Supplementary Material

Synthesis of N3-Substituted Carboranyl Thymidine Bioconjugates and their Evaluation as Substrates of Recombinant Human Thymidine Kinase 1

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1. HPLC methods.

Preparative HPLC was performed with a Gemini 5μ C18 column (21.20 mm x 250 mm, 5 μm particle size) supplied by Phenomenex Inc. CA, USA on a Hitachi HPLC system (L-2130) with a Windows based data acquisition and a Hitachi Diode array detector (L-2455). Purification was accomplished using a water (0.1% trifluoroacetic acid)/methanol (0.1% trifluoroacetic acid) gradient at 7 mL/min flow rate (method: 100:0 to 50:50 over 70 min followed by 50:50 to 0:100 over 40 min).

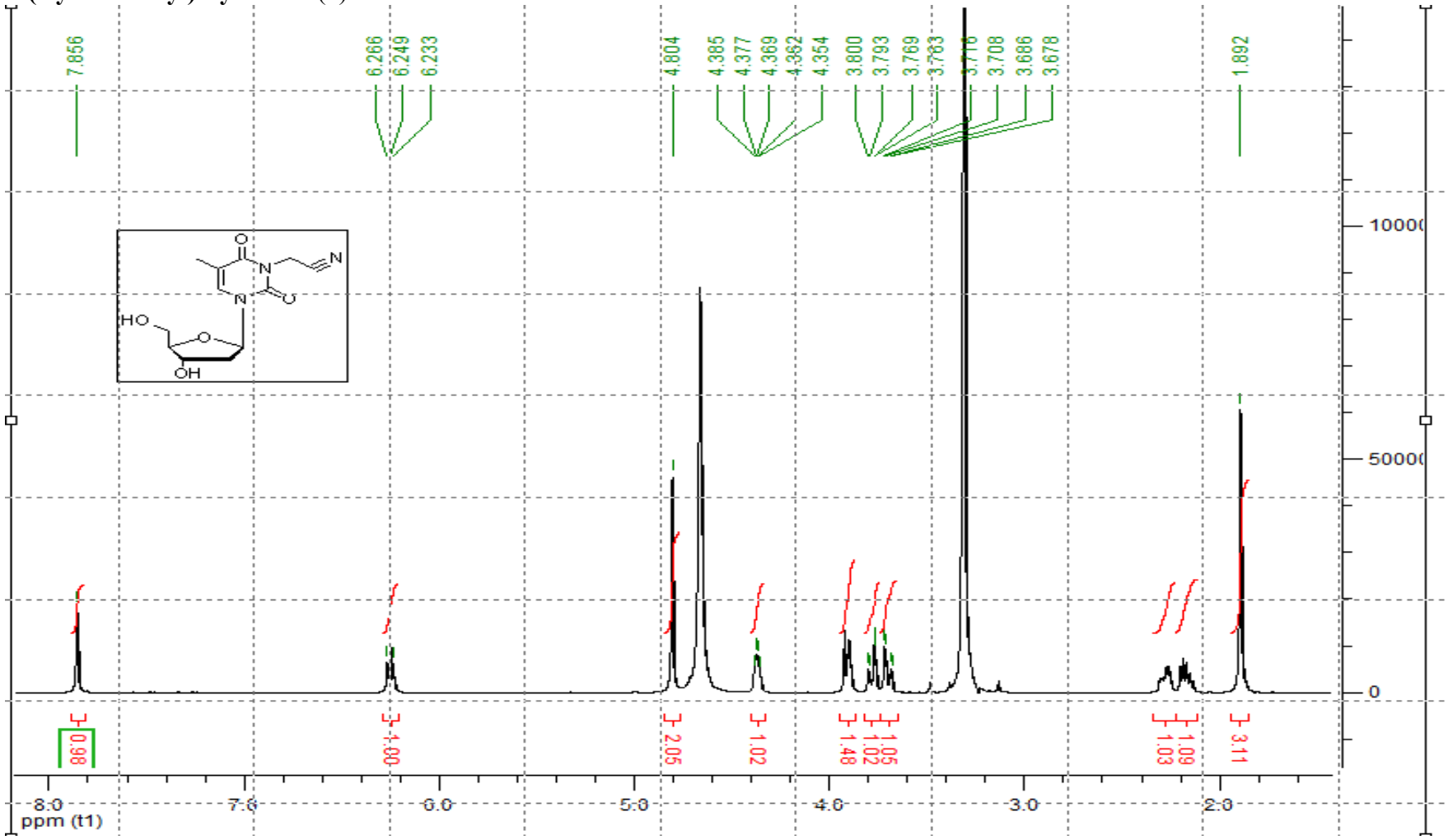
Table S1. HPLC method used for the purification of the compounds.

Time (minutes)	Water Concentration A (%)	Acetonitrile Concentration B (%)	Flow rate (mL/min)
0.00	100.0	0.0	1.0
1.0	100.0	0.0	7.0
70.0	0.0	50.0	7.0
110.0	0.0	100.0	7.0
119.0	100.0	0.0	7.0
120.0	100.0	0.0	1.0

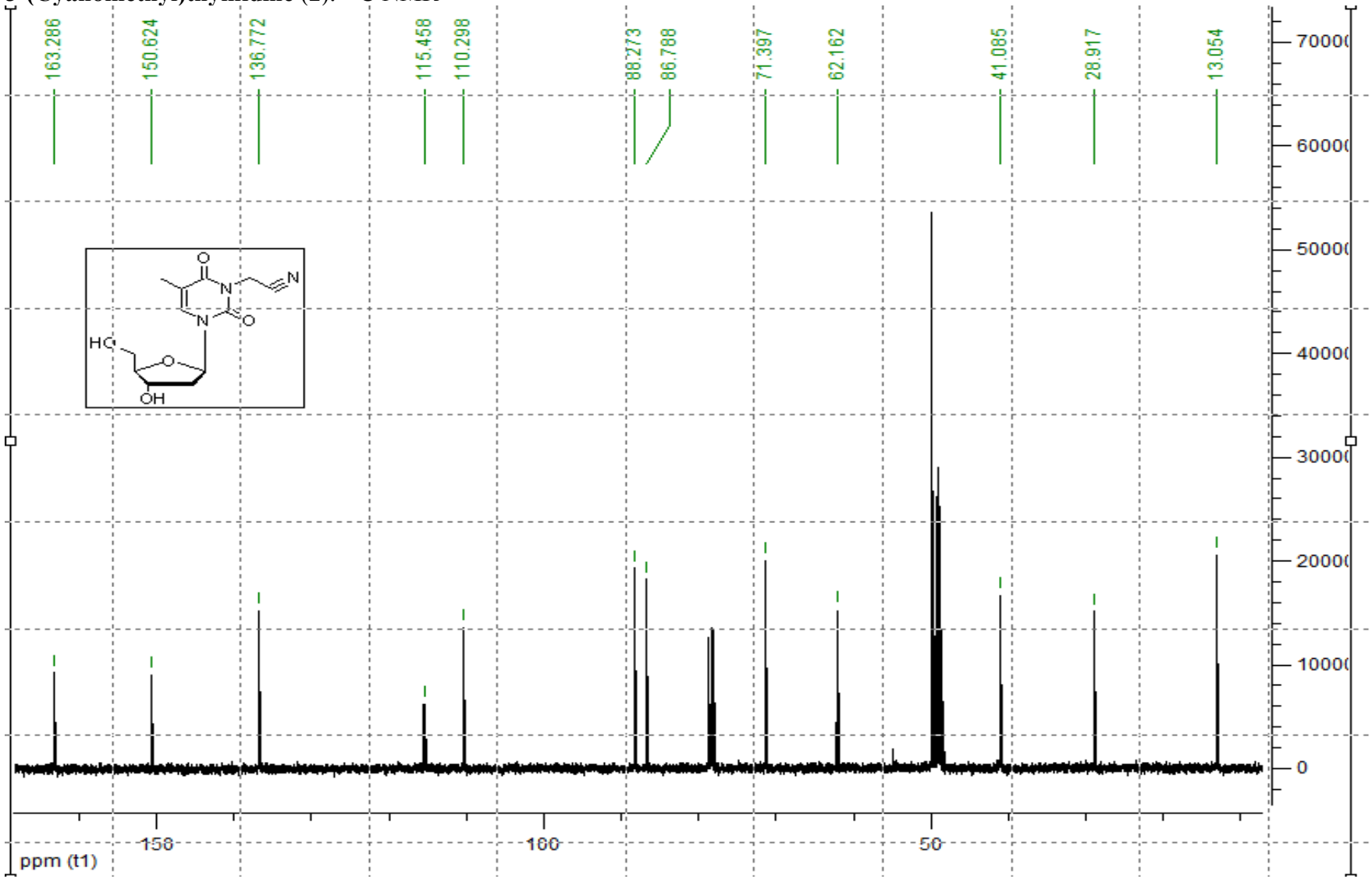
Analytical HPLC was carried out with a Gemini 5μ C18 110A Column (250 x 4.6 mm) supplied by Phenomenex Inc. CA, USA using the HPLC system above. Two different gradients [water (0.1% trifluoroacetic acid)/acetonitrile (0.1% trifluoroacetic acid) and water (0.1% trifluoroacetic acid)/methanol (0.1% trifluoroacetic acid)] were used at 1 mL/min flow rate (method: 100:0 to 75:25 over 20 min followed by 75:25 to 100:0 over 10 min).

