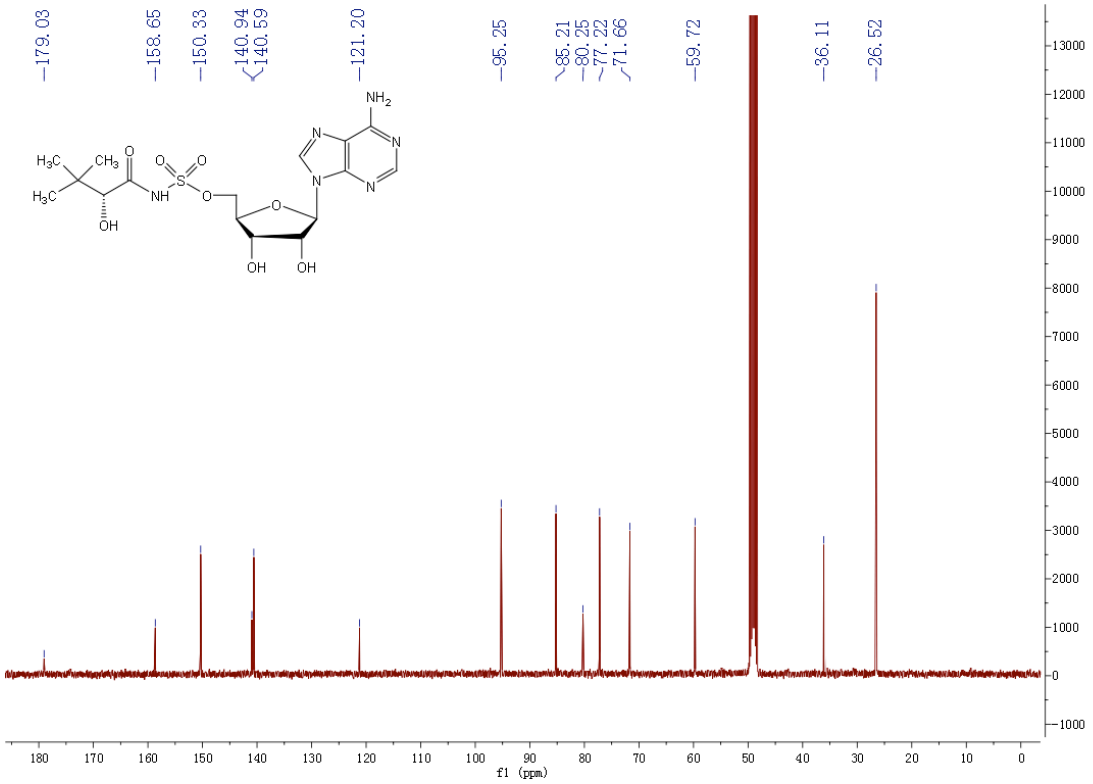
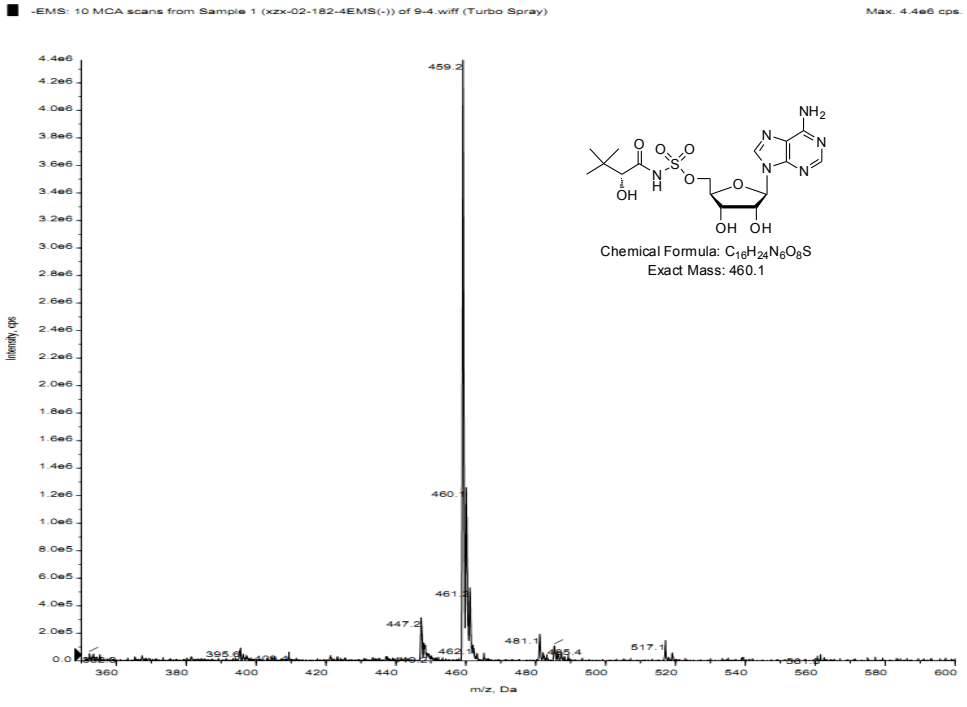
化合物 **11**(MS)



化合物 **1**(^{1}H NMR ^{13}C NMR MS)




179.03
158.65
150.33
140.94
140.59
121.20
95.25
85.21
80.25
77.22
71.66
59.72
36.11
26.52
f1 (ppm)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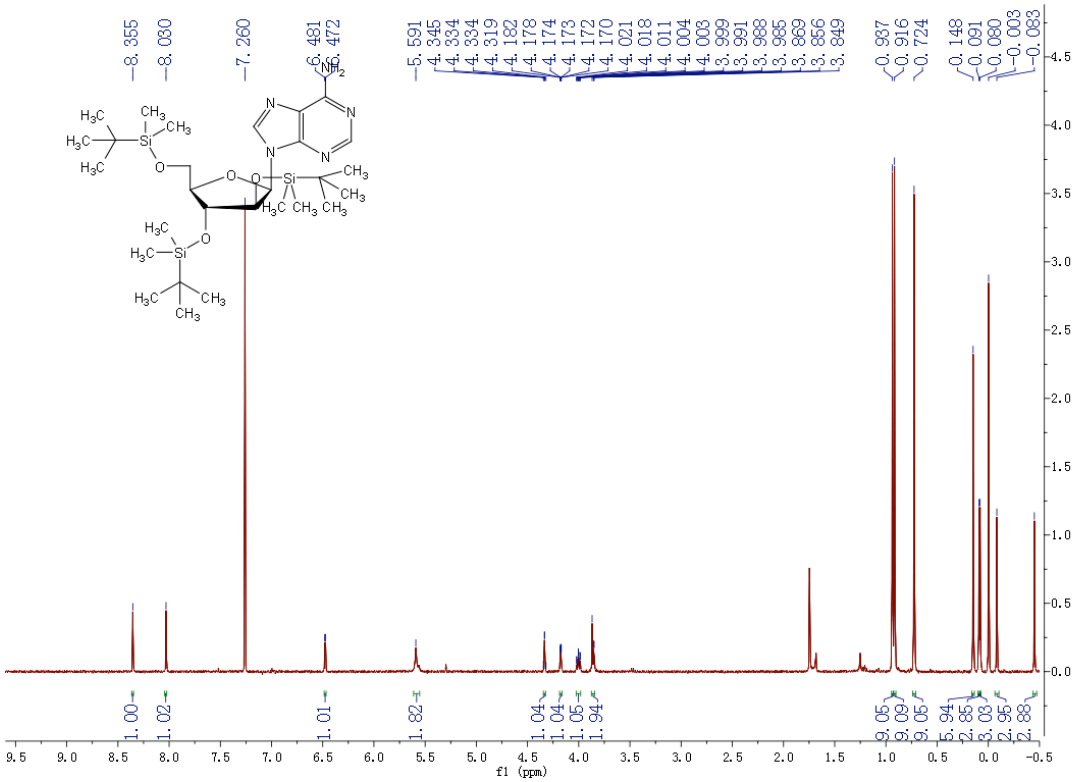
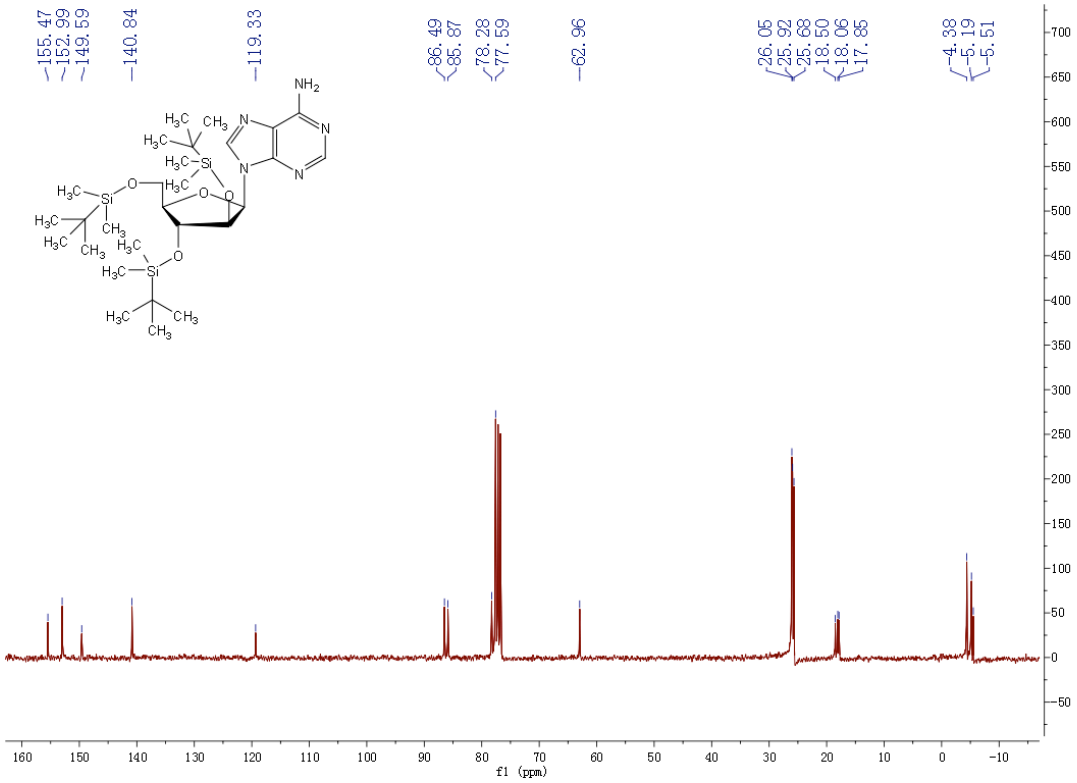
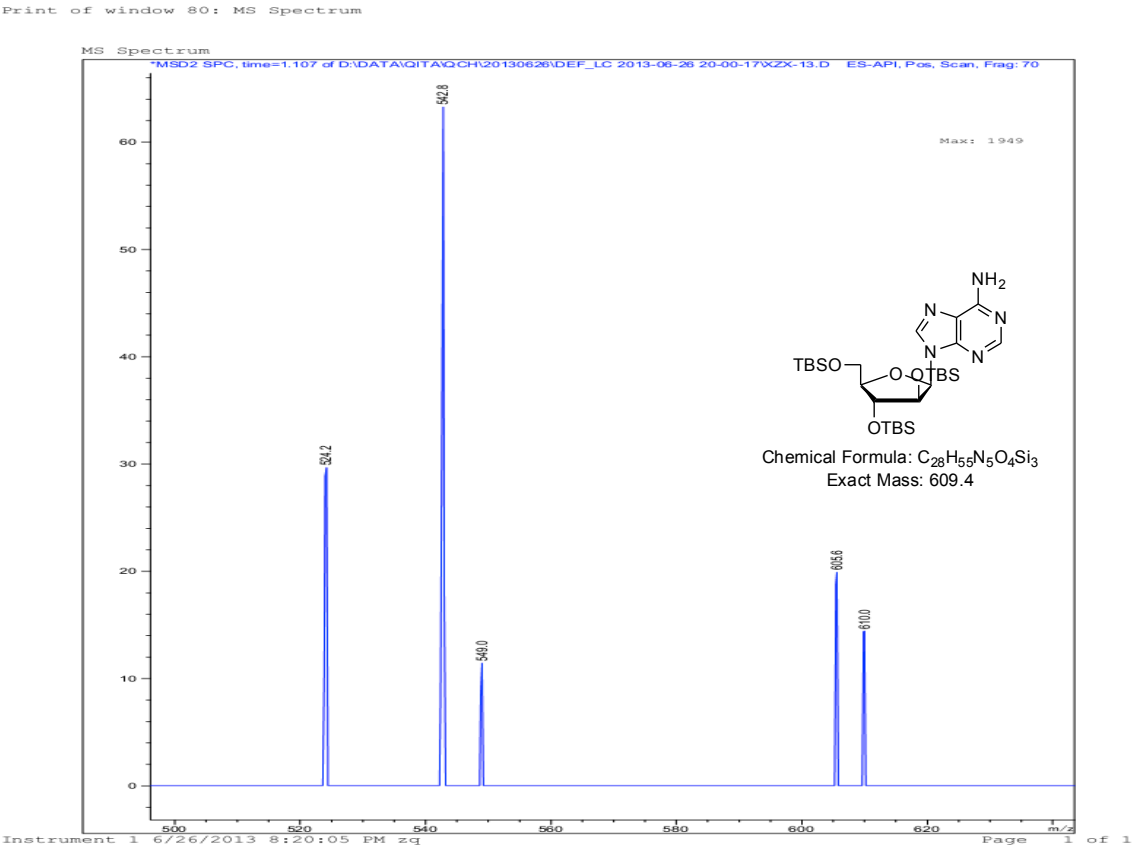
Max. 4.4e6 cps.
Intensity, cps
m/z, Da
459.2
460.1
461.2
447.2
481.1
517.1
Chemical Formula: C16H24N6O8S
Exact Mass: 460.1

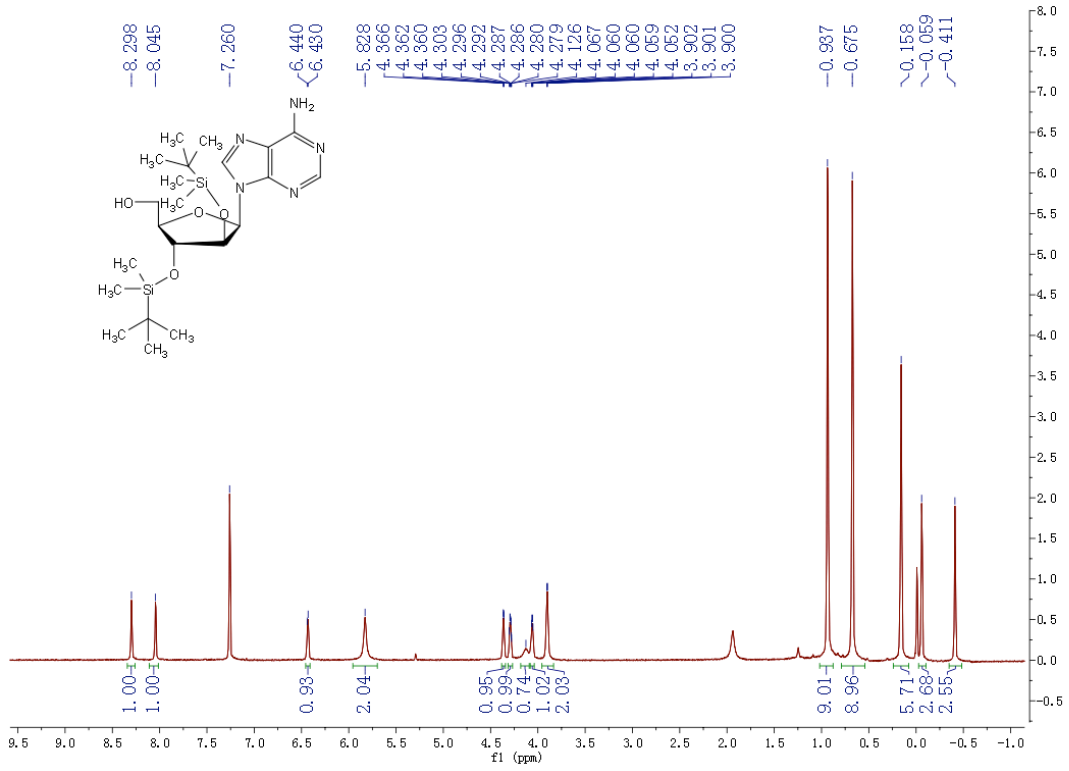
化合物 **13**(^{1}H NMR ^{13}C NMR MS)

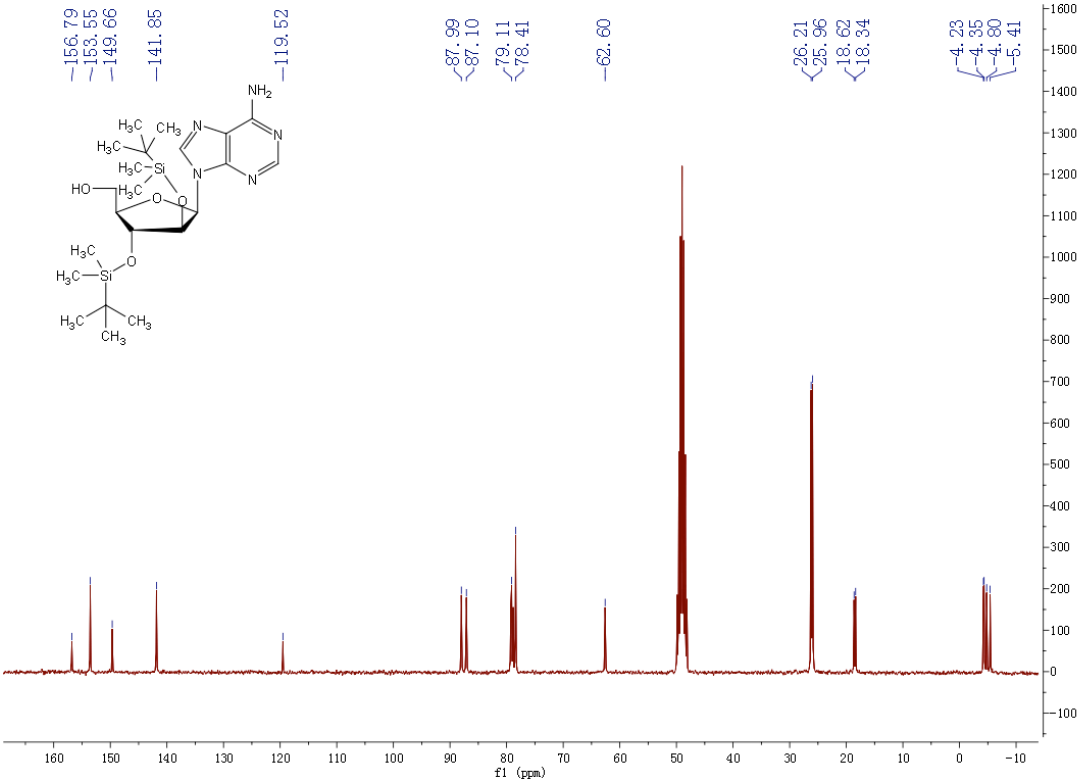




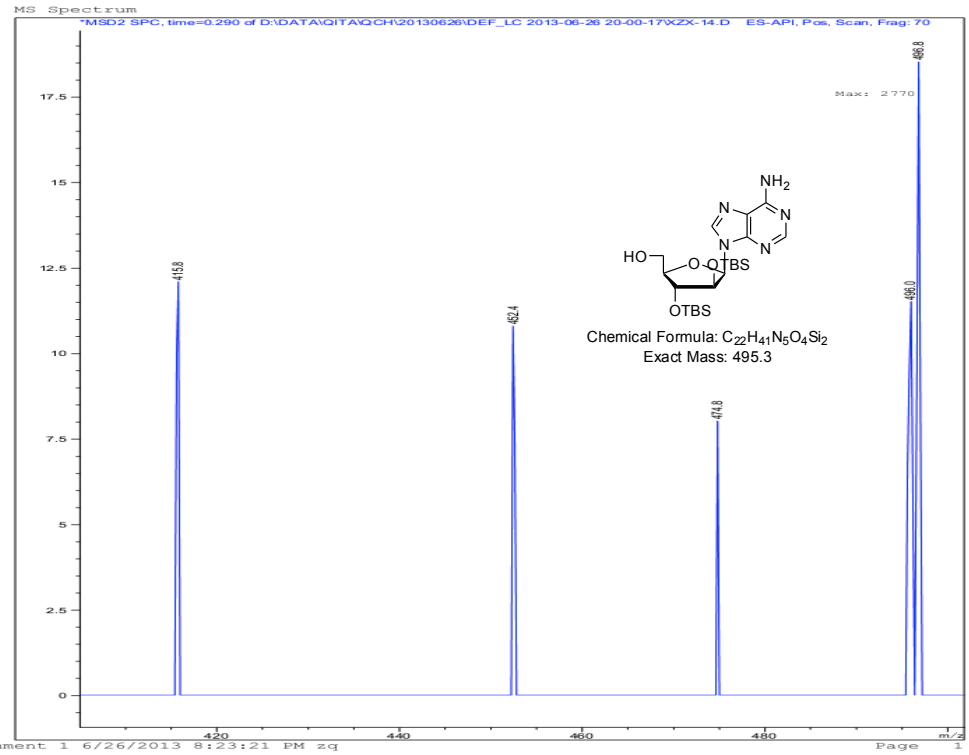


化合物 **14**(^{1}H NMR ^{13}C NMR MS)



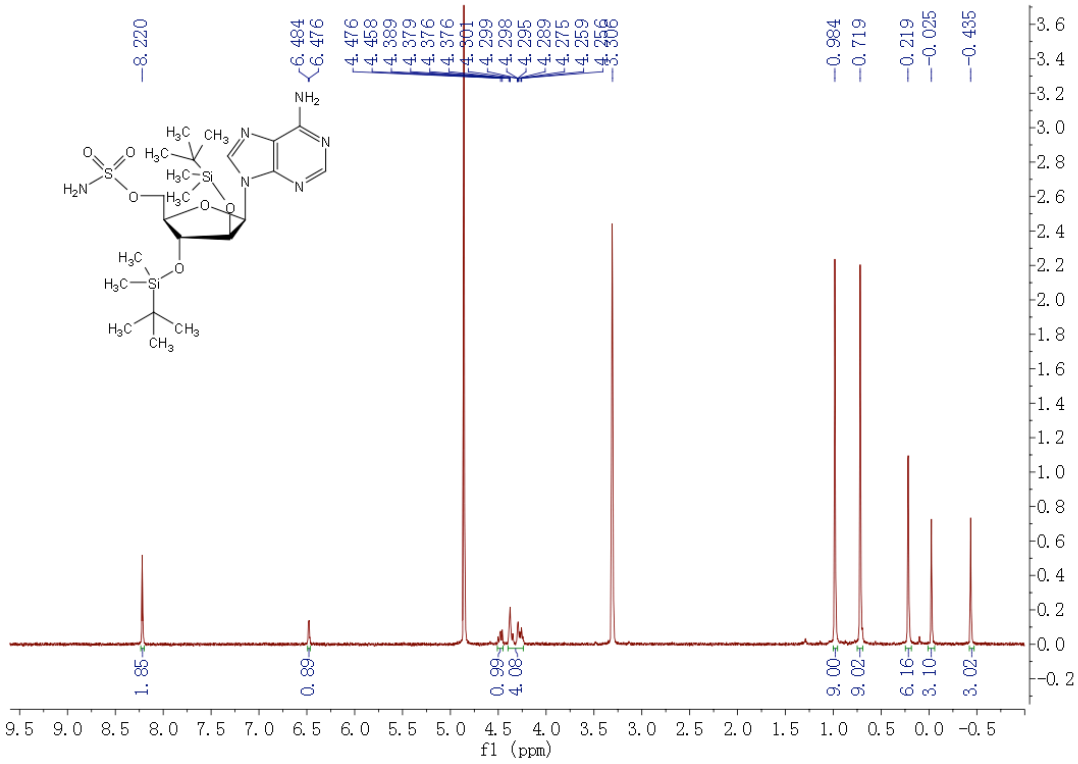


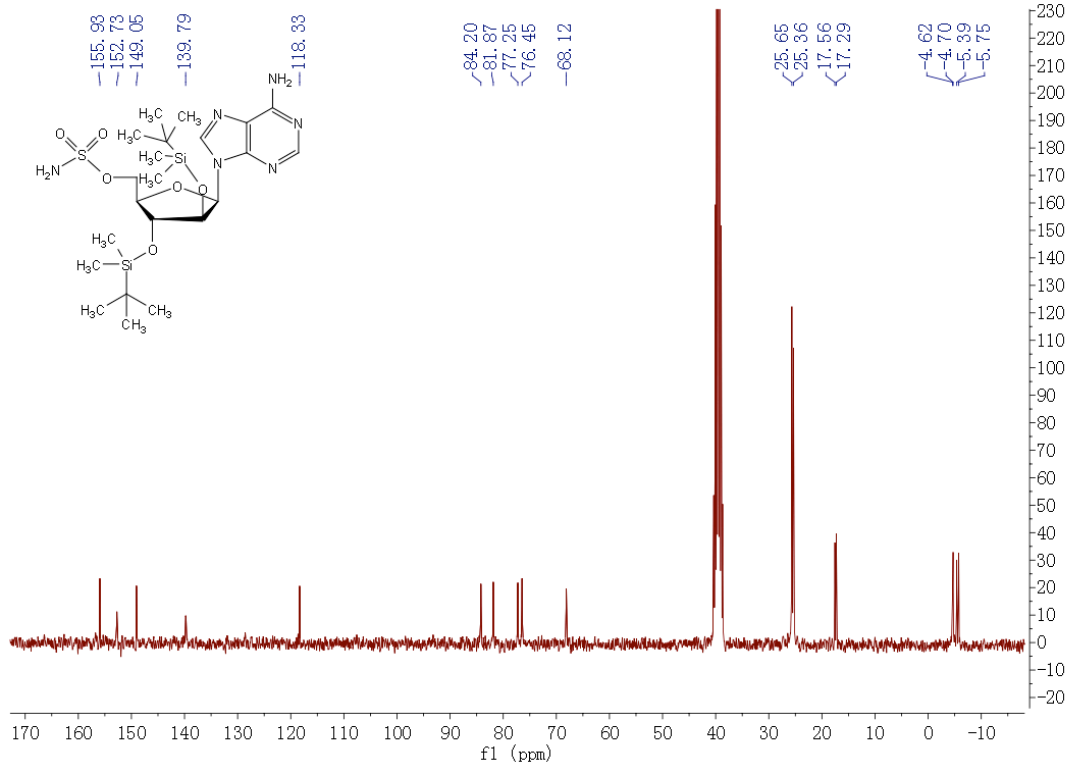
Print of window 80: MS Spectrum

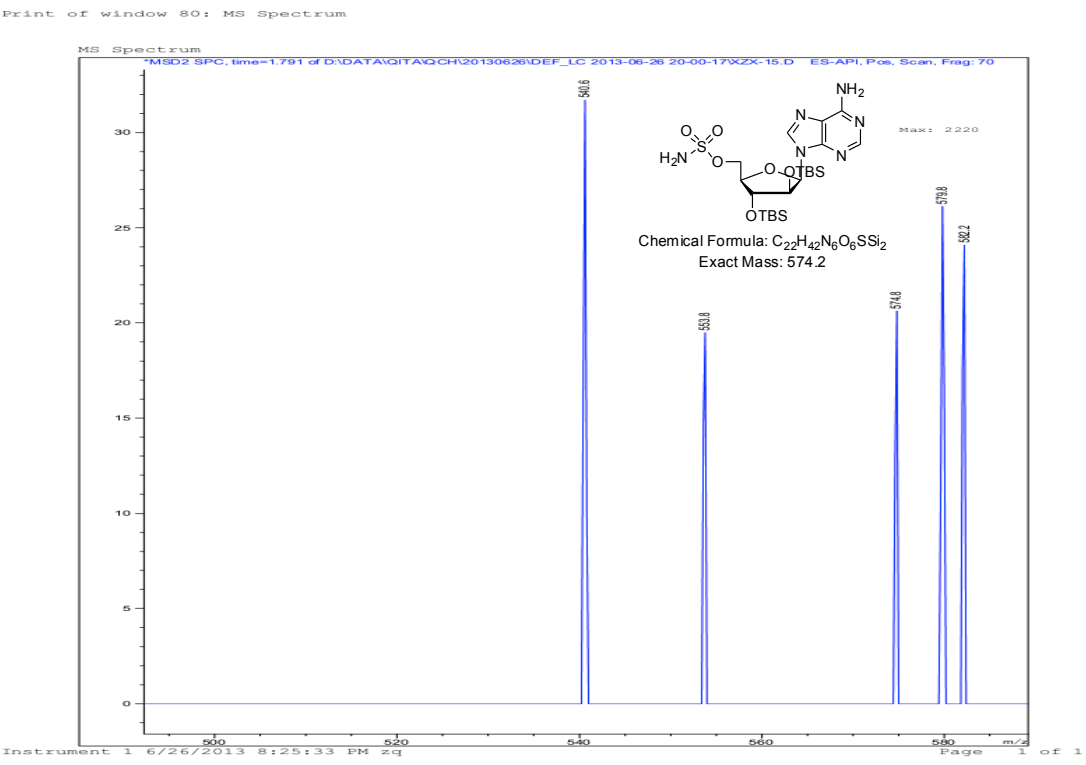


Instrument 1 6/26/2013 8:23:21 PM zq Page 1 of 1

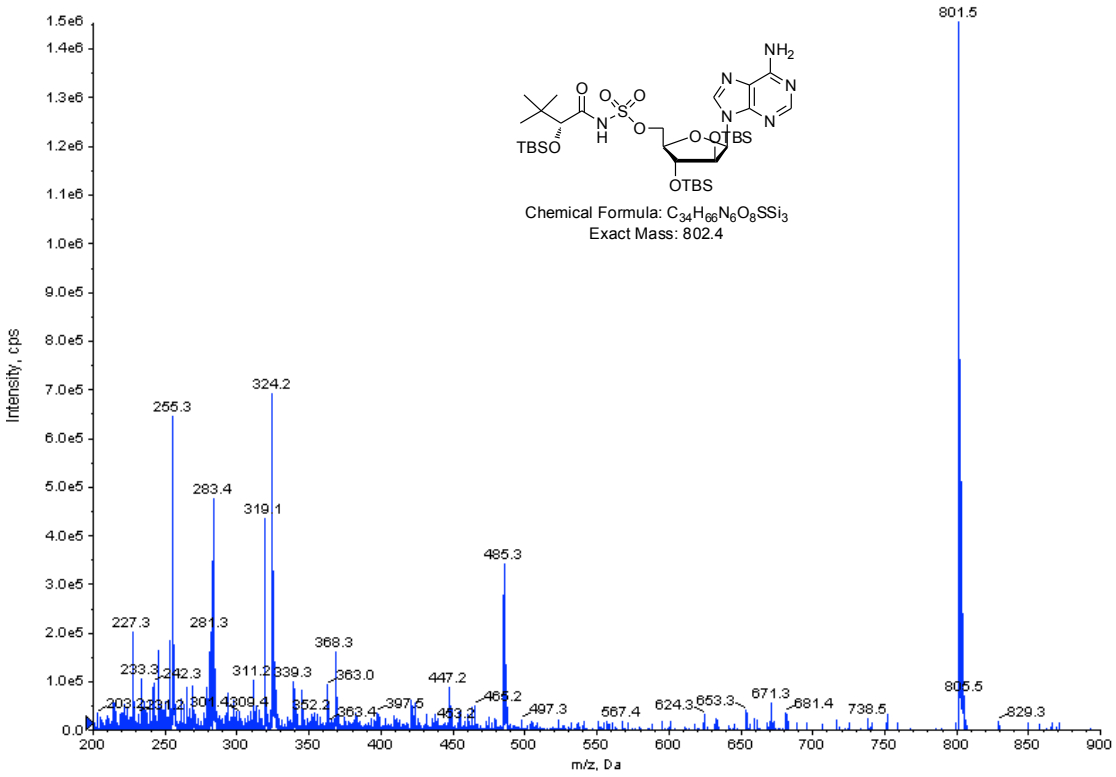
化合物 **15**(^{1}H NMR ^{13}C NMR MS)



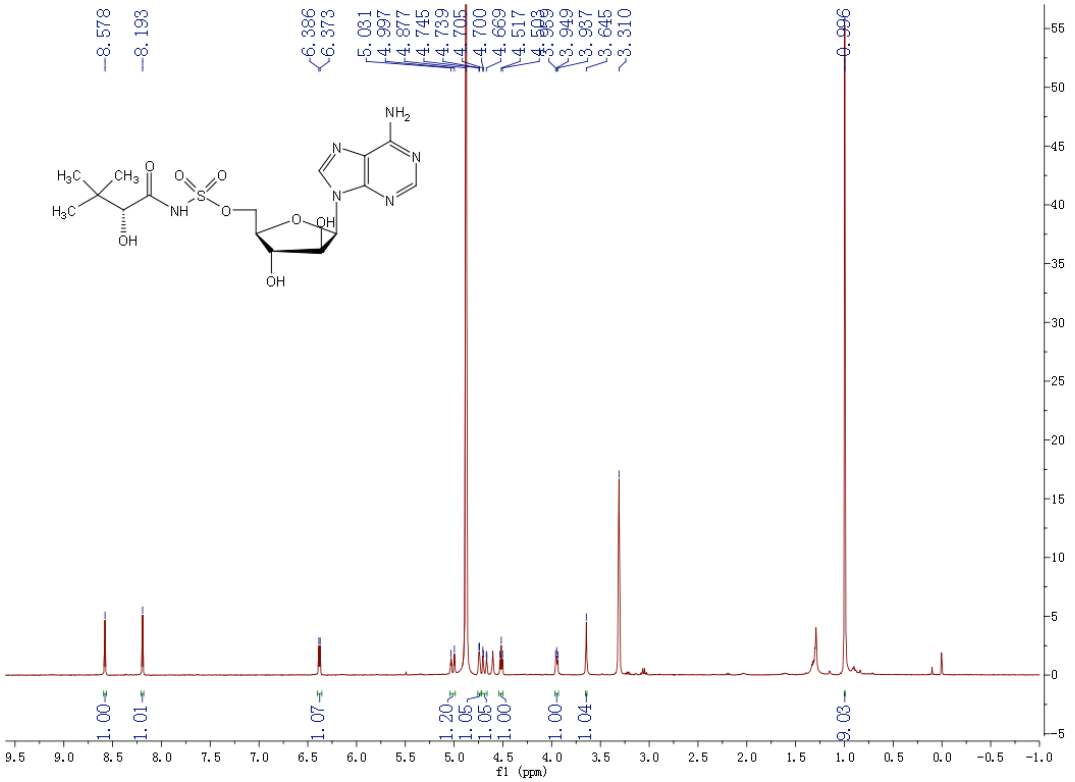


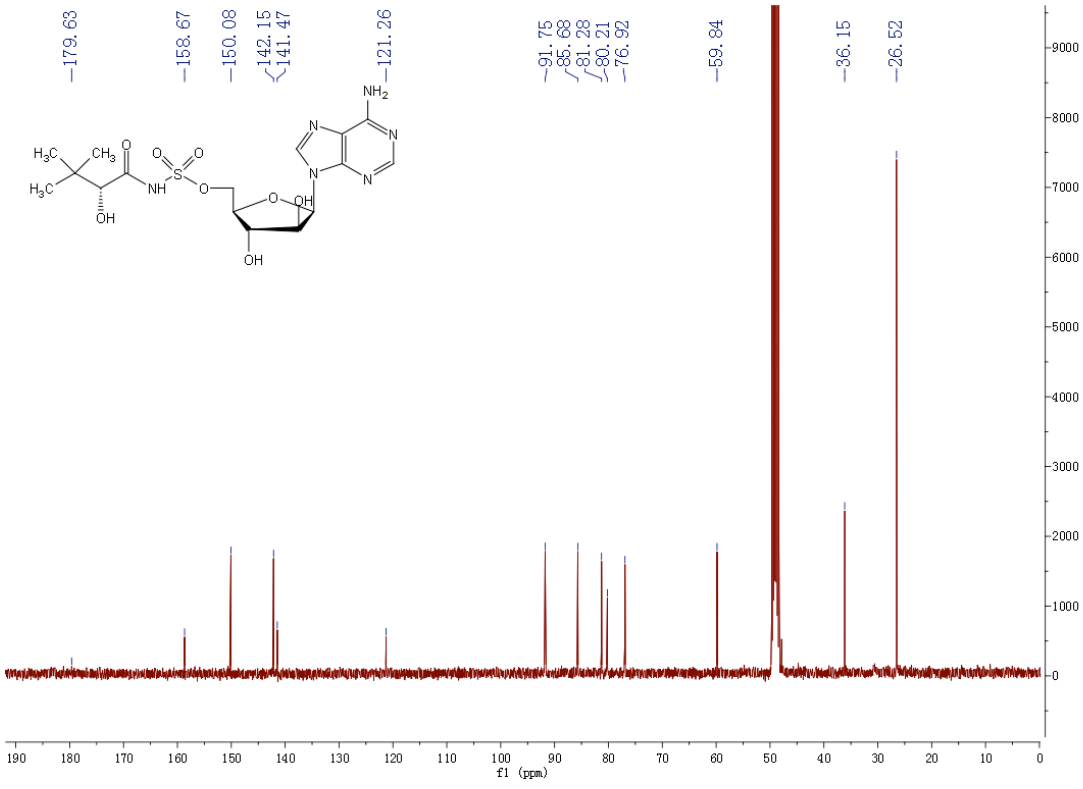

Print of window 80: MS Spectrum
MS Spectrum
*MSD2 SPC, time=1.791 of D:\DATA\QITA\QCH\20130626\DEF_LC 2013-06-26 20-00-17\XZX-15.D ES-API, Pos, Scan, Frag: 70
Max: 2220
540.6
553.8
574.8
578.8
582.2
Chemical Formula: C22H42N6O6SSi2
Exact Mass: 574.2
Instrument 1 6/26/2013 8:25:33 PM zq
Page 1 of 1