2. High resolution mass-, ^{1}H-NMR-, and ^{13}C NMR spectra and analytical HPLC traces in two different solvent systems

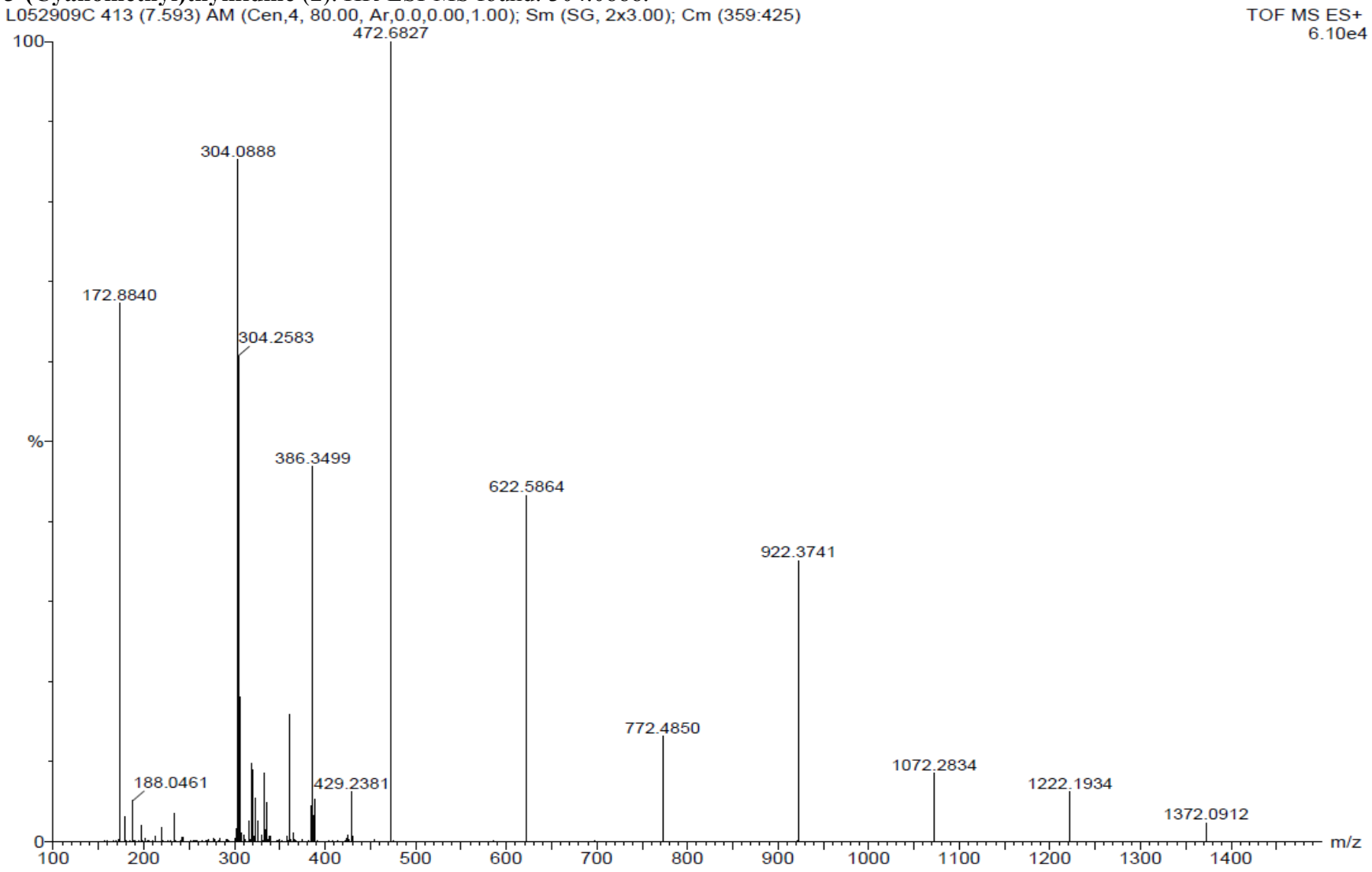
3-(Cyanomethyl)thymidine (2). ^{1}H NMR



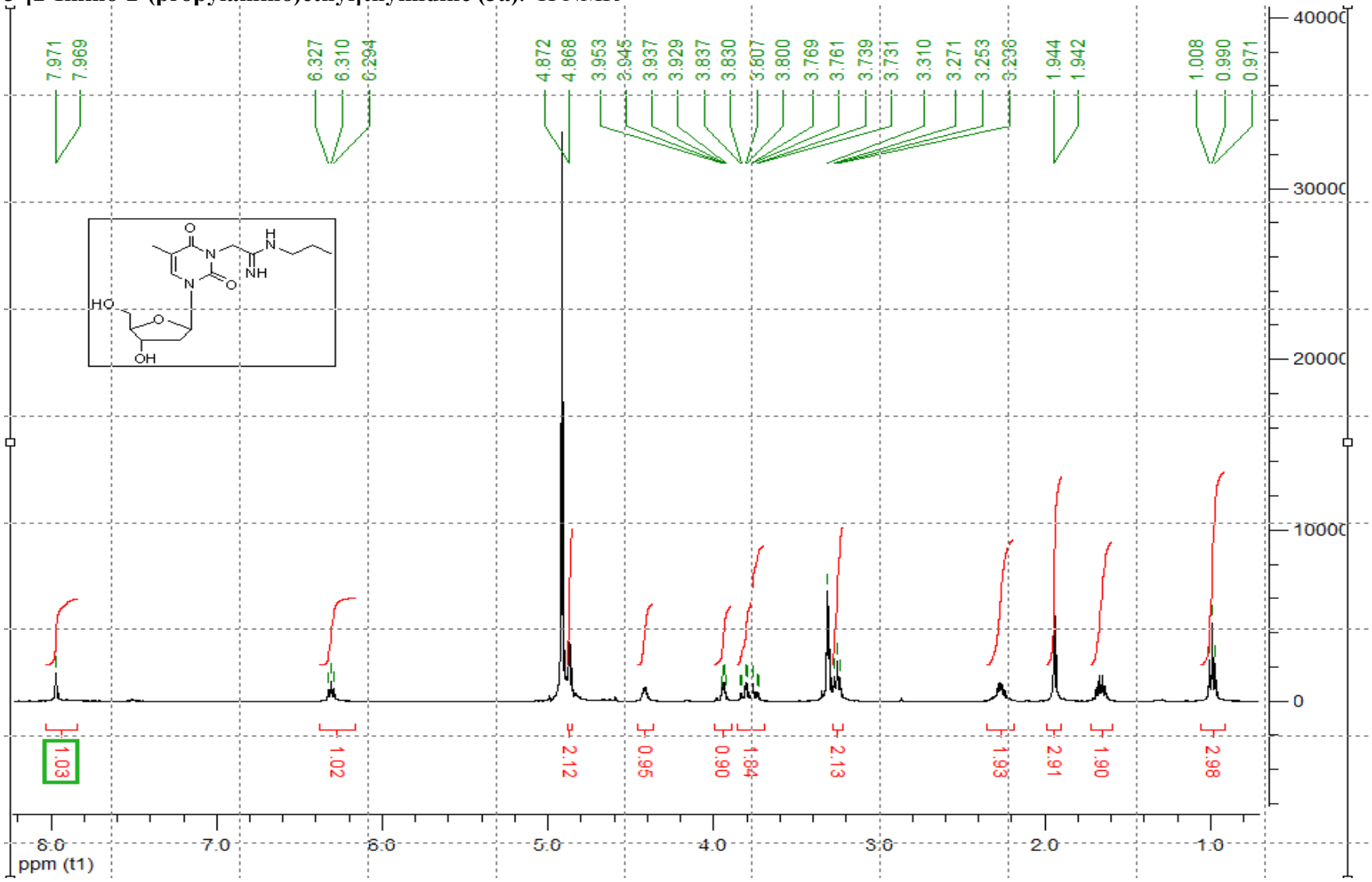
3-(Cyanomethyl)thymidine (**2**). ^{13}C NMR



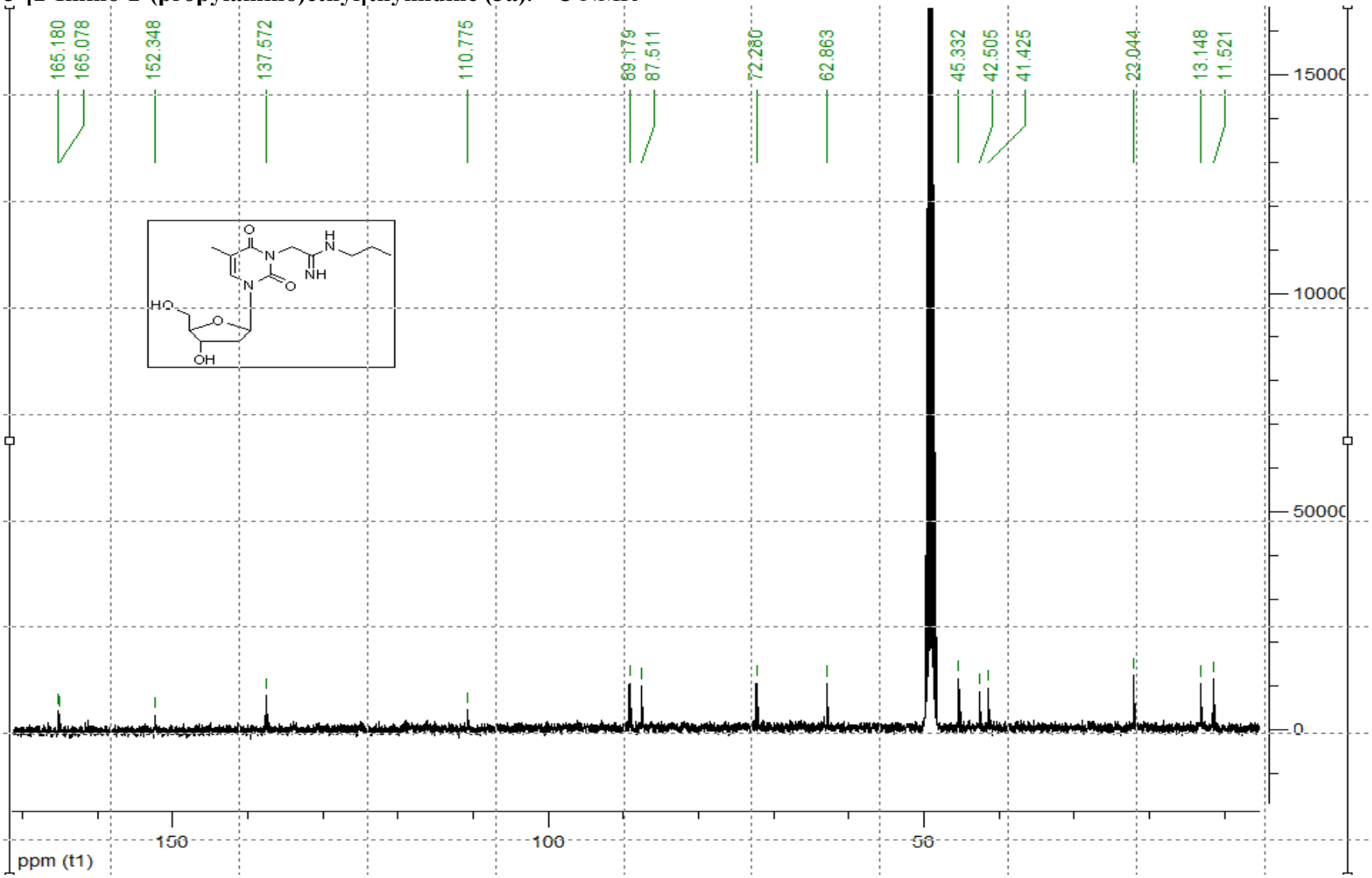
3-(Cyanomethyl)thymidine (**2**). HR-ESI-MS found: 304.0888.



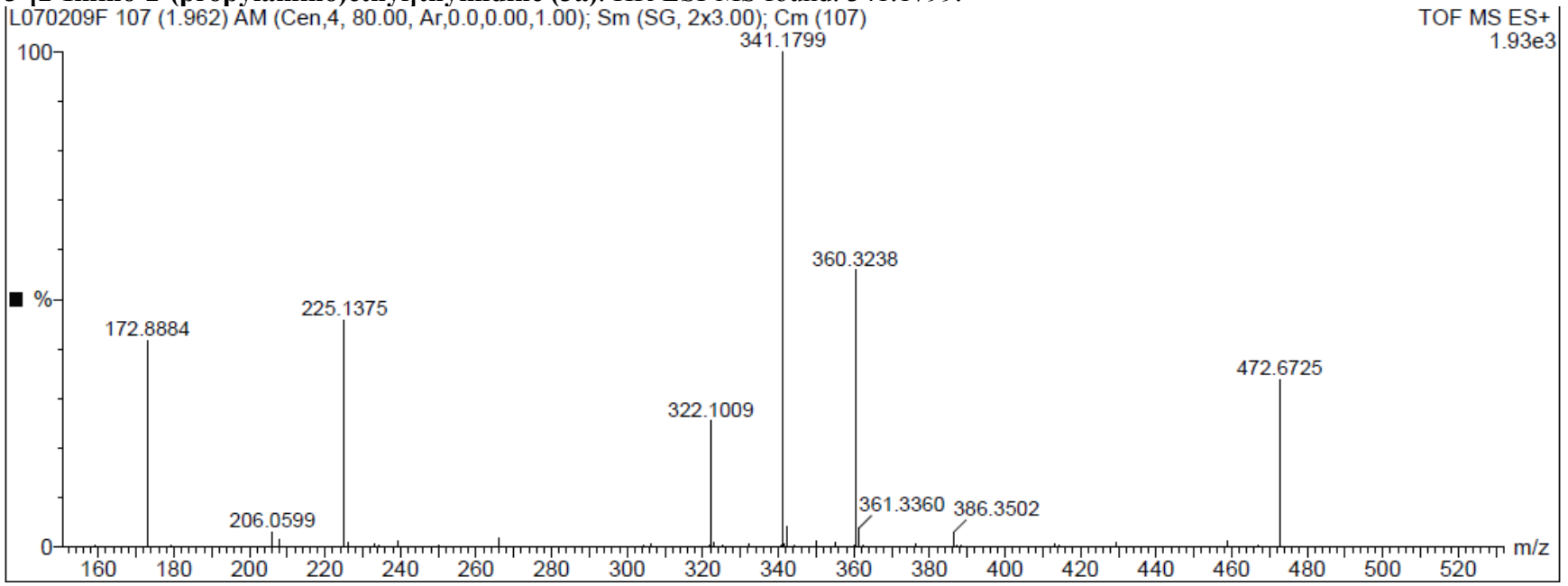
3-[2-Imino-2-(propylamino)ethyl]thymidine (3a). ^{1}H NMR