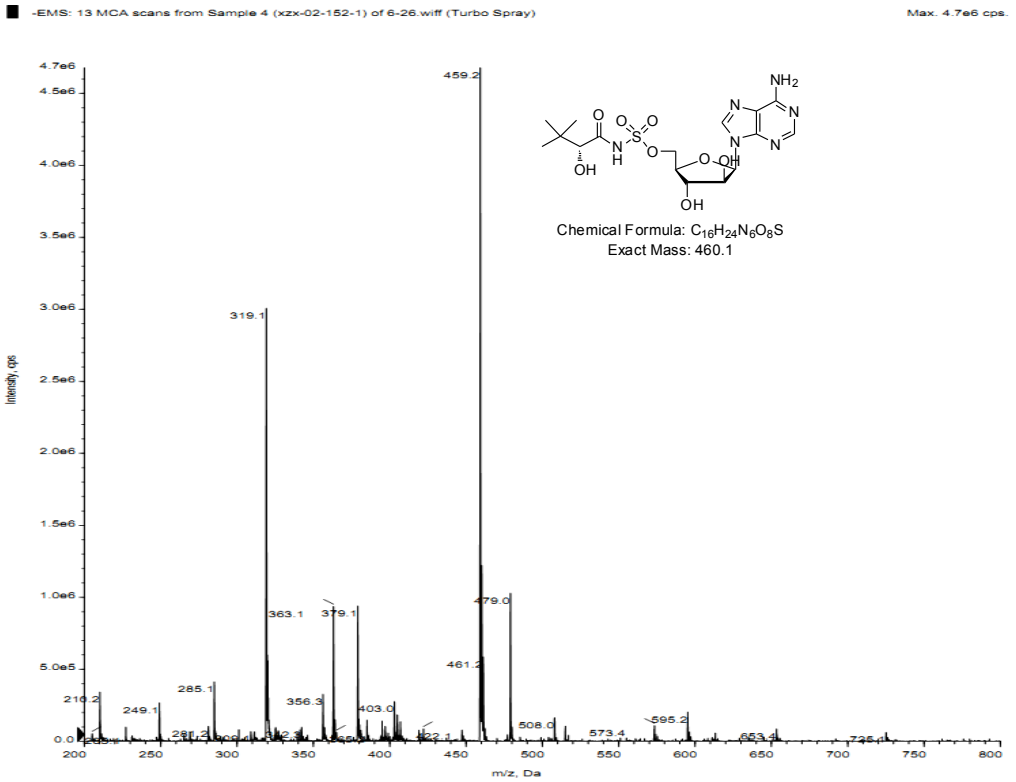
化合物 **16**(MS)


Intensity, cps
m/z, Da
801.5
324.2
255.3
283.4
319.1
485.3
227.3
281.3
368.3
Chemical Formula: C34H66N6O8SSi3
Exact Mass: 802.4

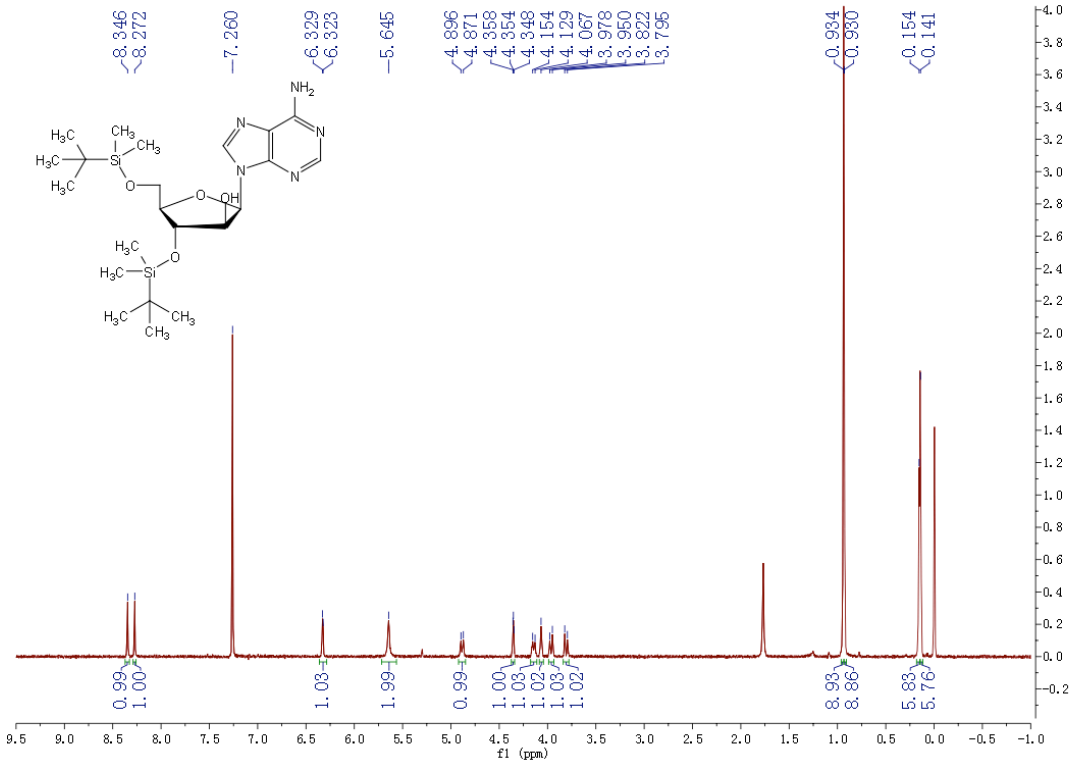
化合物 **2**(^{1}H NMR ^{13}C NMR MS)

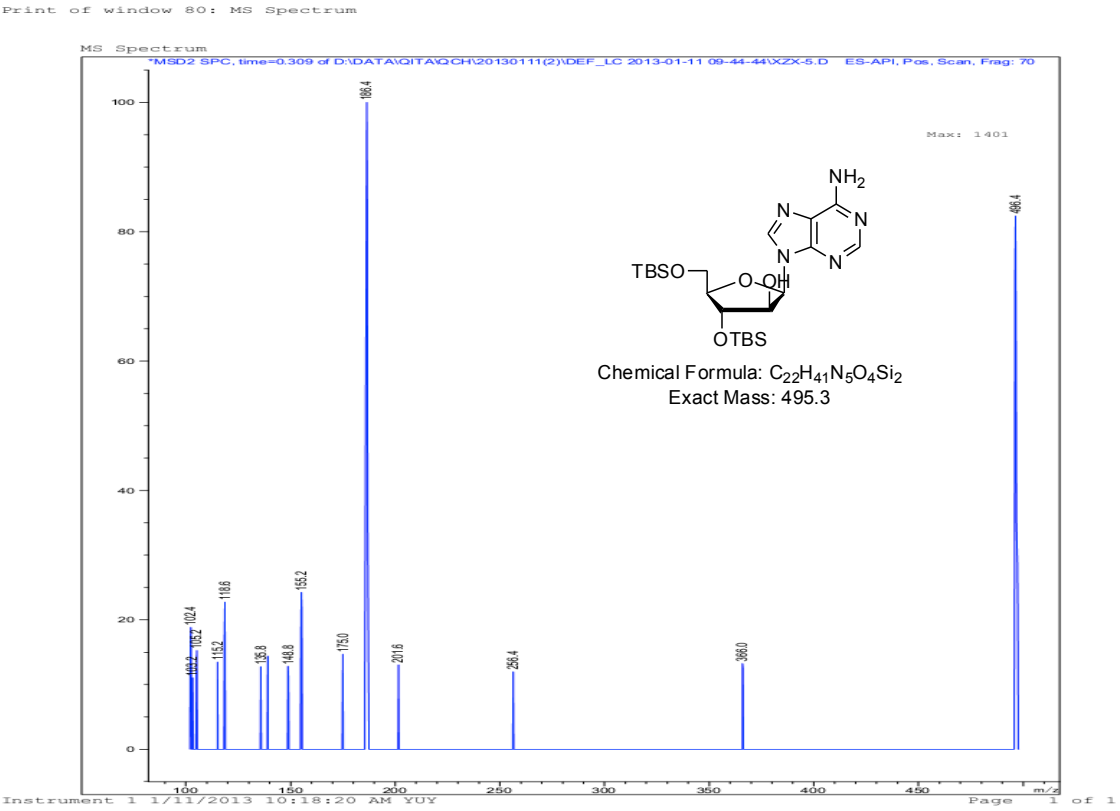




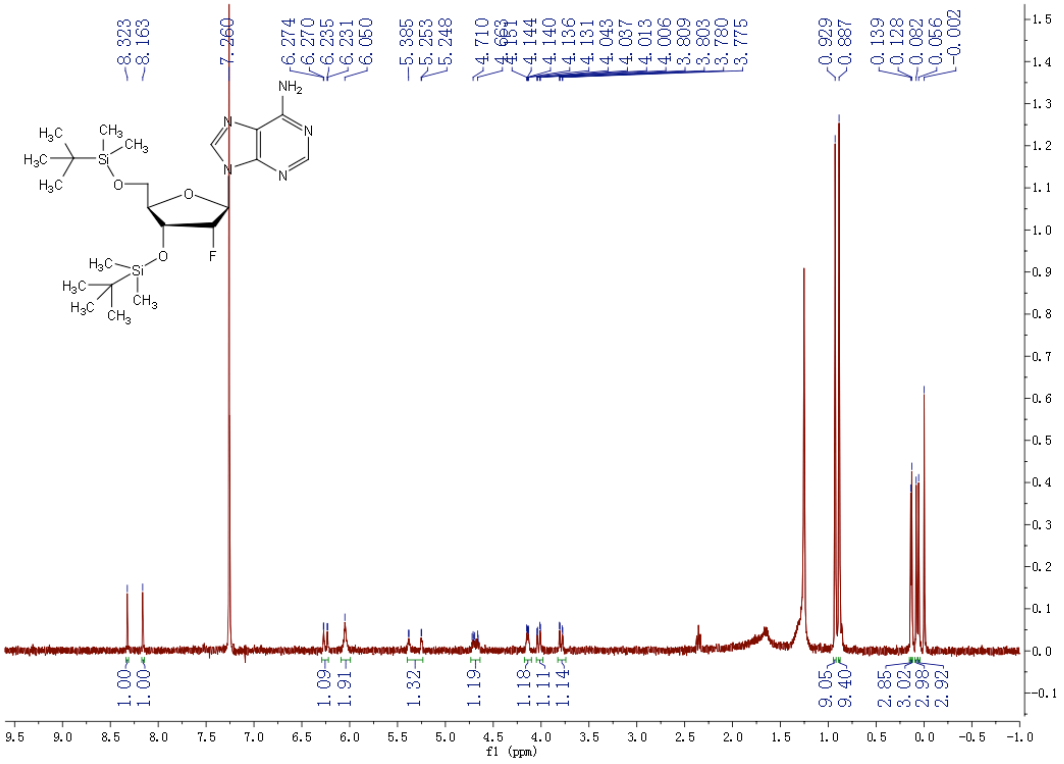


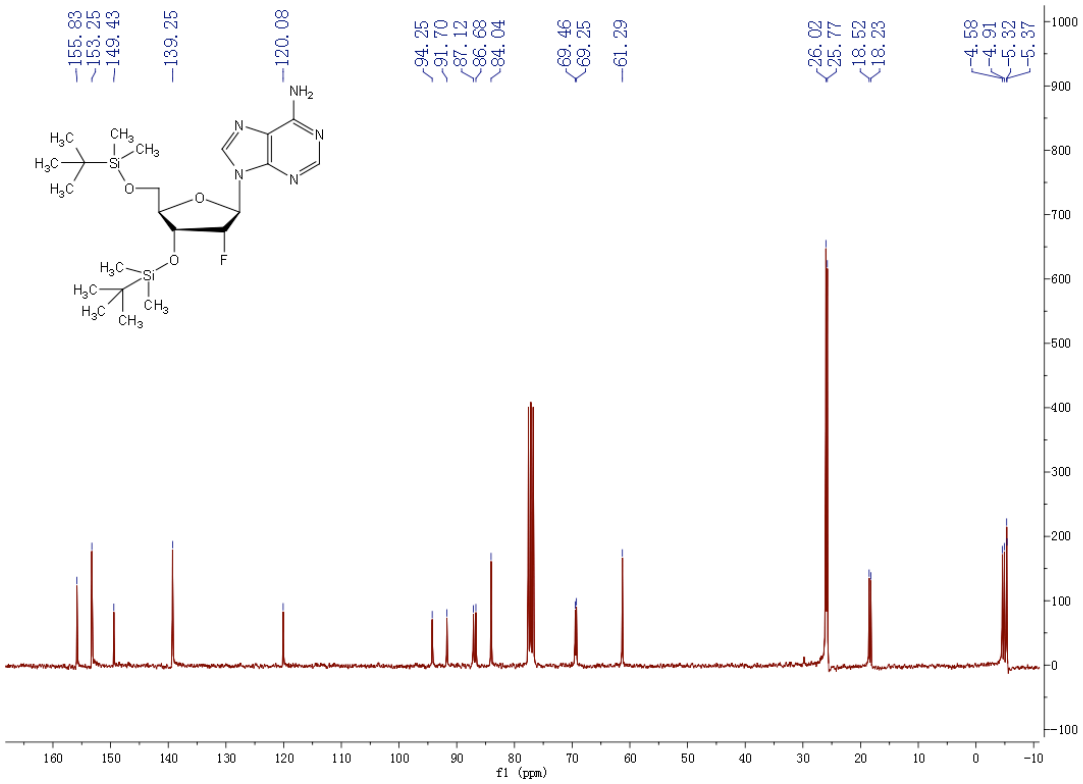
化合物 **17**(^{1}H NMR MS)

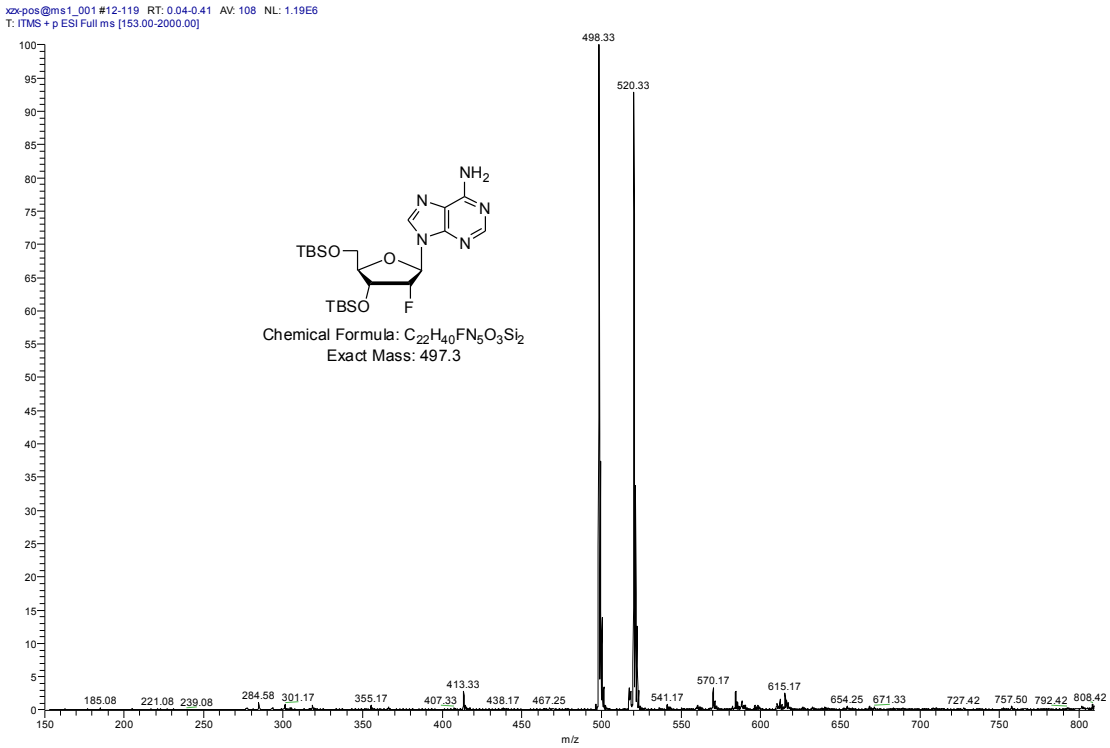




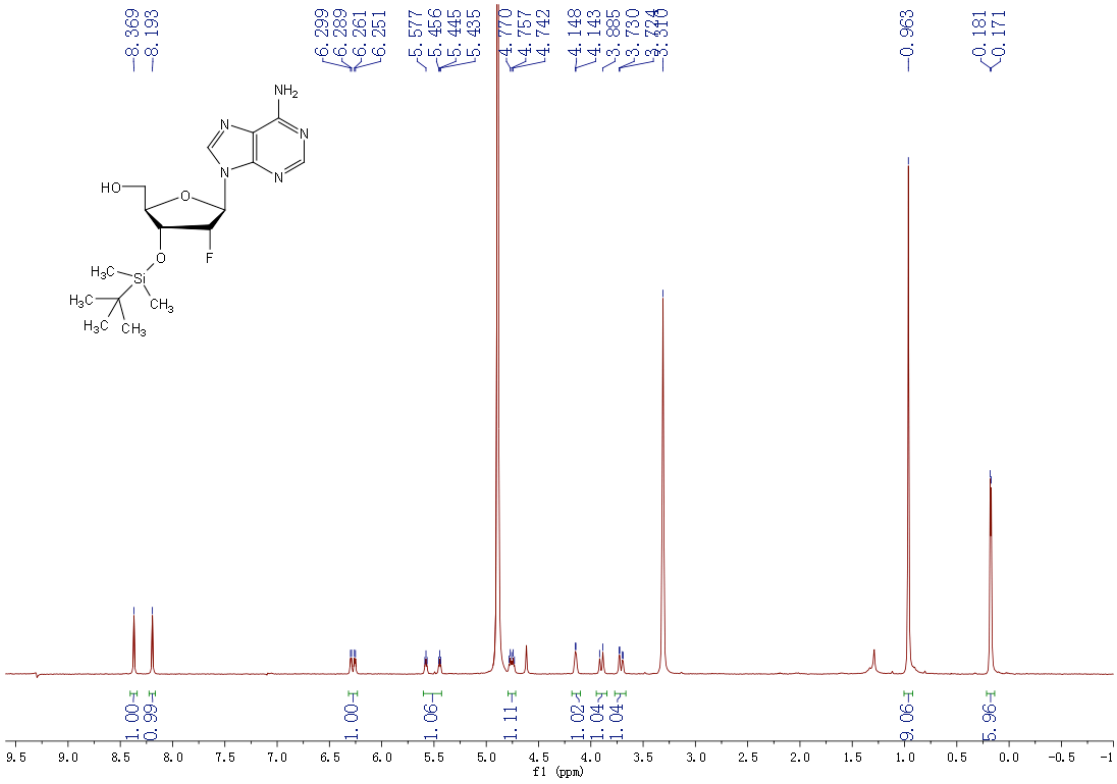
化合物 **18**(^{1}H NMR ^{13}C NMR MS)