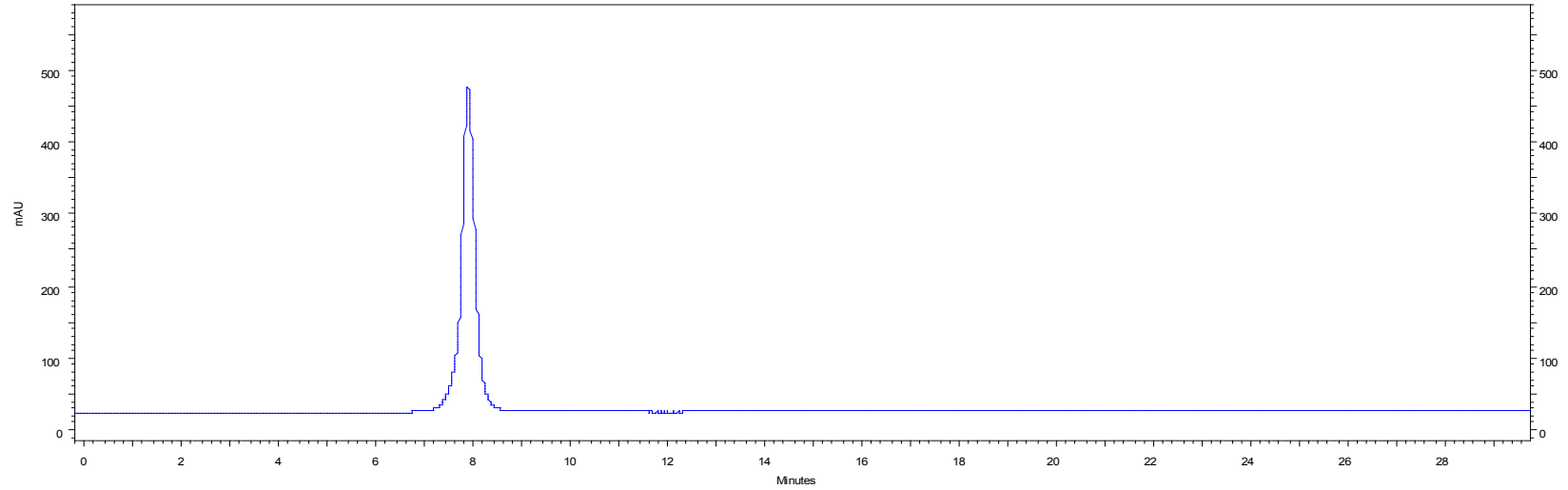
3-[2-Imino-2-(propylamino)ethyl]thymidine (3a). ^{13}C NMR



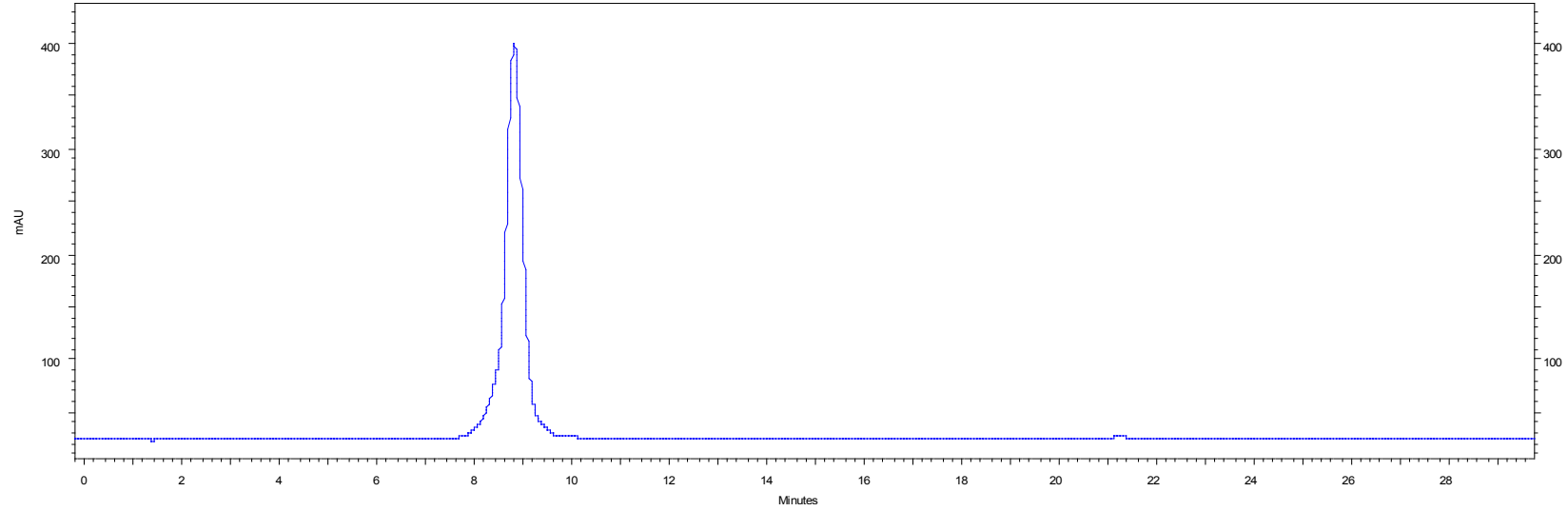
3-[2-Imino-2-(propylamino)ethyl]thymidine (3a). HR-ESI-MS found: 341.1799.



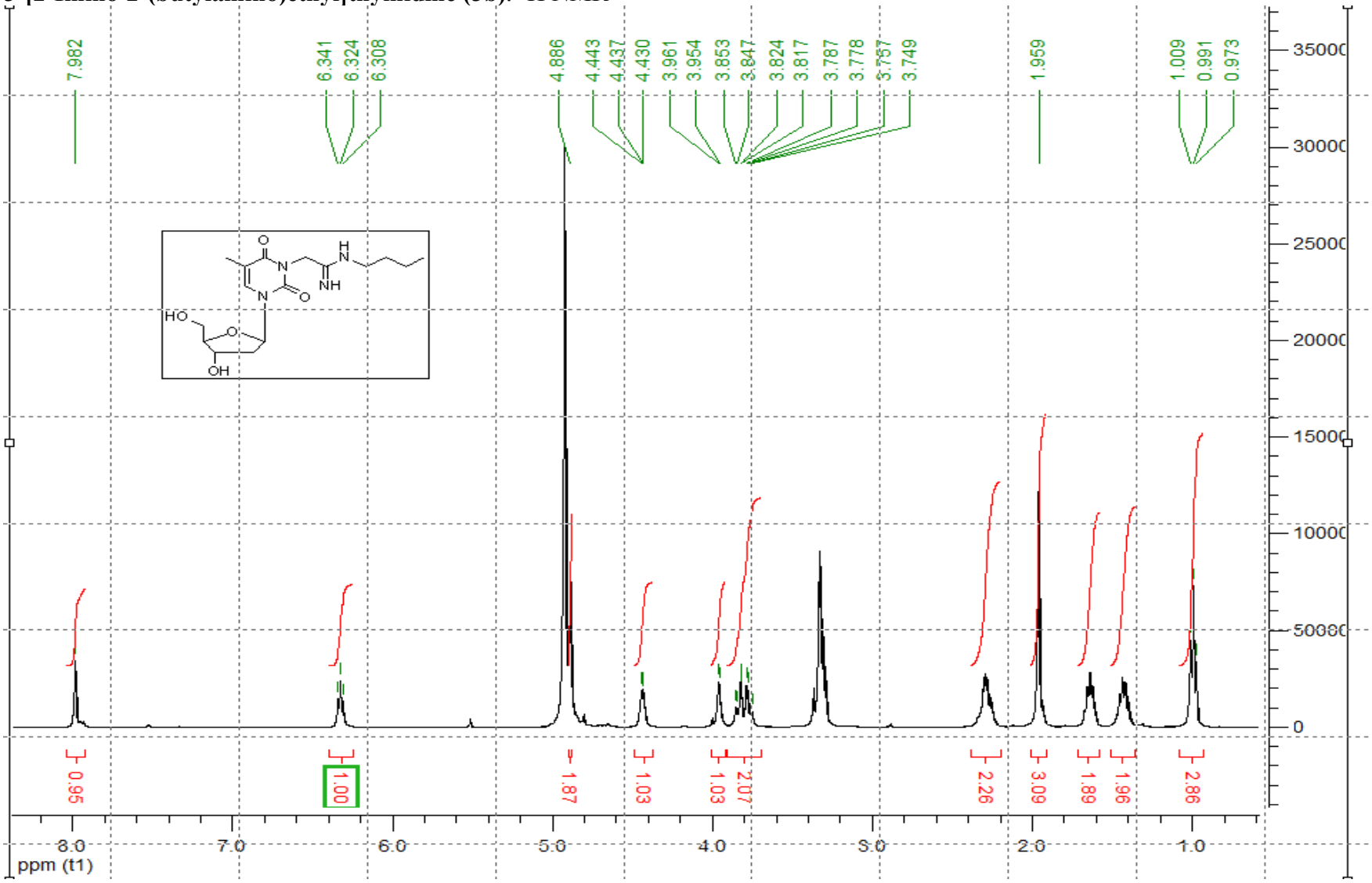
3-[2-Imino-2-(propylamino)ethyl]thymidine (3a). Analytical traces in Water:Acetonitrile gradient