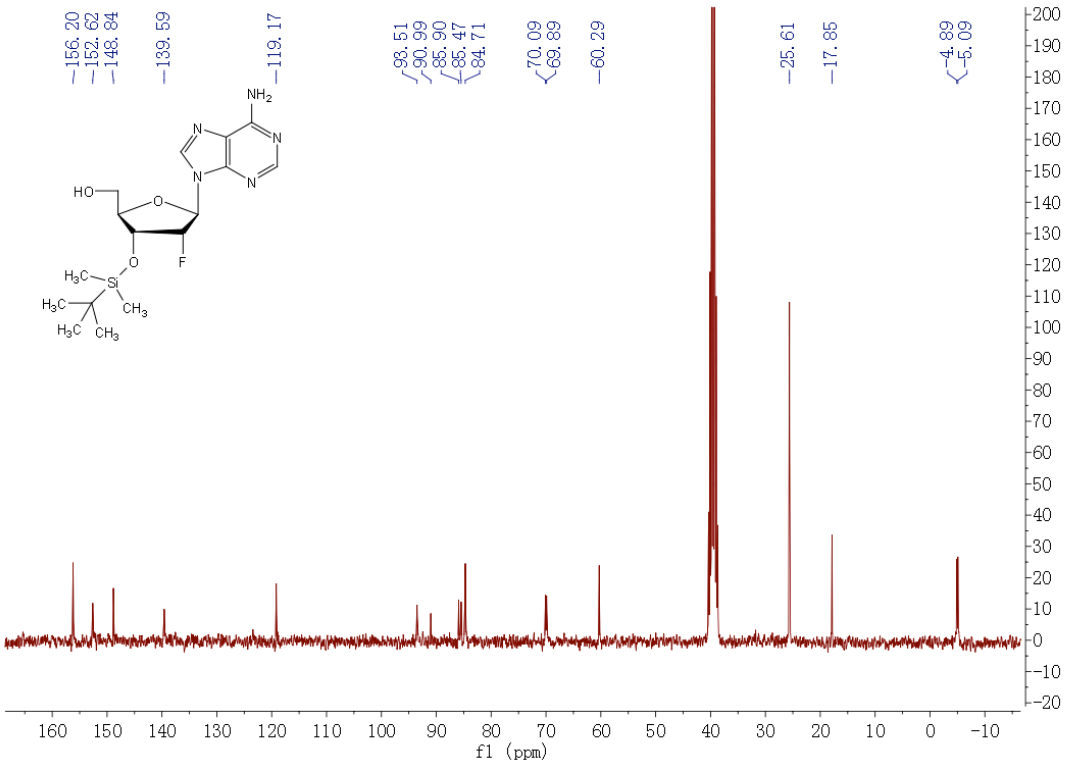


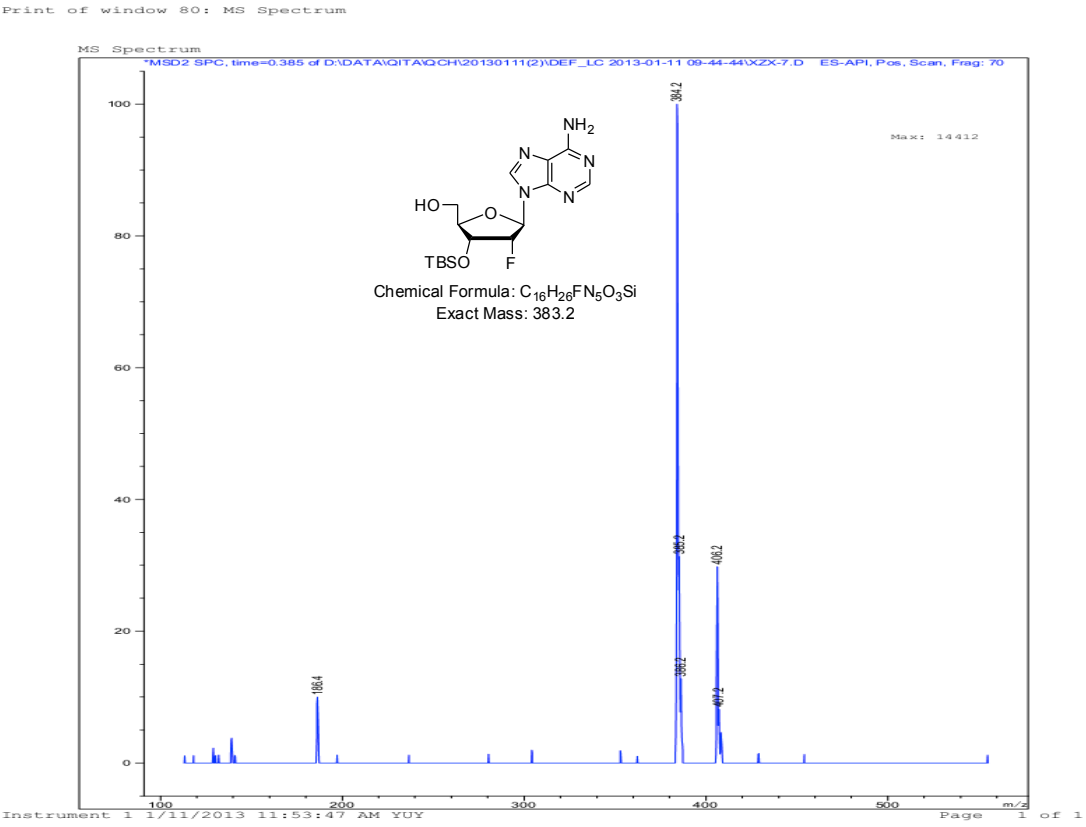

155.83
153.25
149.43
139.25
120.08
94.25
91.70
87.12
86.68
84.04
69.46
69.25
61.29
26.02
25.77
18.52
18.23
-4.58
-4.91
-5.32
-5.37
NH2
N
N
N
N
O
O
F
Si
Si
f1 (ppm)


xzx-pos@ms1_001 #12-119 RT: 0.04-0.41 AV: 108 NL: 1.19E6
T: ITMS + p ESI Full ms [153.00-2000.00]
498.33
520.33
NH2
TBSO
TBSO
F
Chemical Formula: C22H40FN5O3Si2
Exact Mass: 497.3
413.33
570.17
615.17
m/z

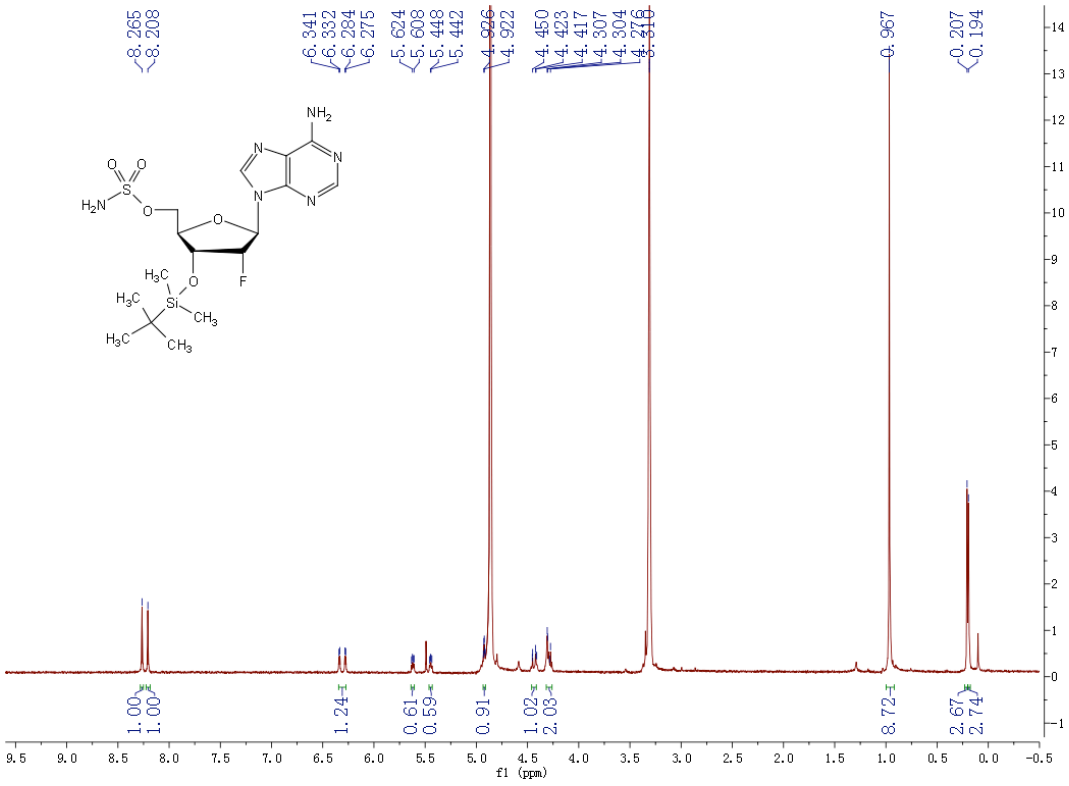
化合物 **19**(^{1}H NMR ^{13}C NMR MS)

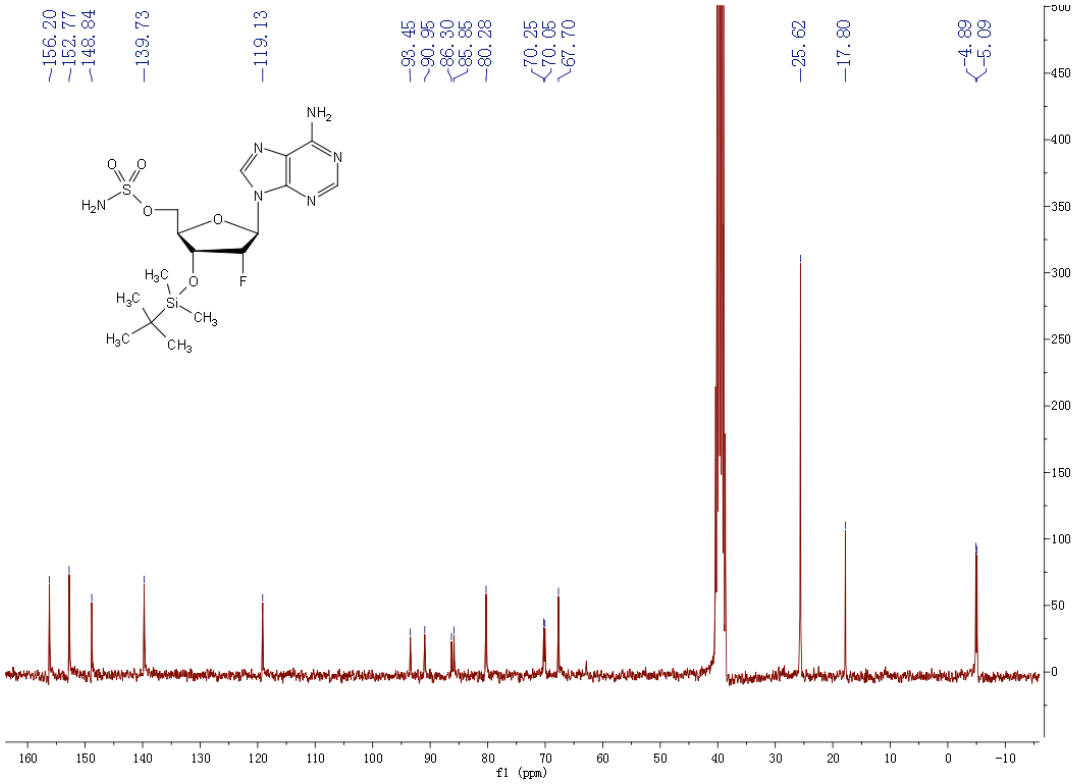




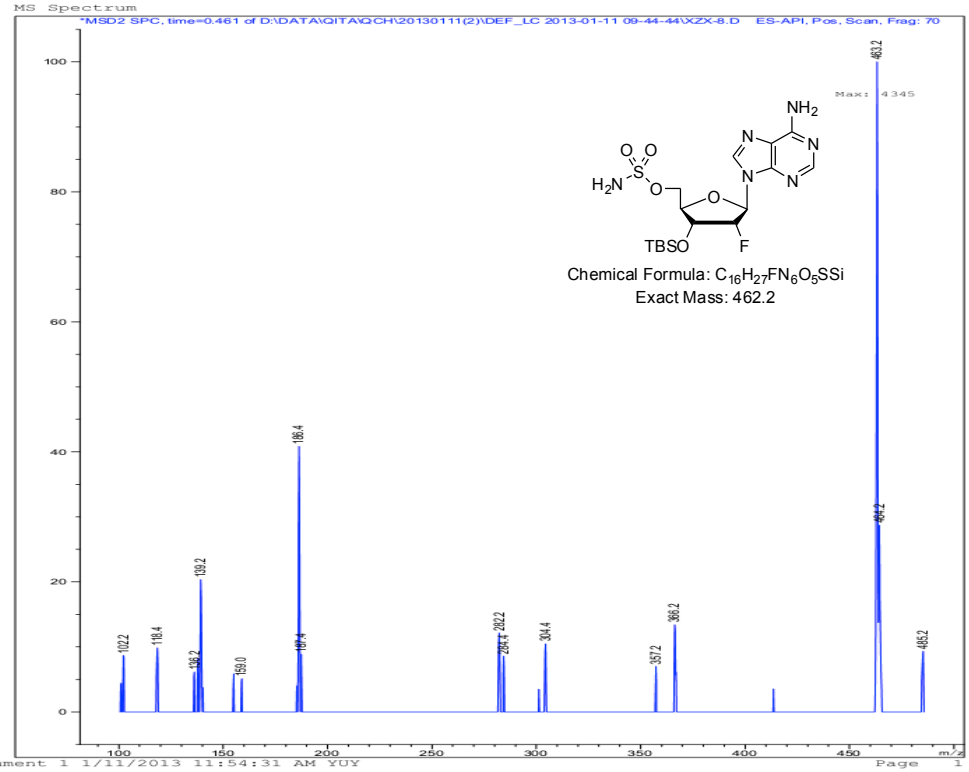


化合物 **20**(^{1}H NMR ^{13}C NMR MS)

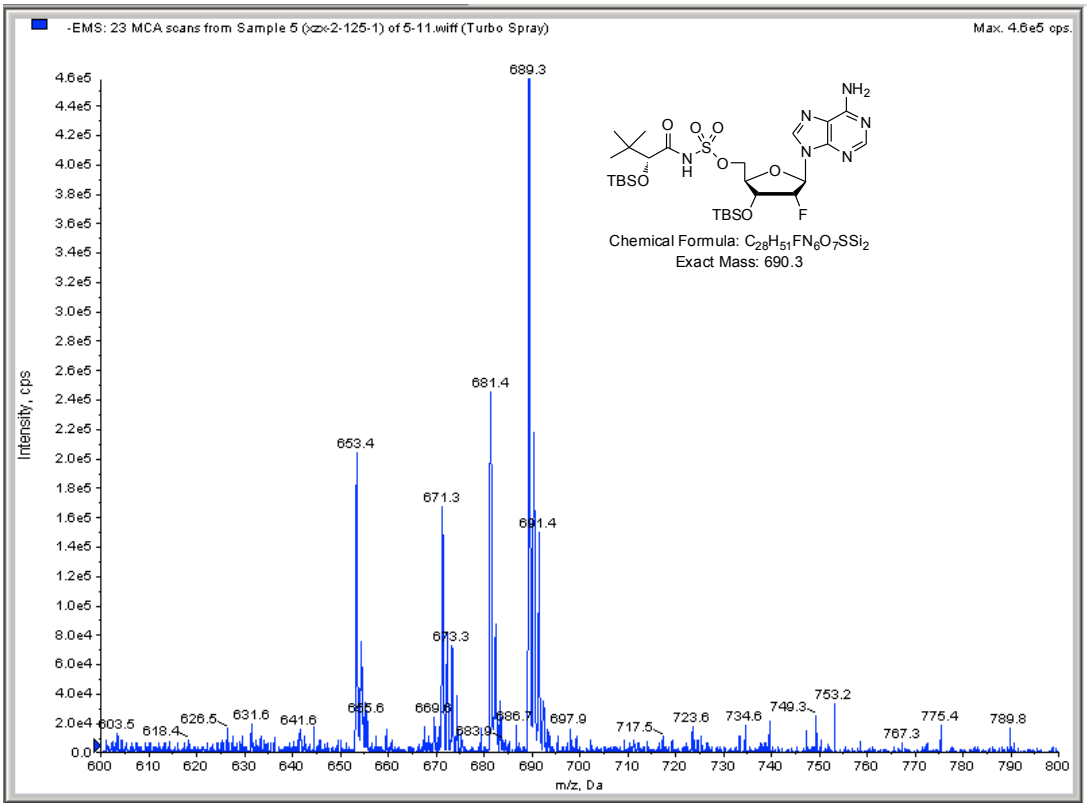




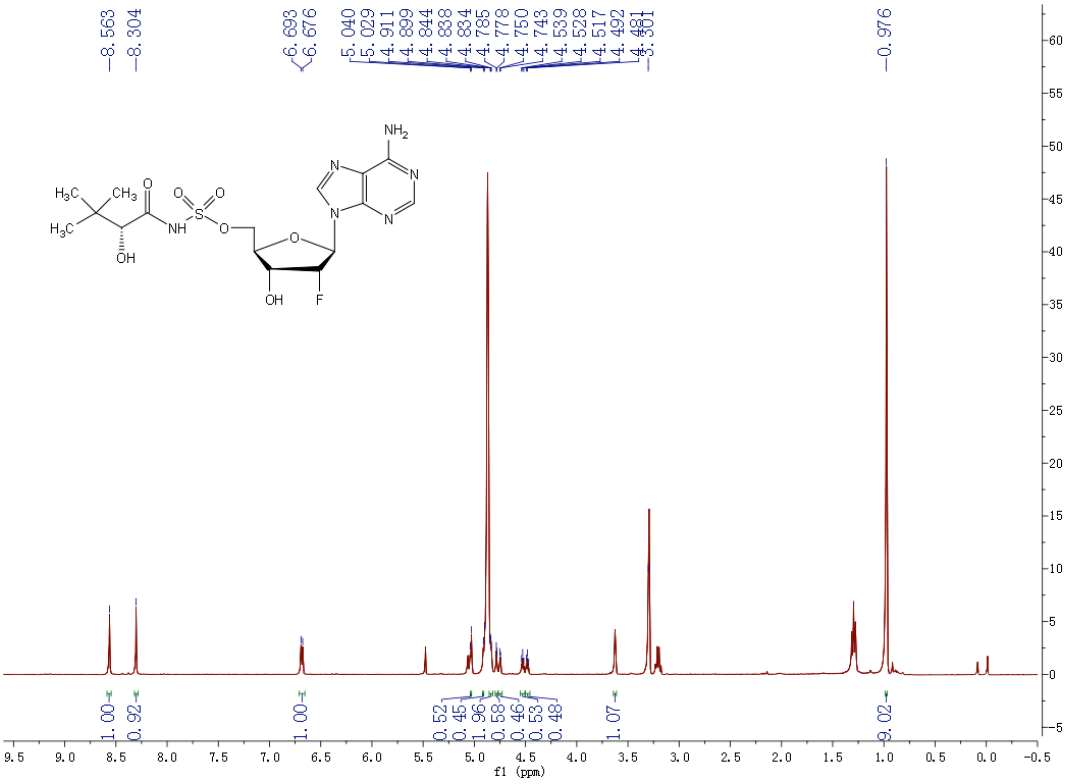
Print of window 80: MS Spectrum

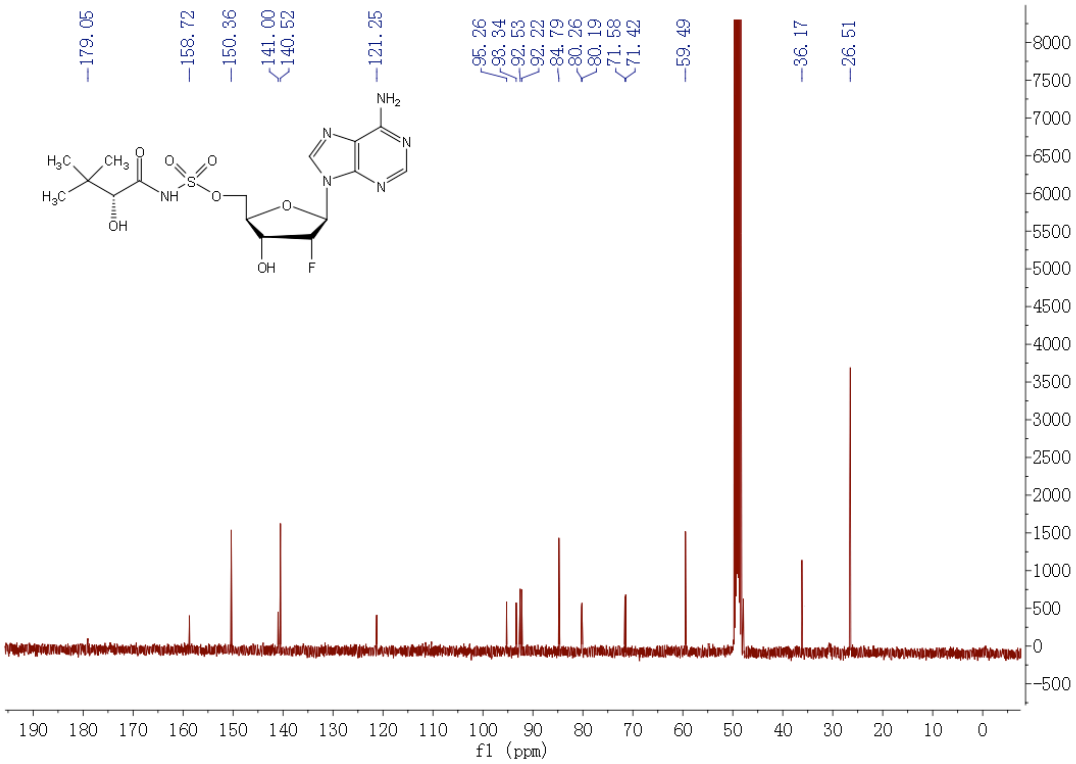


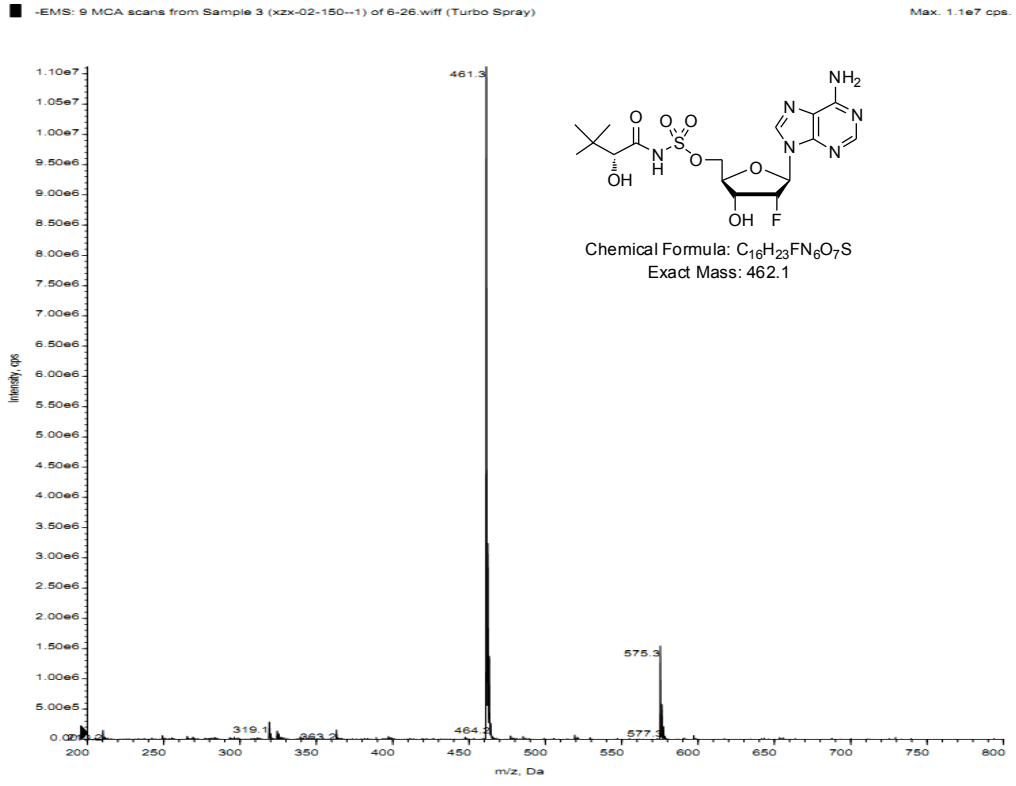
化合物 **21**(MS)

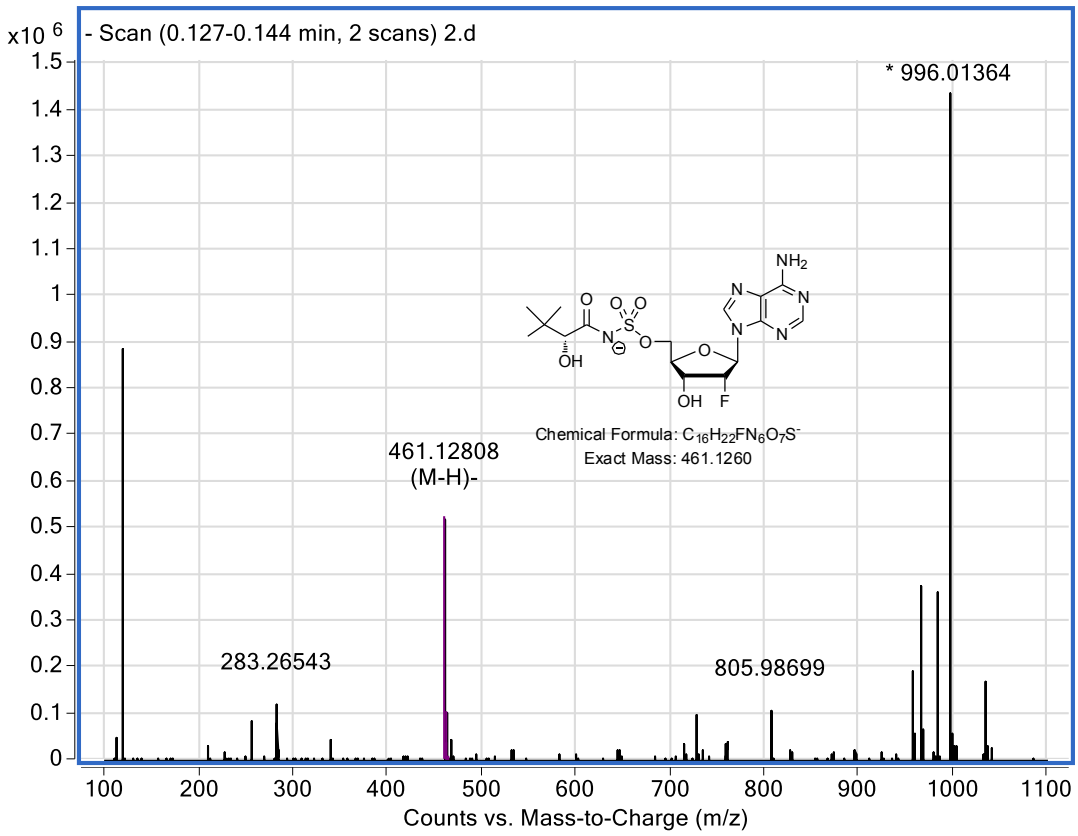


化合物 **3** (^{1}H NMR ^{13}C NMR MS HRMS)

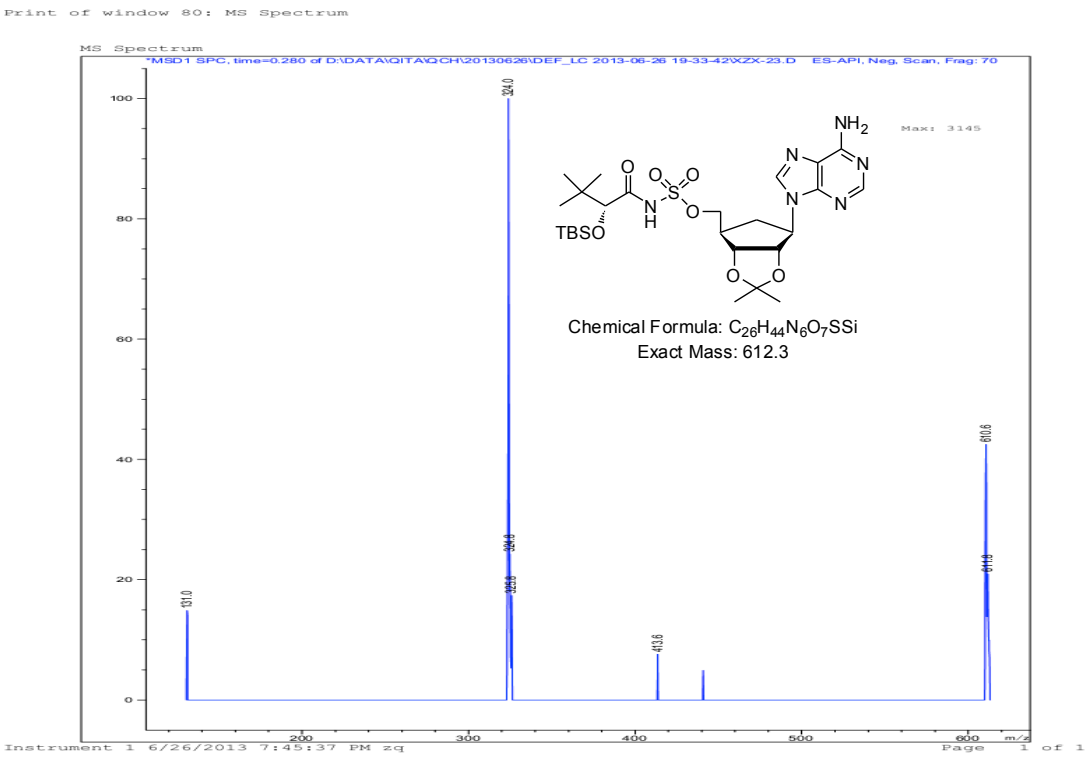



179.05
158.72
150.36
141.00
140.52
121.25
96.26
93.34
92.53
92.22
84.79
80.26
80.19
71.58
71.42
59.49
36.17
26.51
f1 (ppm)

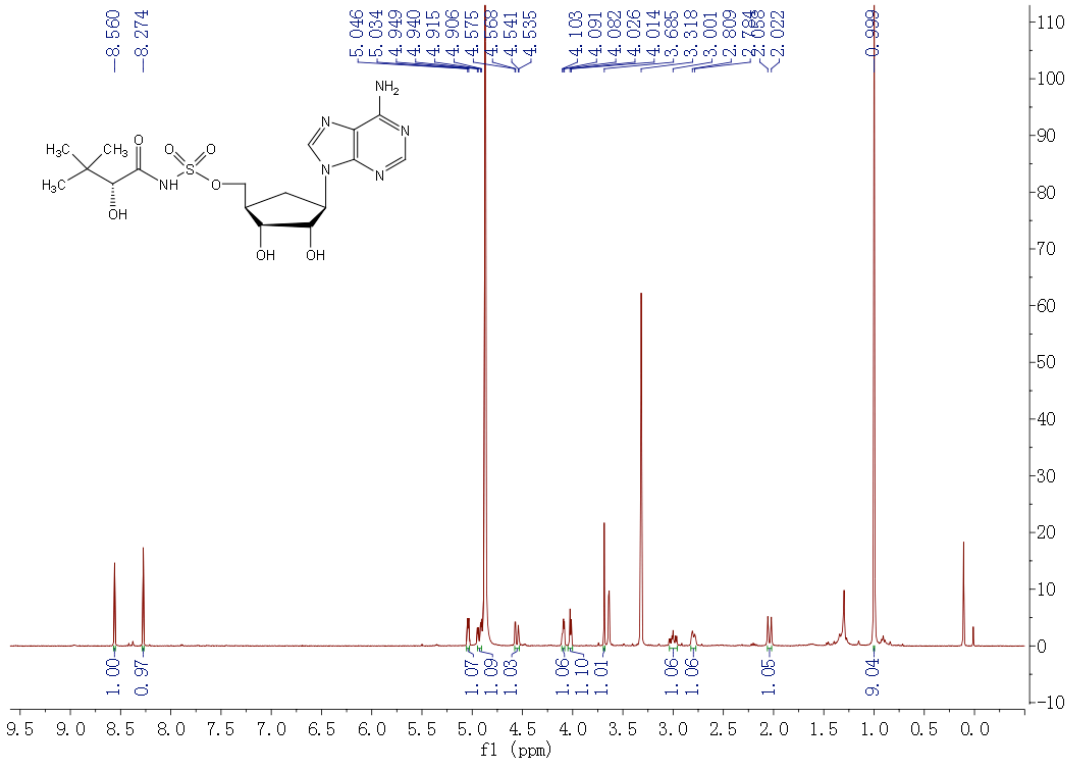

-EMS: 9 MCA scans from Sample 3 (xzx-02-150--1) of 6-26.wiff (Turbo Spray)
Max. 1.1e7 cps.
Intensity, cps
m/z, Da
461.3
575.3
319.1
464.3
577.3
Chemical Formula: C16H23FN6O7S
Exact Mass: 462.1

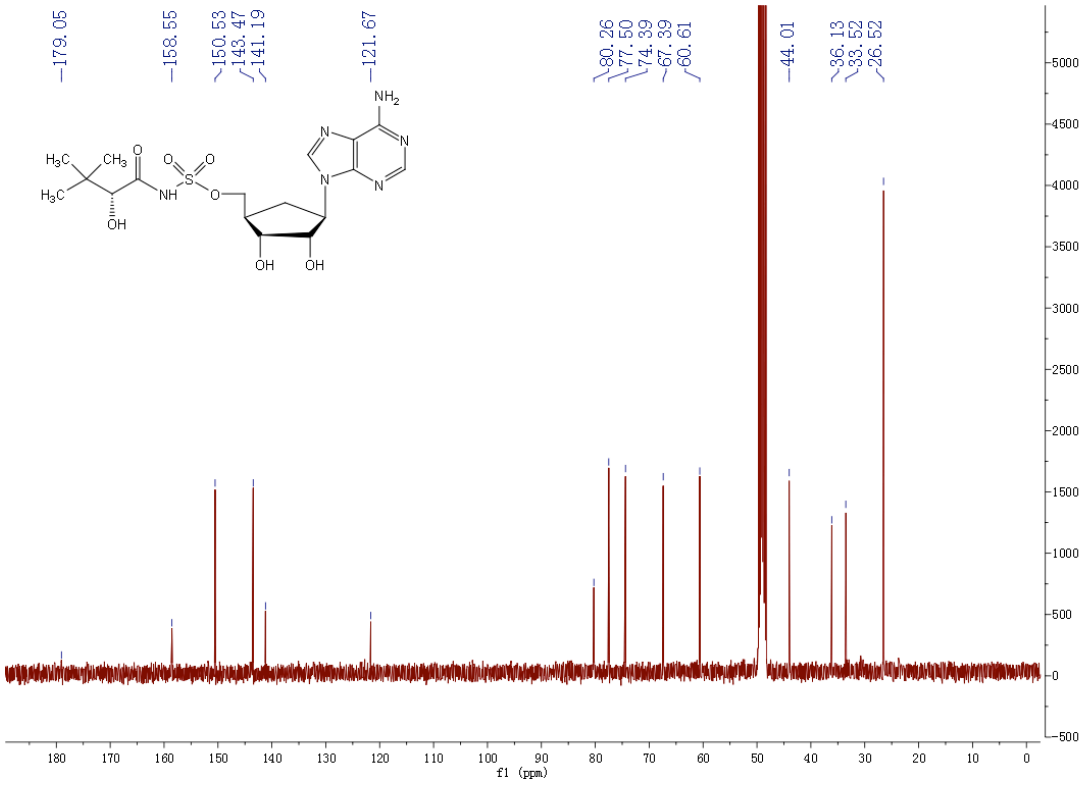

x10 6
- Scan (0.127-0.144 min, 2 scans) 2.d
* 996.01364
461.12808
(M-H)-
283.26543
805.98699
Chemical Formula: C16H22FN6O7S-
Exact Mass: 461.1260
Counts vs. Mass-to-Charge (m/z)