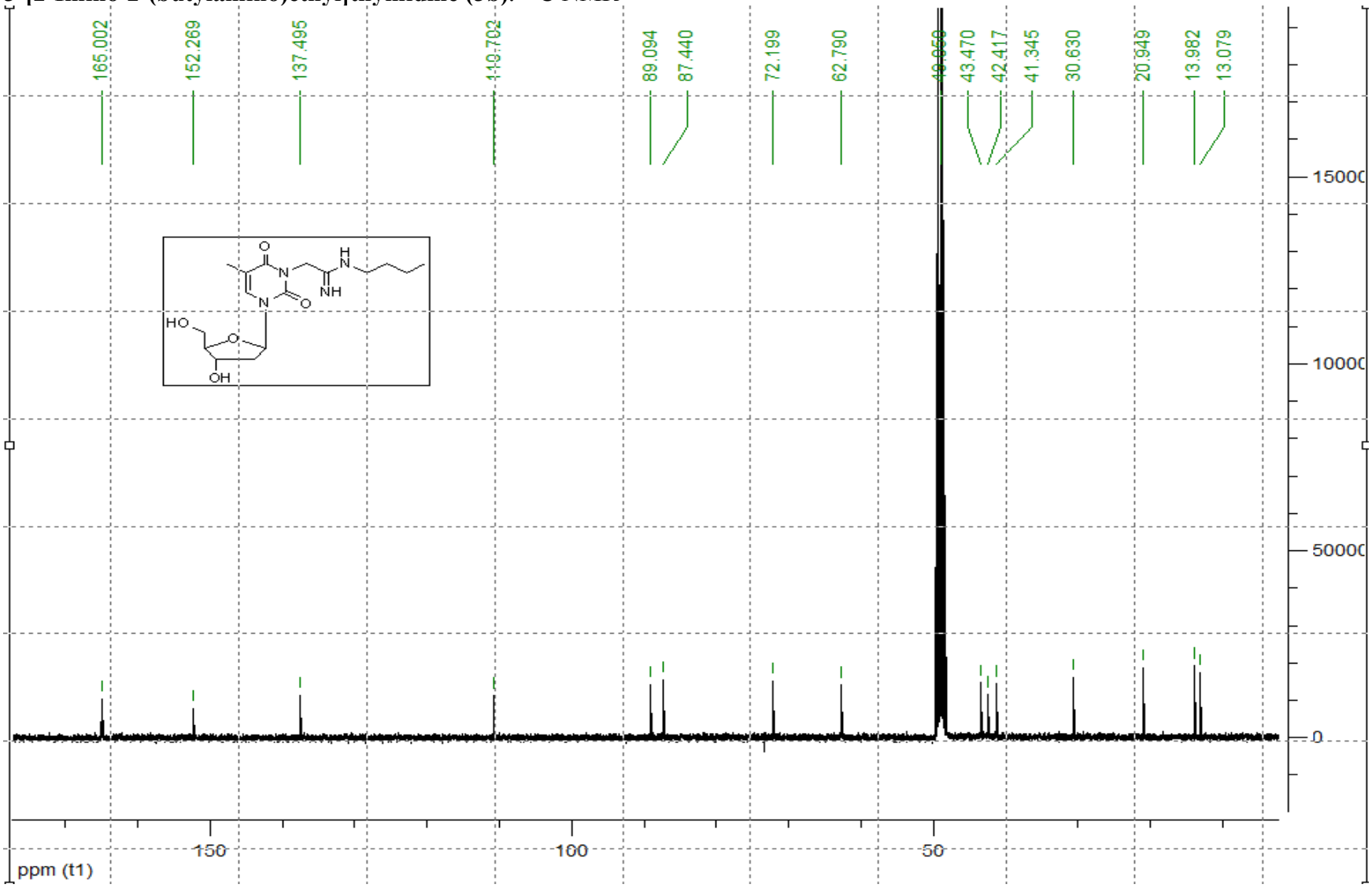
Analytical traces in Water:Methanol gradient



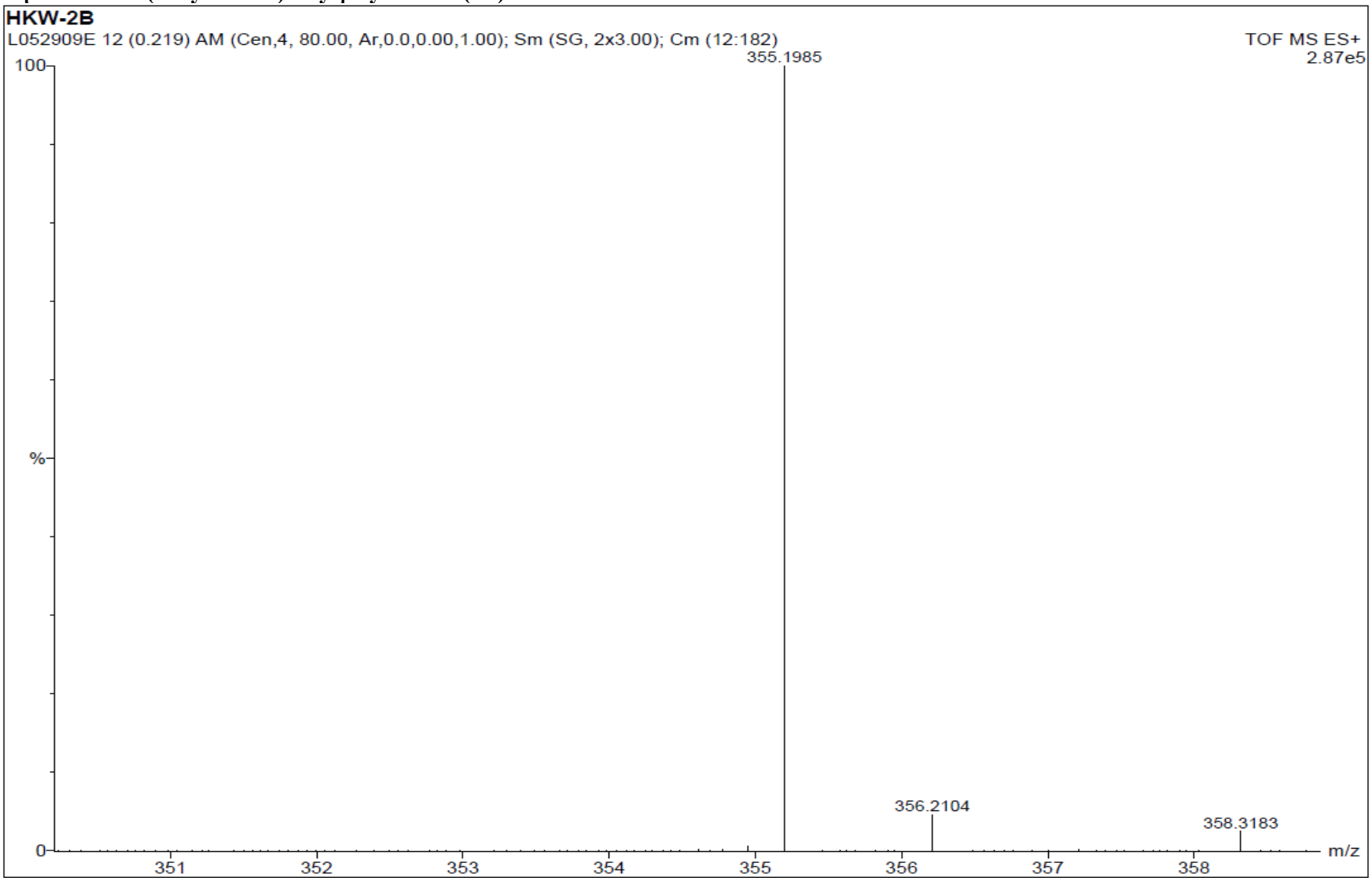
3-[2-Imino-2-(butylamino)ethyl]thymidine (3b). ^{1}H NMR