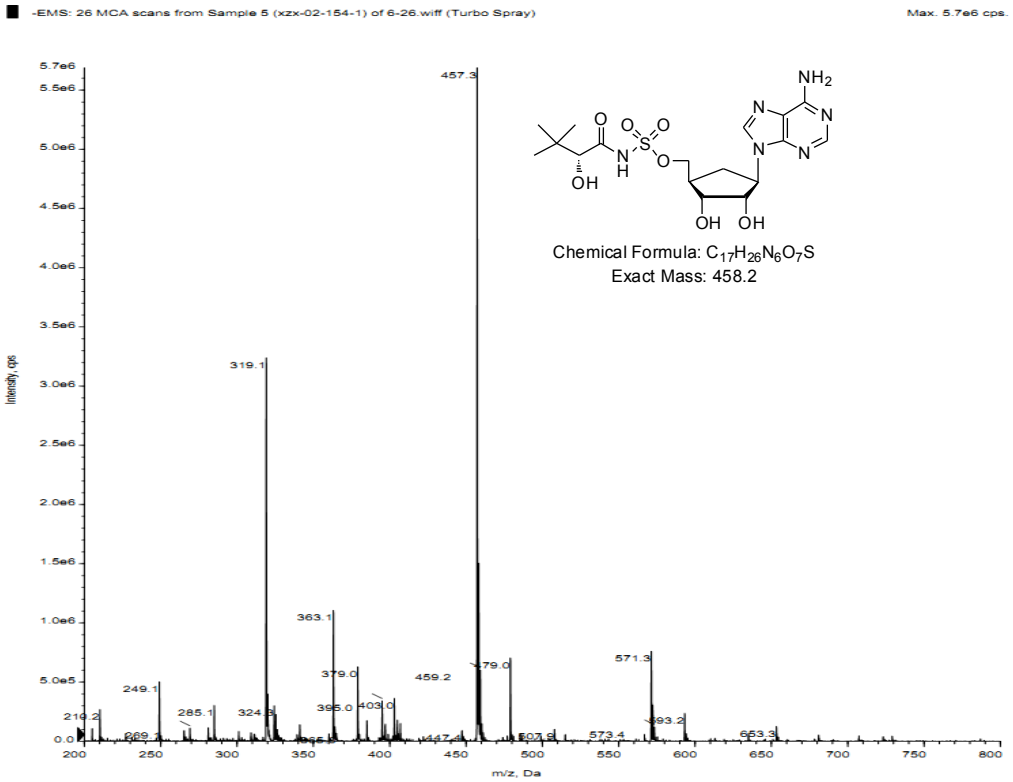
化合物 **23** (MS)


Print of window 80: MS Spectrum
MS Spectrum
*MSD1 SPC, time=0.280 of D:\DATA\QITA\QCH\20130626\DEF_LC 2013-06-26 19-33-42\XZX-23.D ES-API, Neg, Scan, Frag: 70
Max: 3145
TBSO
Chemical Formula: C26H44N6O7SSi
Exact Mass: 612.3
Instrument 1 6/26/2013 7:45:37 PM zq
Page 1 of 1

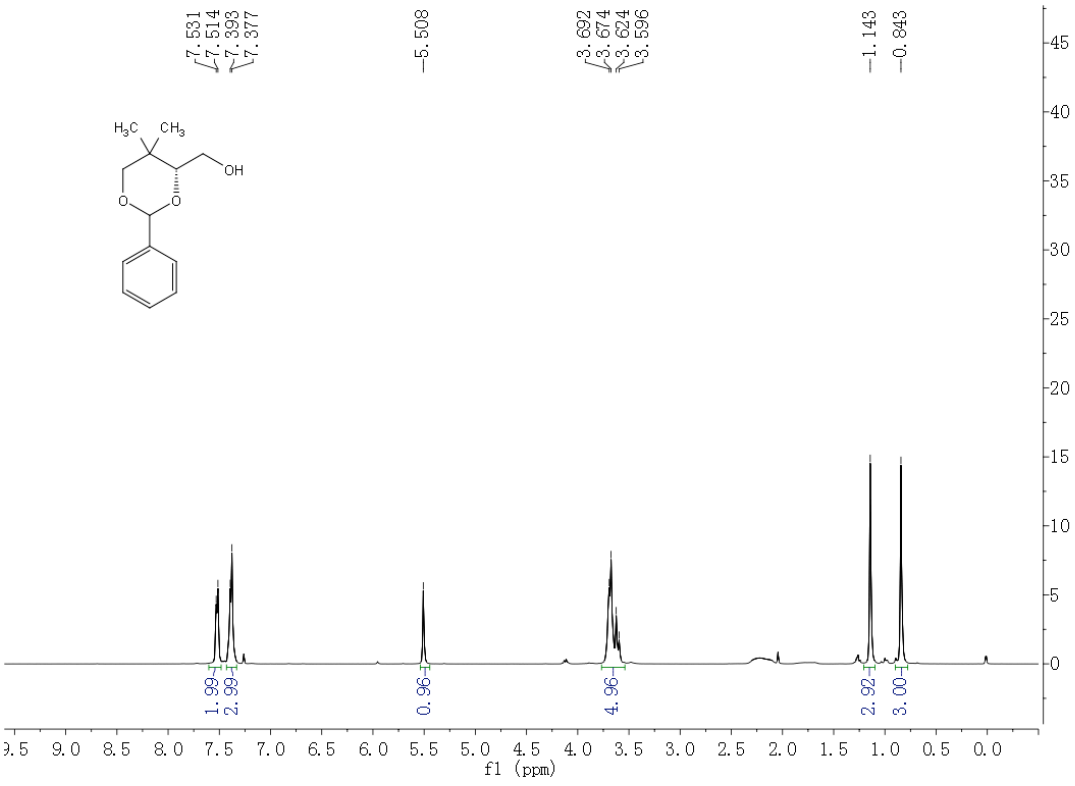
化合物 **4**(^{1}H NMR ^{13}C NMR MS)

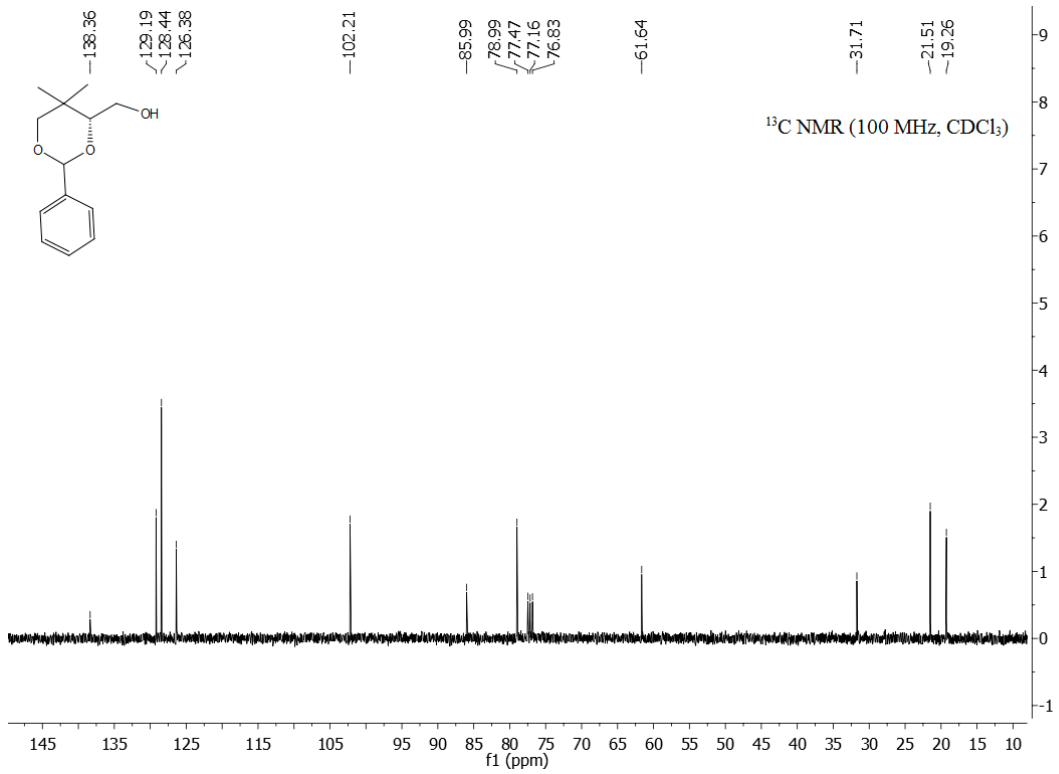




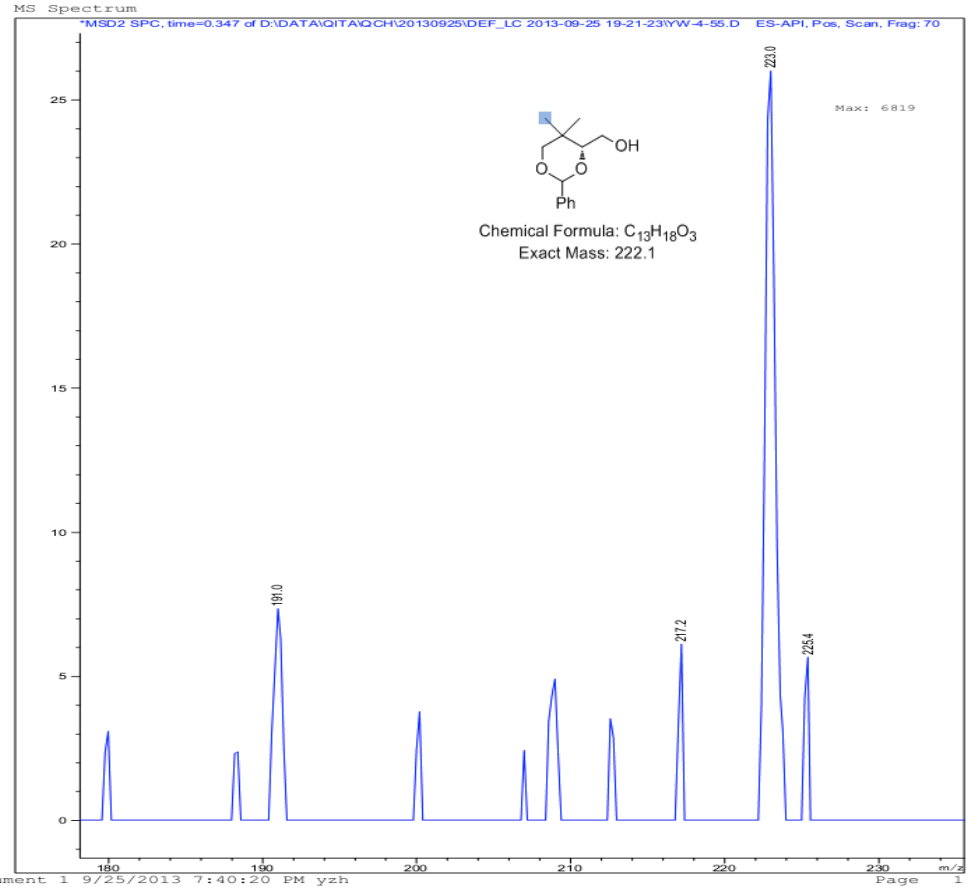


化合物 **26**（^{1}H NMR ^{13}C NMR MS）



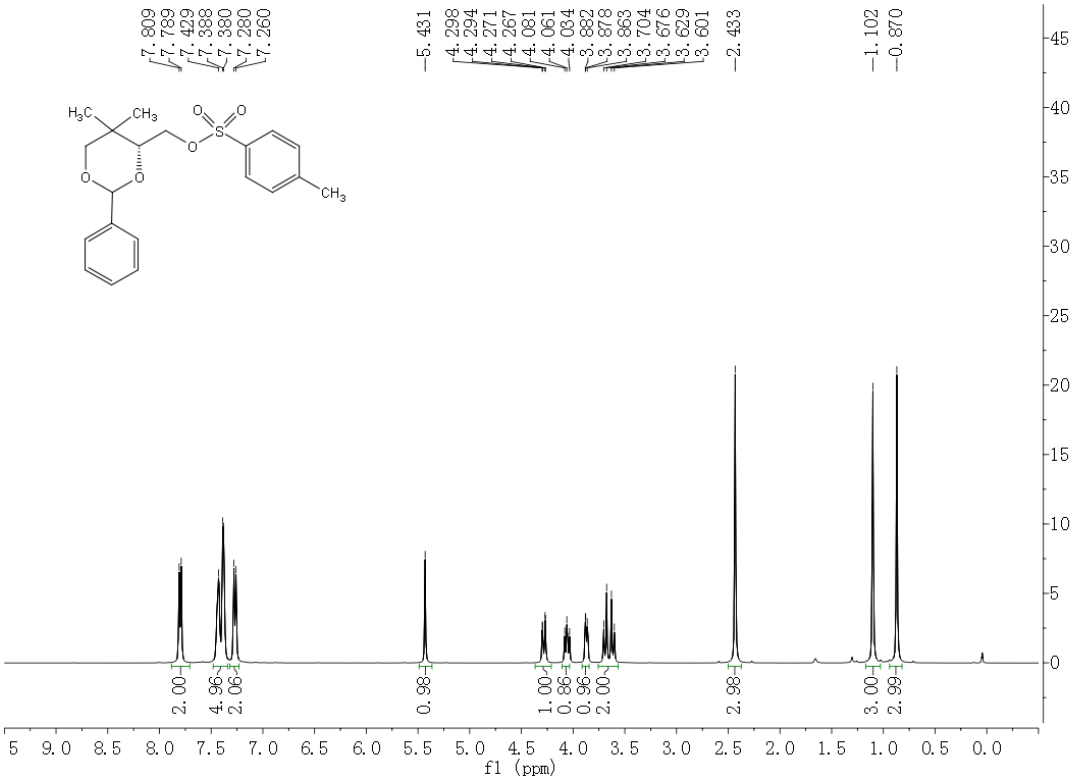


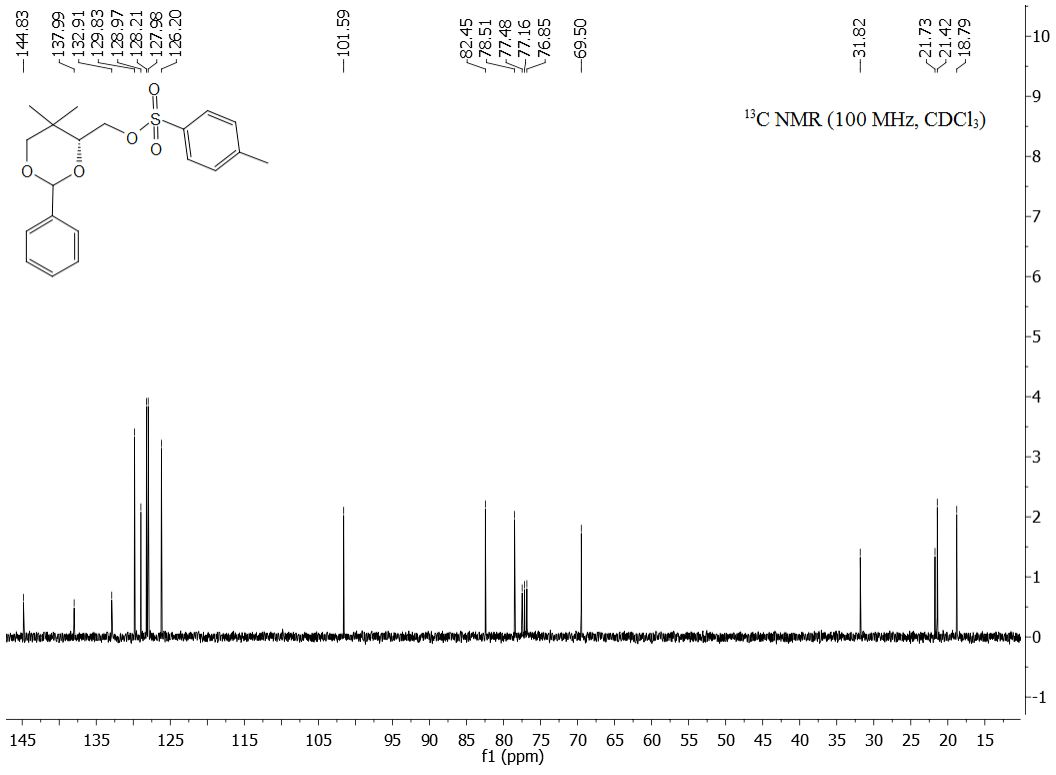
Print of window 80: MS Spectrum

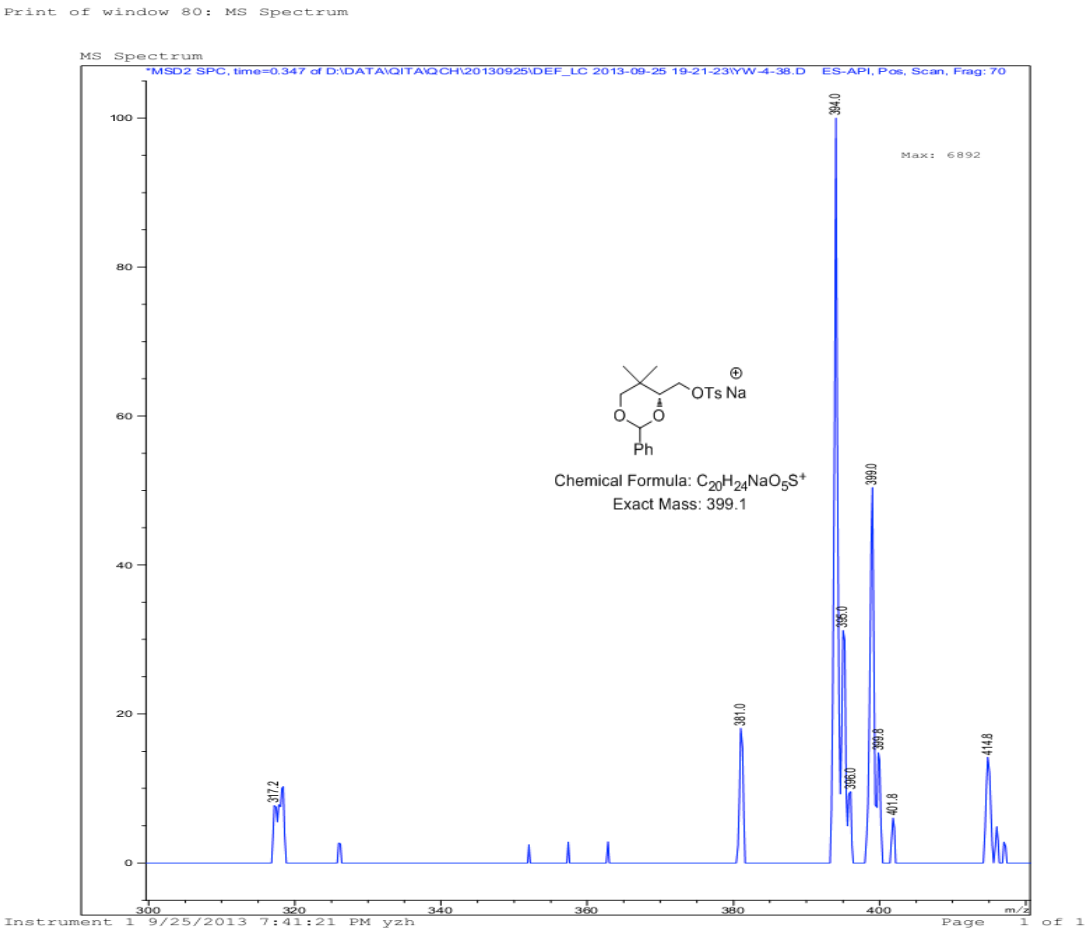


Instrument 1 9/25/2013 7:40:20 PM yzh Page 1 of 1

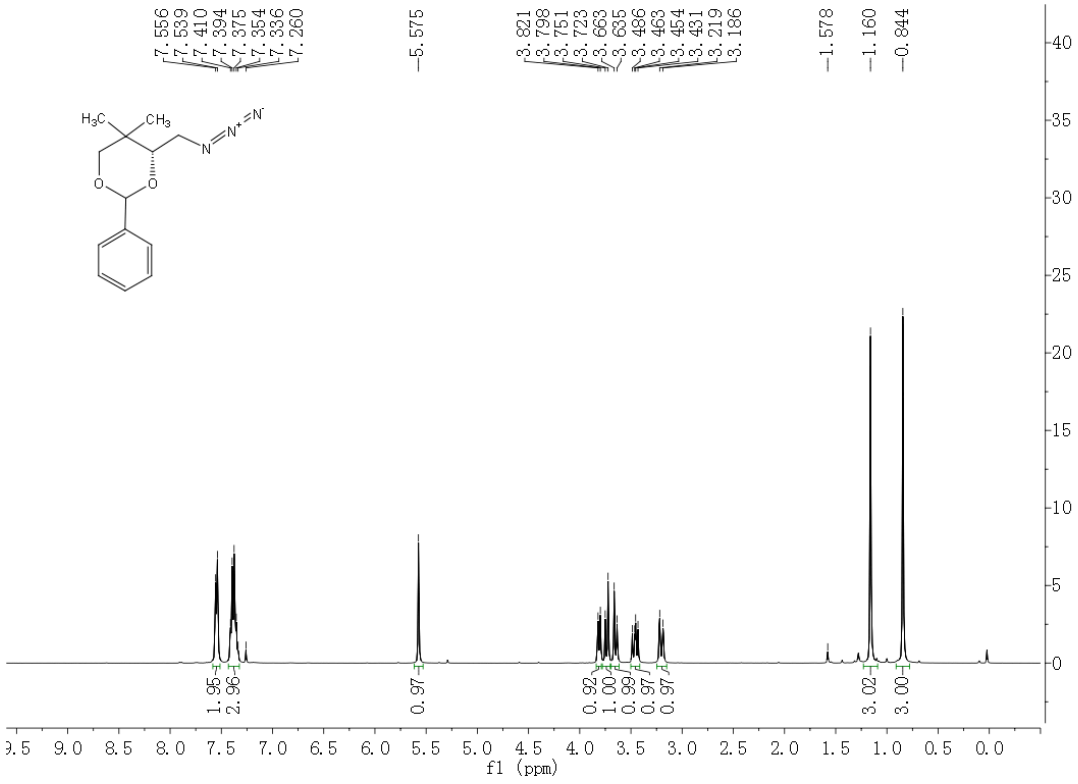
化合物 **27**（^{1}H NMR ^{13}C NMR MS）

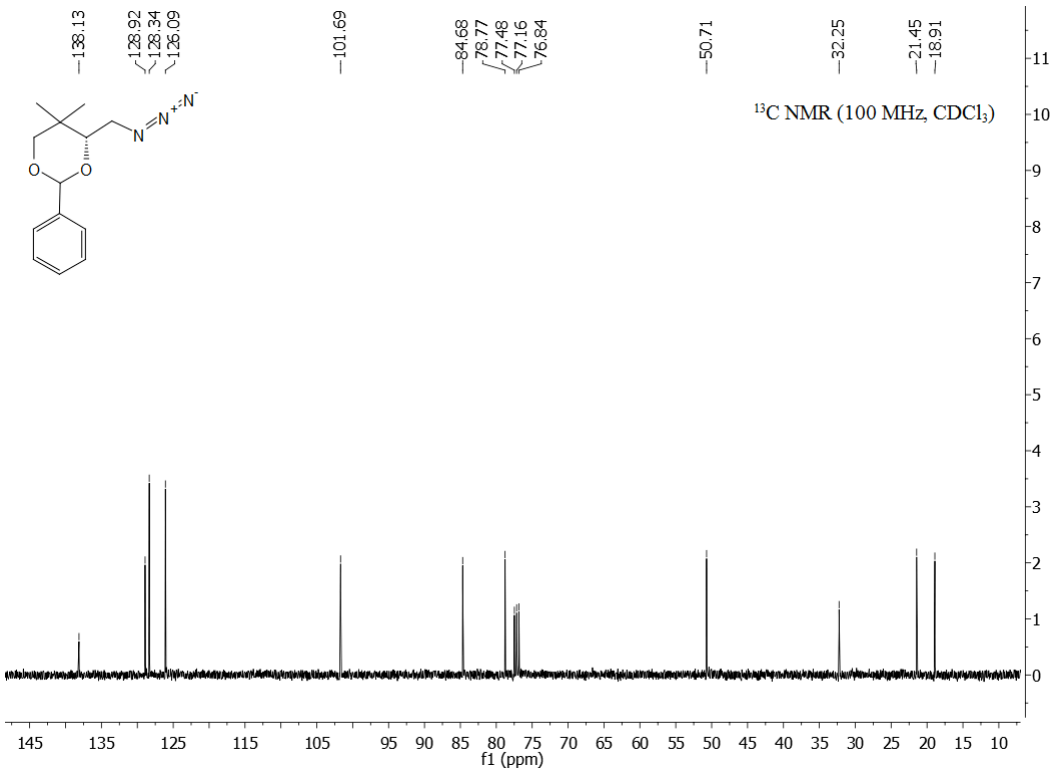




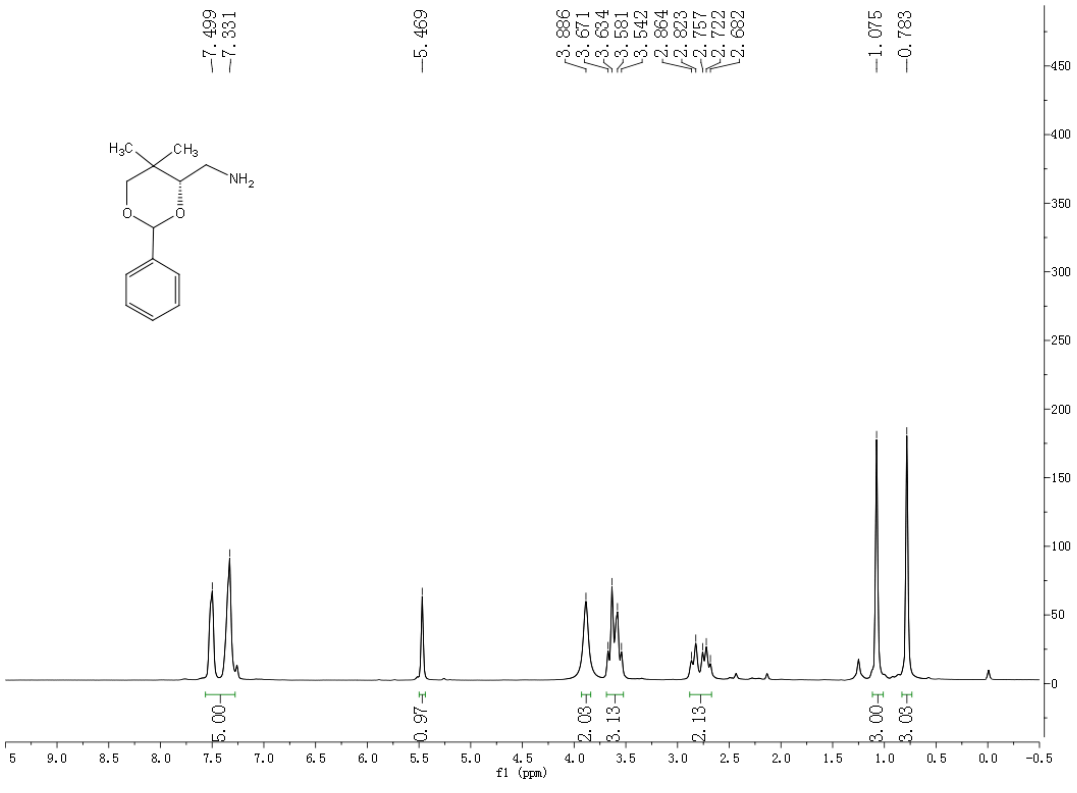


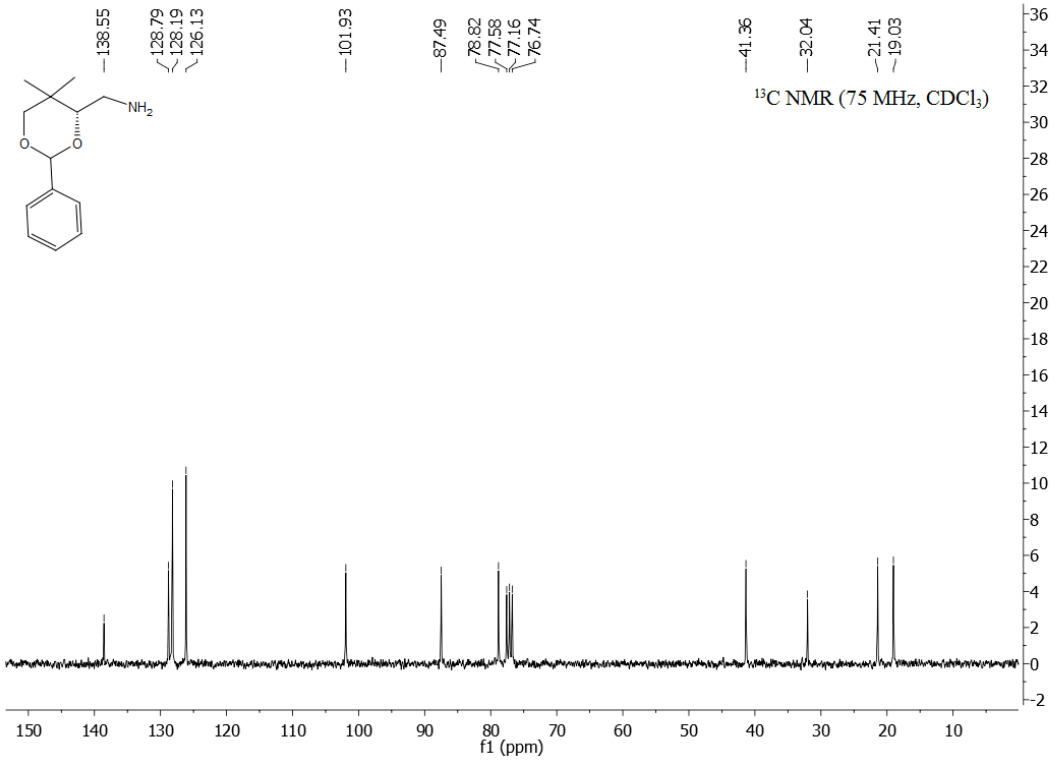
化合物 **28**（^{1}H NMR，^{13}C NMR）



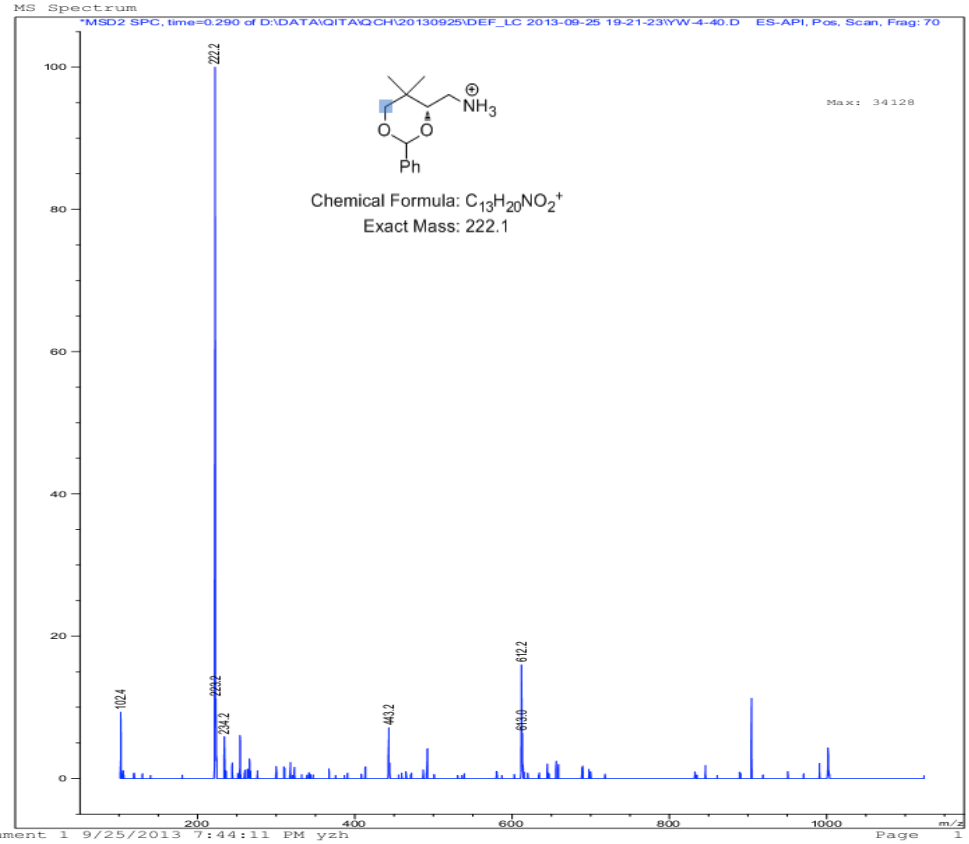


化合物 **29**（^{1}H NMR，^{13}C NMR）



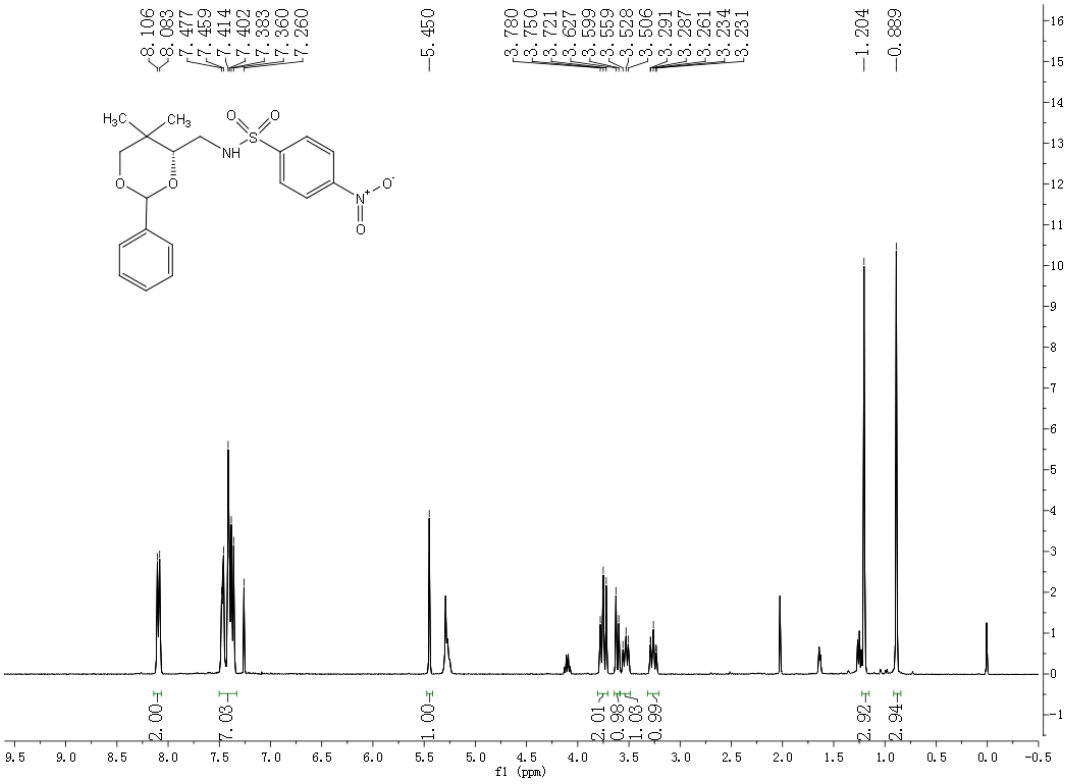


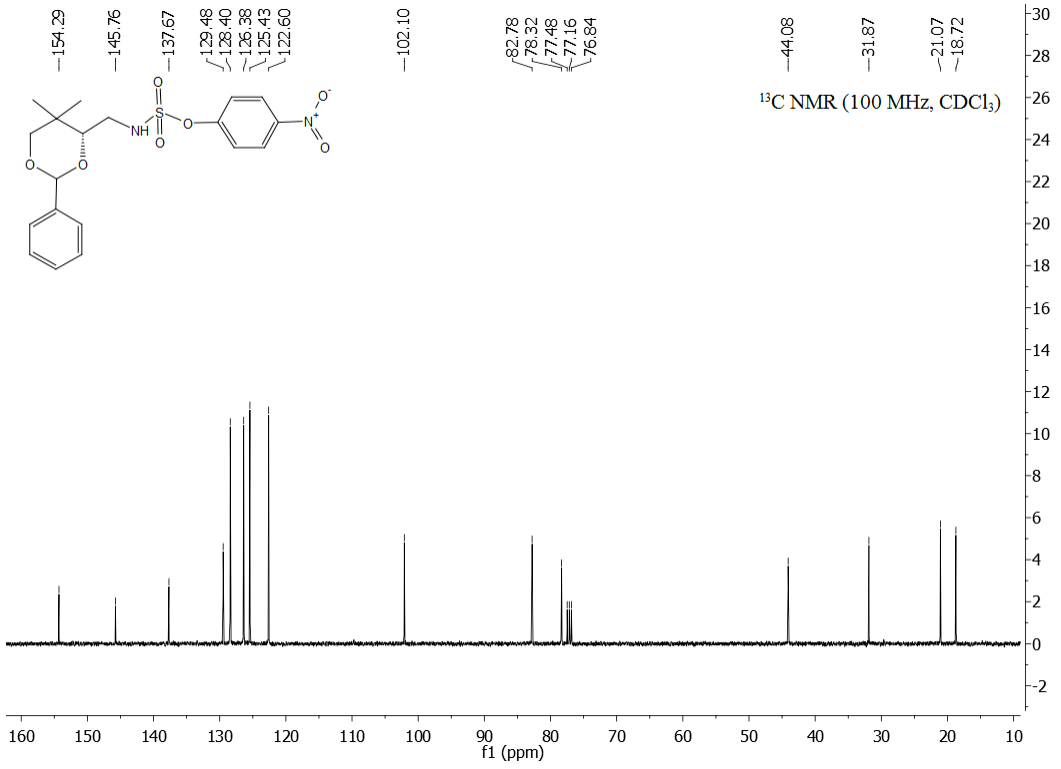
Print of window 80: MS Spectrum

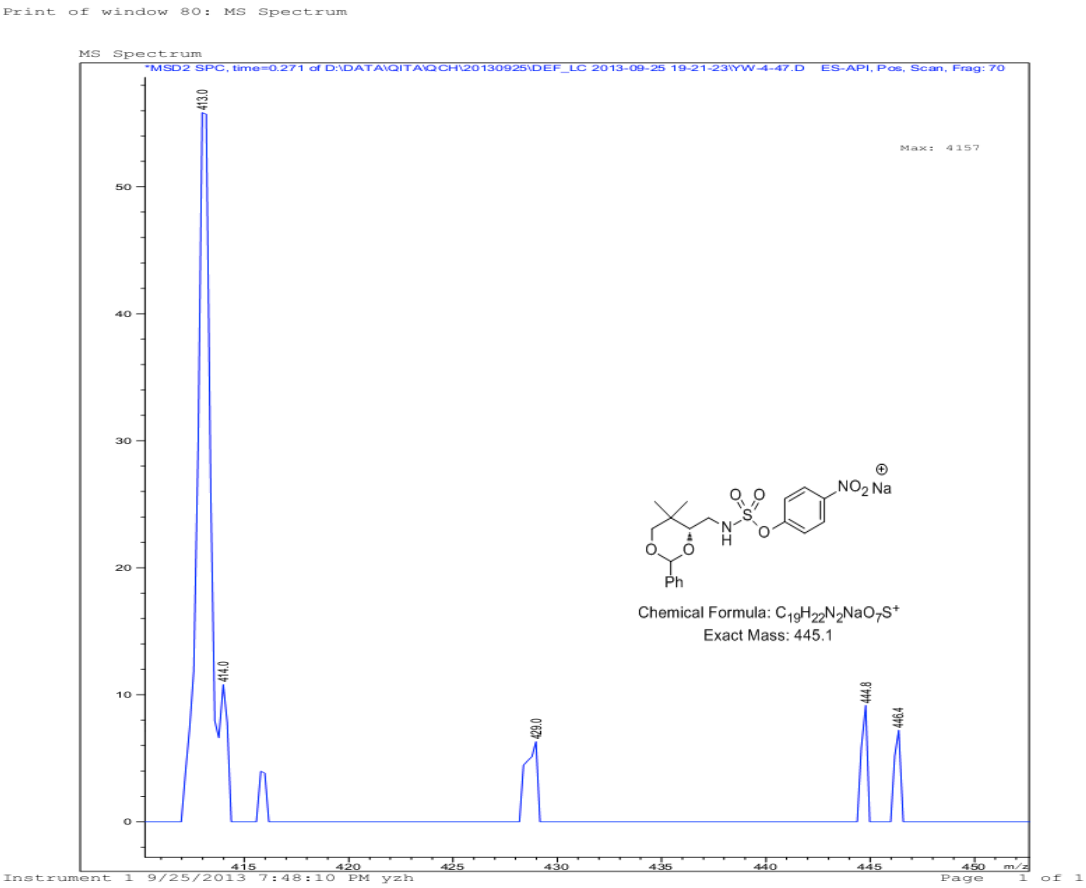


Instrument 1 9/25/2013 7:44:11 PM yzh Page 1 of 1

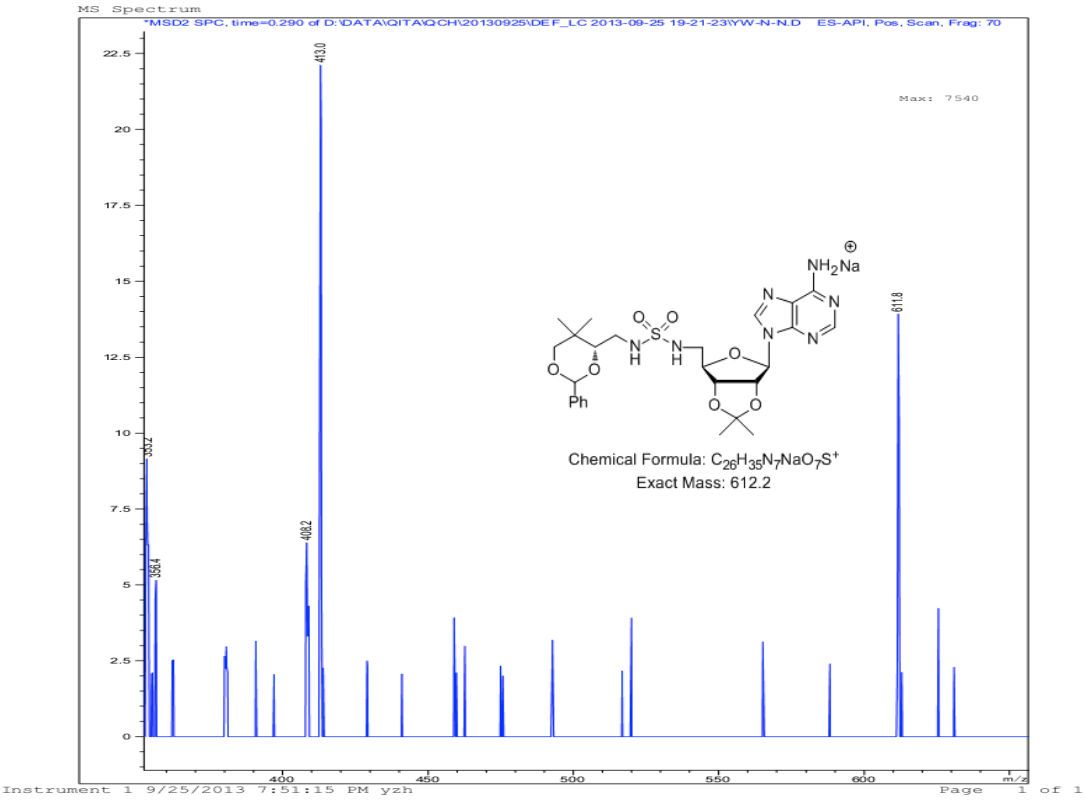
化合物 **30**（^{1}H NMR，^{13}C NMR）



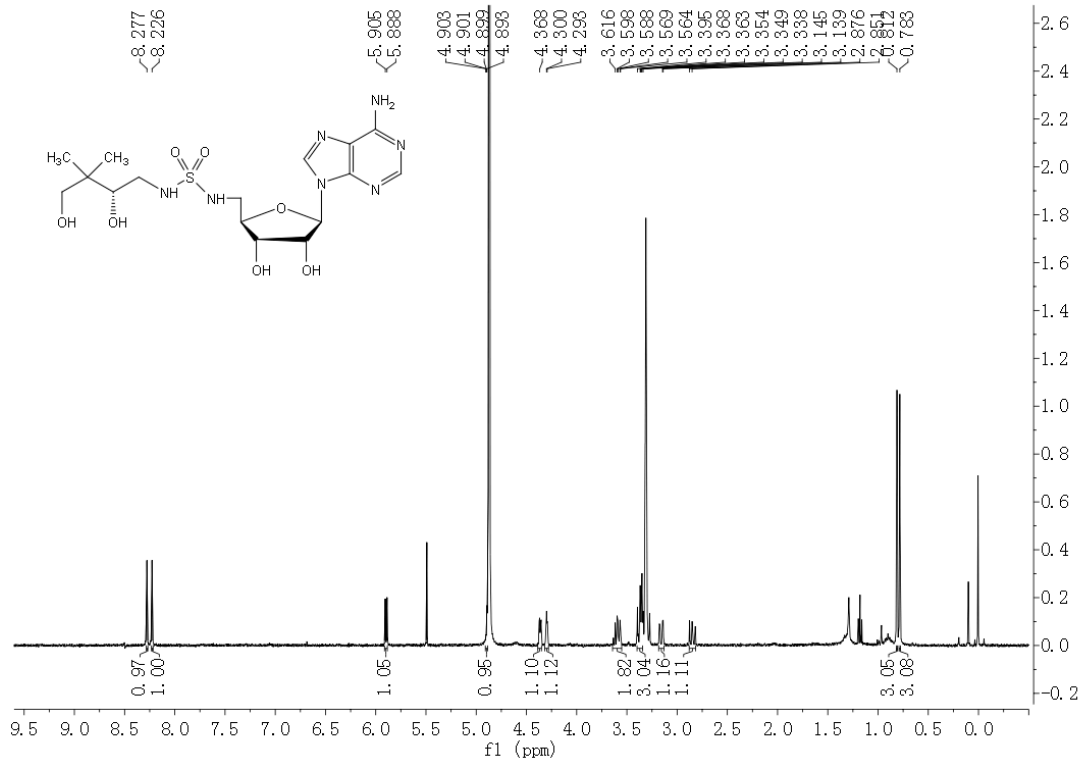


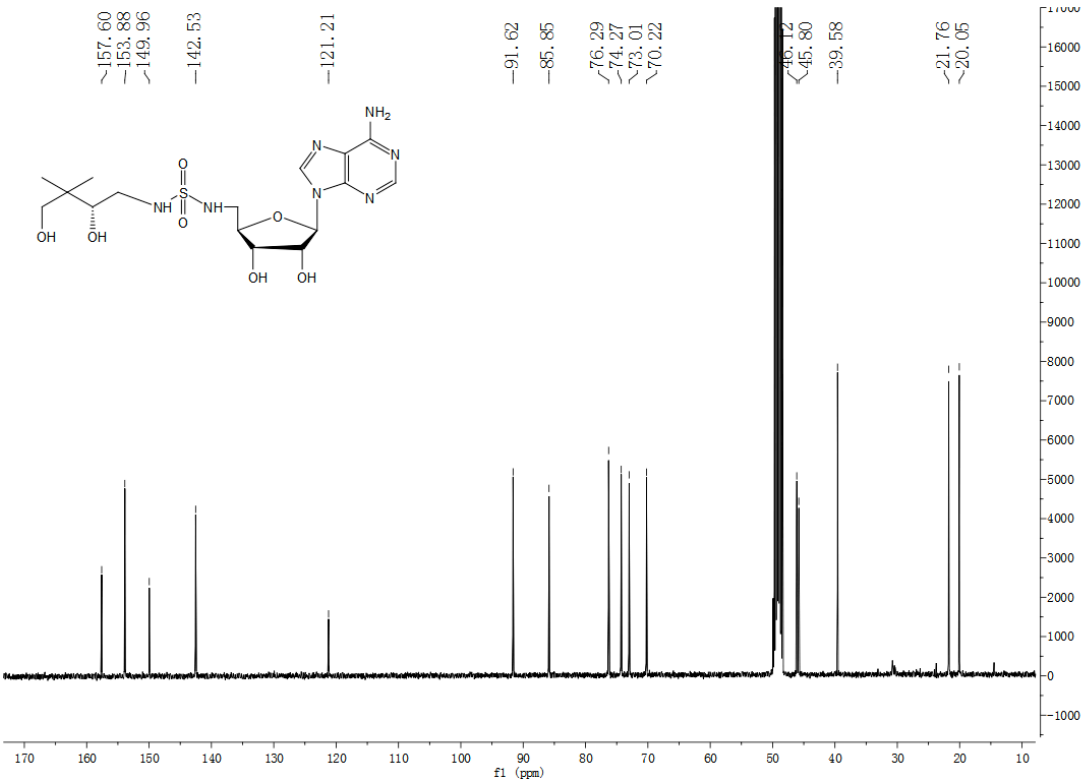