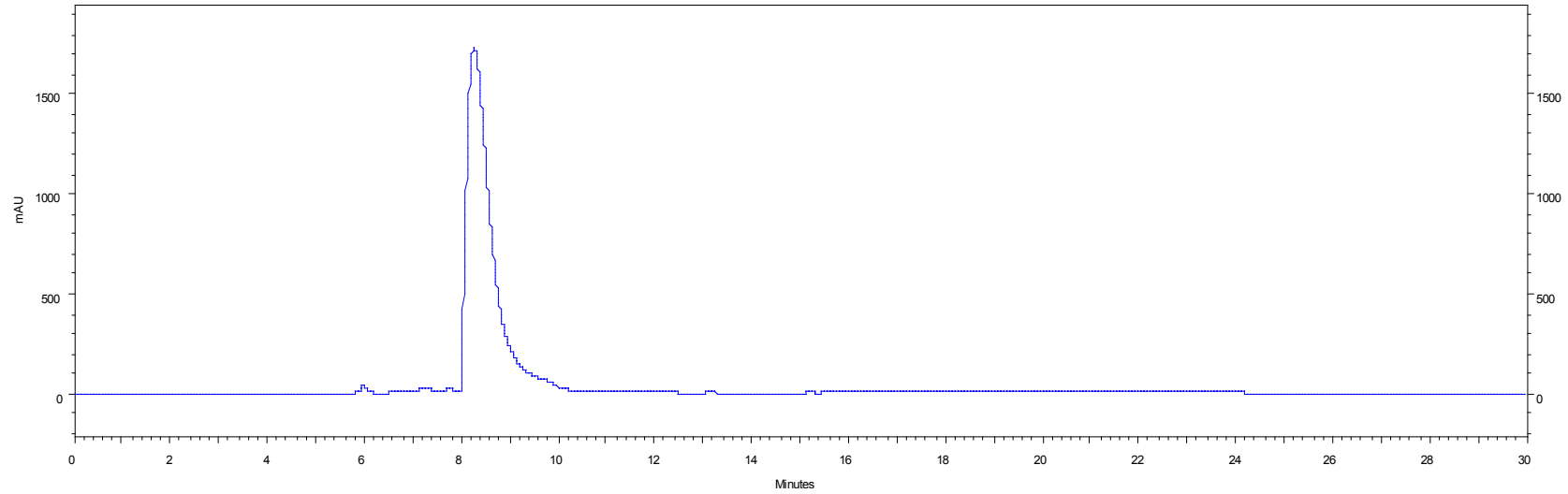
3-[2-Imino-2-(butylamino)ethyl]thymidine (3b). ^{13}C NMR



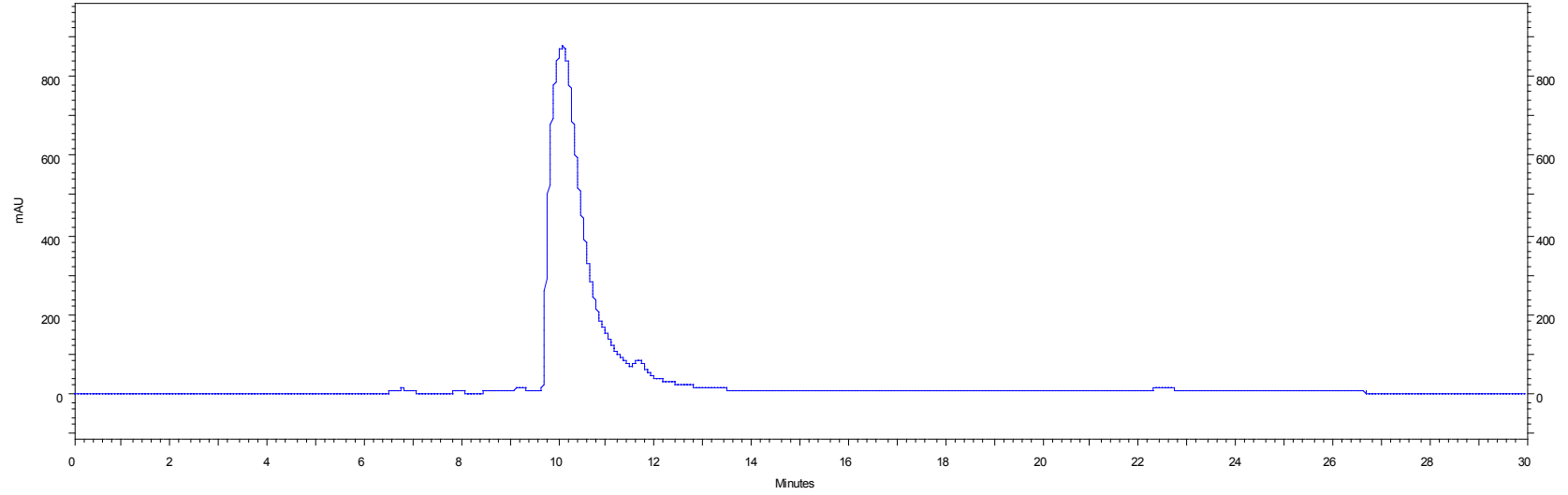
3-[2-Imino-2-(butylamino)ethyl]thymidine (3b). HR-ESI-MS found: 355.1985.



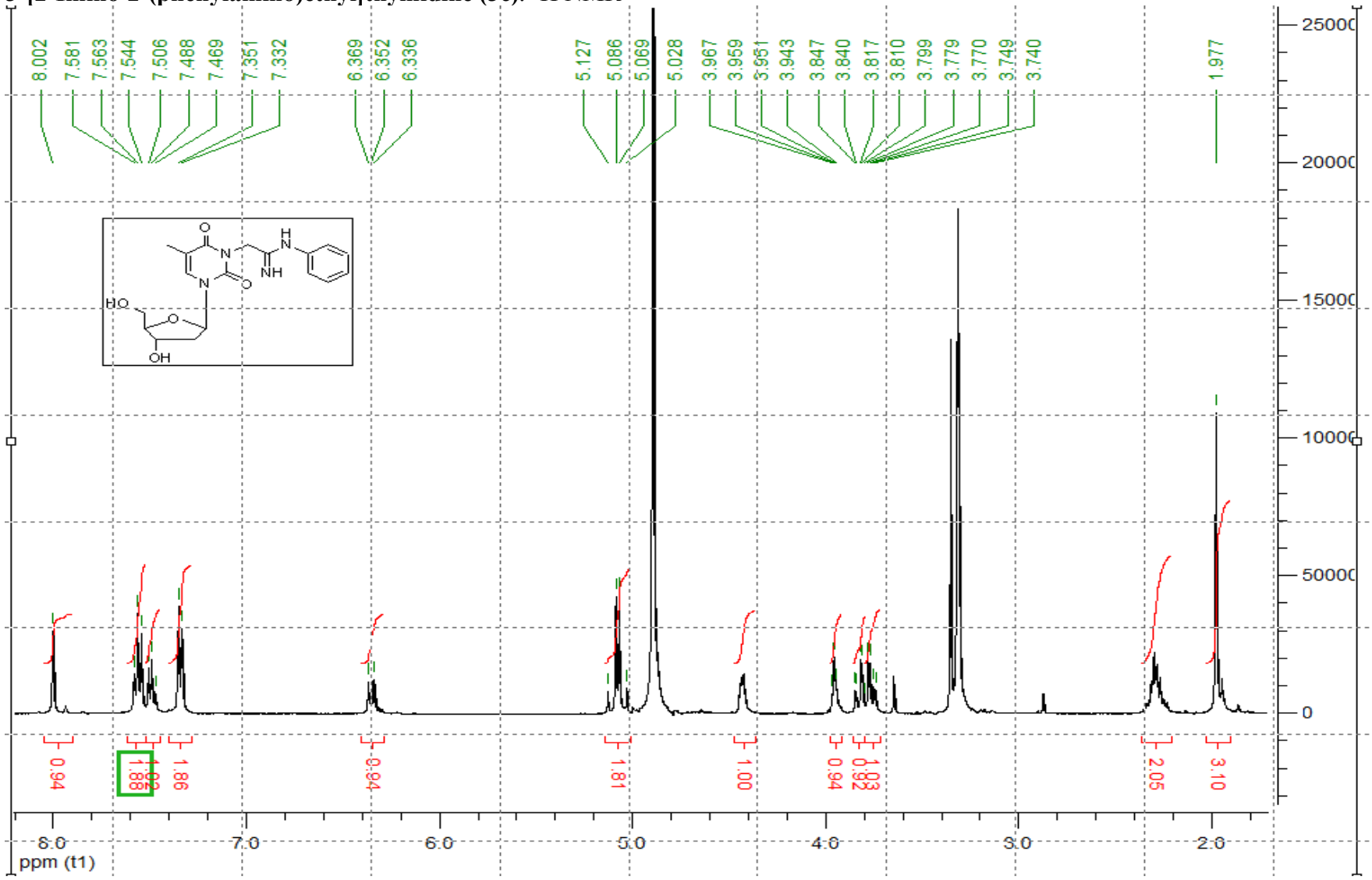
3-[2-Imino-2-(butylamino)ethyl]thymidine (3b). Analytical traces in Water:Acetonitrile gradient