Print of window 80: MS Spectrum
MS Spectrum
*MSD2 SPC, time=0.271 of D:\DATA\QITA\QCH\20130925\DEF_LC 2013-09-25 19-21-23\YW-4-47.D ES-API, Pos, Scan, Frag: 70
Max: 4157
413.0
414.0
429.0
444.8
446.4
Chemical Formula: C19H22N2NaO7S+
Exact Mass: 445.1
Instrument 1 9/25/2013 7:48:10 PM yzh
Page 1 of 1

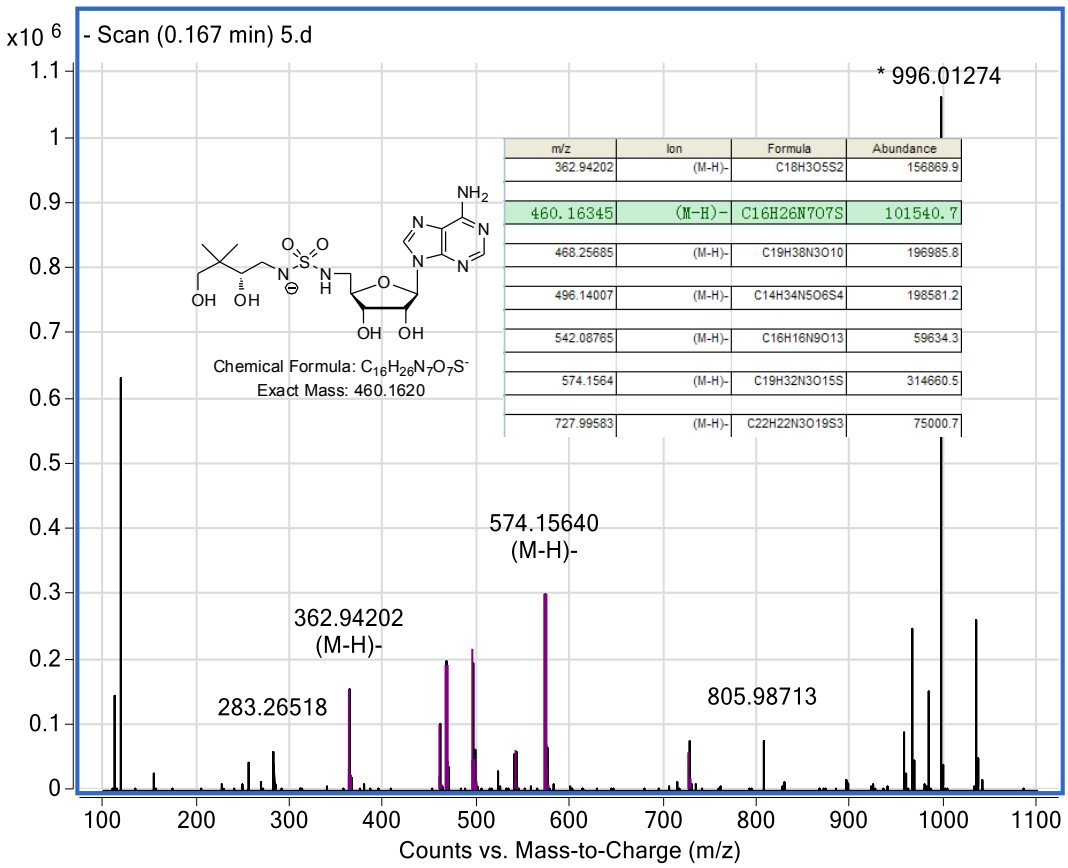
化合物 **32**（MS）


Print of window 80: MS Spectrum
MS Spectrum
*MSD2 SPC, time=0.290 of D:\DATA\QITA\QCH\20130925\DEF_LC 2013-09-25 19-21-23\YW-N-N.D ES-API, Pos, Scan, Frag: 70
Max: 7540
413.0
611.8
352.2
356.4
408.2
Chemical Formula: C26H35N7NaO7S+
Exact Mass: 612.2
Instrument 1 9/25/2013 7:51:15 PM yzh
Page 1 of 1

化合物 **5**（^{1}H NMR ^{13}C NMR HRMS）







m/z	Ion	Formula	Abundance
362.94202	(M-H)-	C18H3O5S2	156869.9
460.16345	(M-H)-	C16H26N7O7S	101540.7
468.25685	(M-H)-	C19H38N3O10	196985.8
496.14007	(M-H)-	C14H34N5O6S4	198581.2
542.08765	(M-H)-	C16H16N9O13	59634.3
574.1564	(M-H)-	C19H32N3O15S	314660.5
727.99583	(M-H)-	C22H22N3O19S3	75000.7