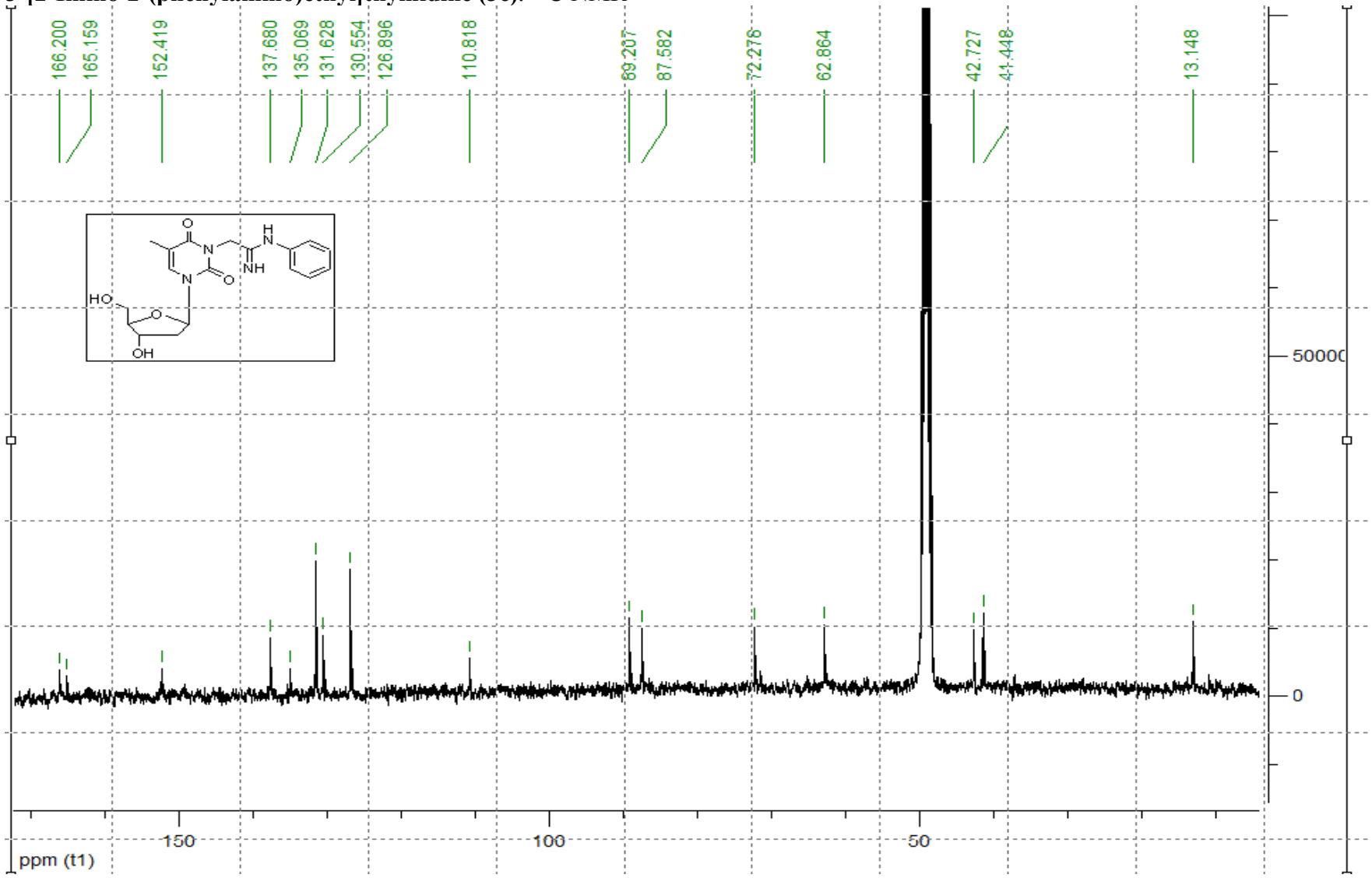
Analytical traces in Water:Methanol gradient



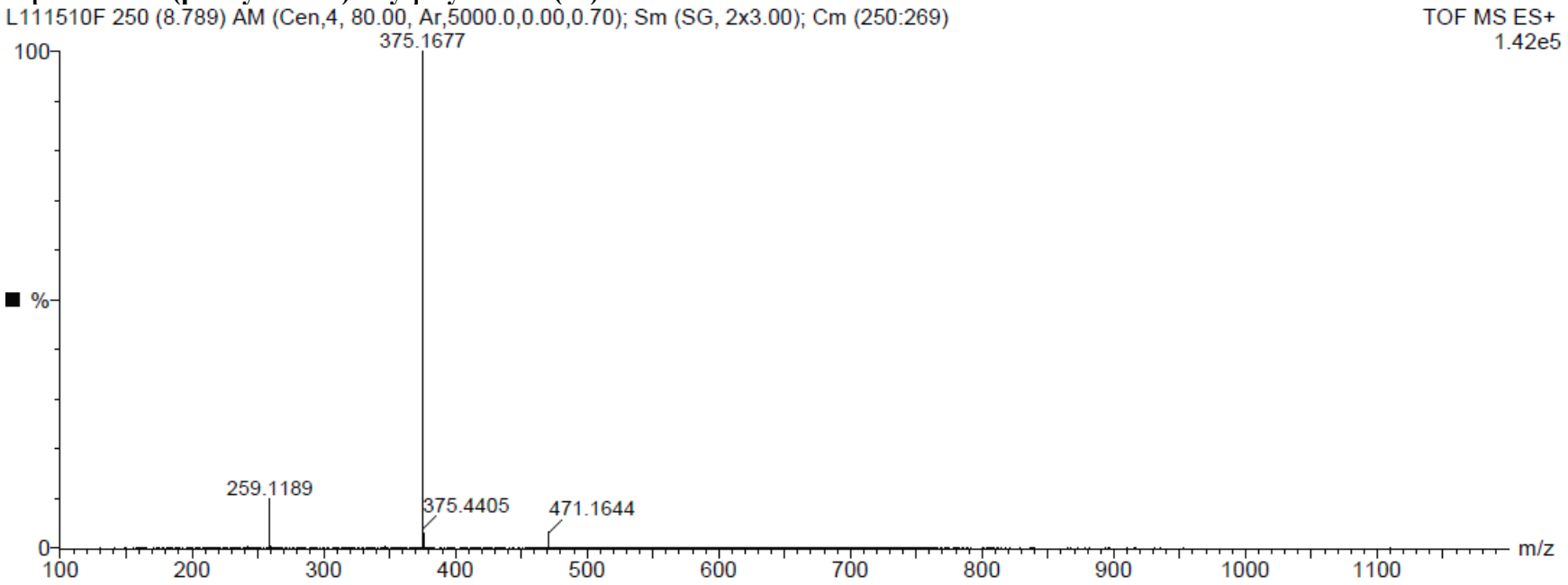
3-[2-Imino-2-(phenylamino)ethyl]thymidine (3c). ^{1}H NMR



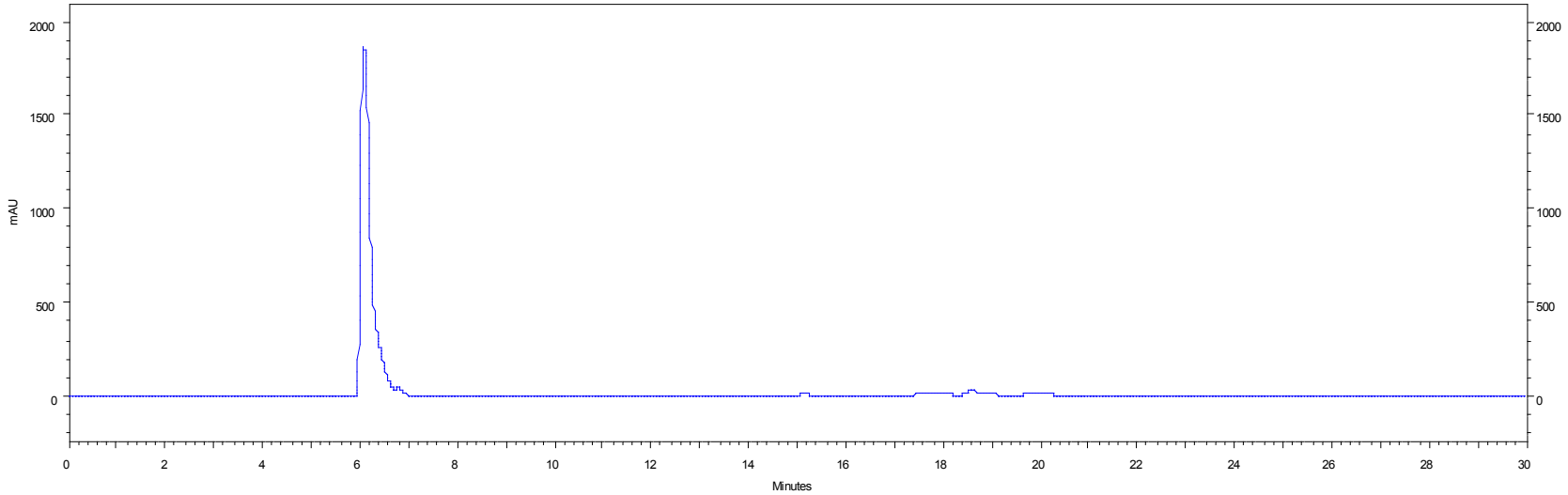
3-[2-Imino-2-(phenylamino)ethyl]thymidine (3c). ^{13}C NMR



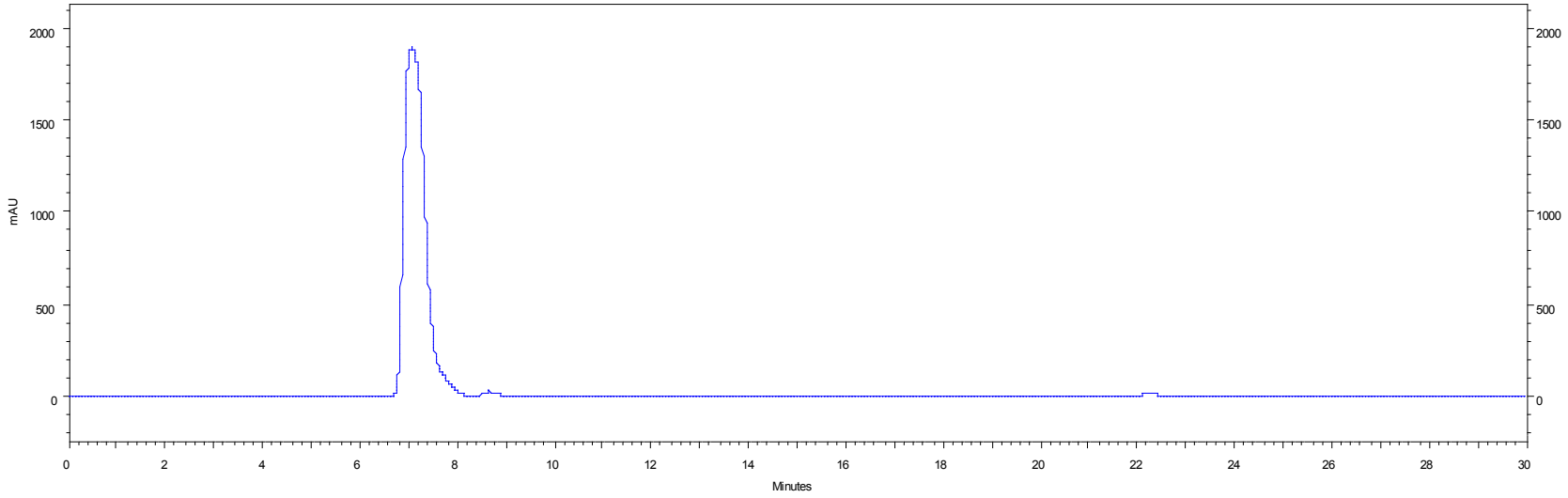
3-[2-Imino-2-(phenylamino)ethyl]thymidine (3c). HR-ESI-MS found: 375.1677.



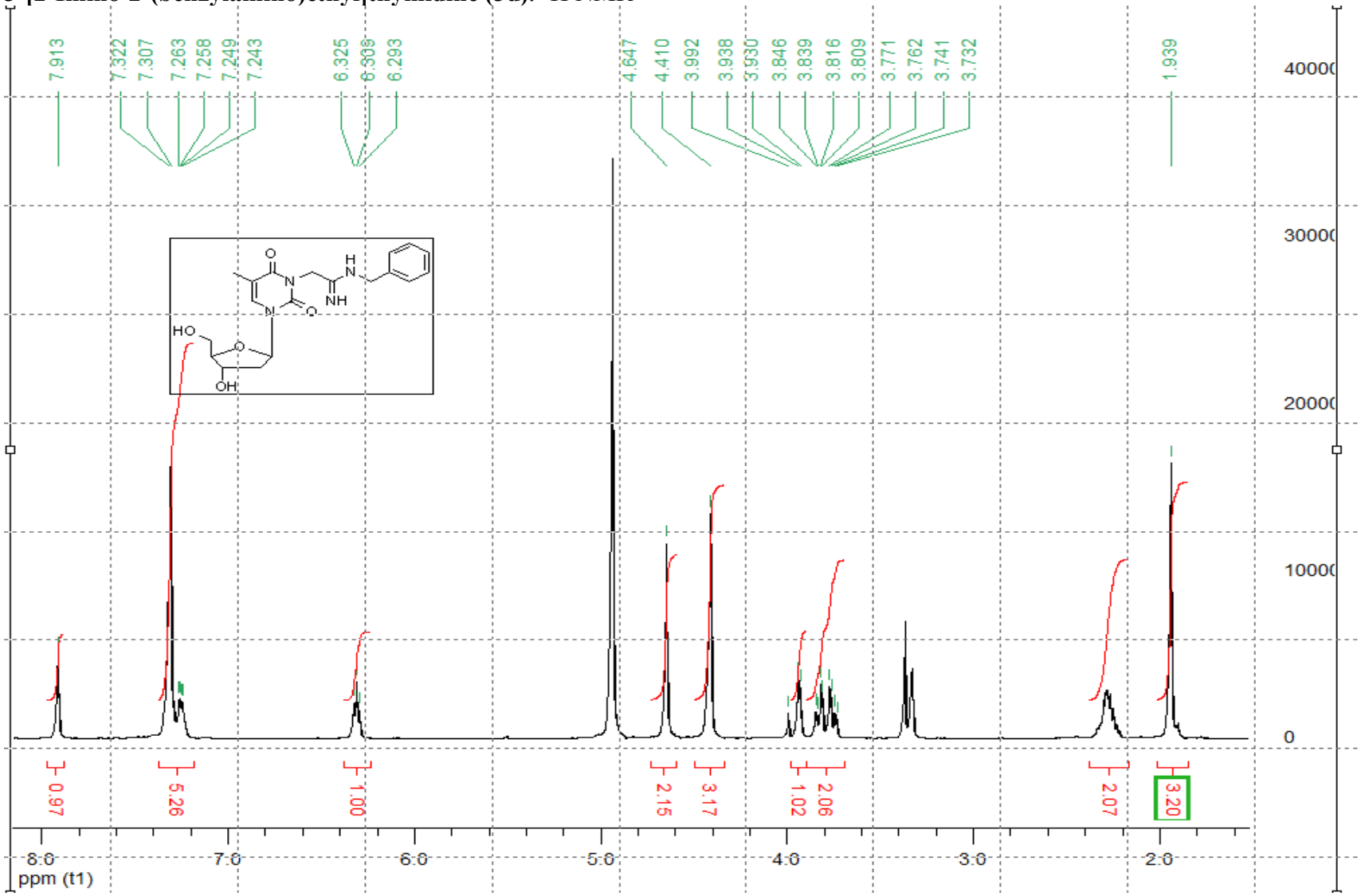
3-[2-Imino-2-(phenylamino)ethyl]thymidine (3c). Analytical traces in Water:Acetonitrile gradient



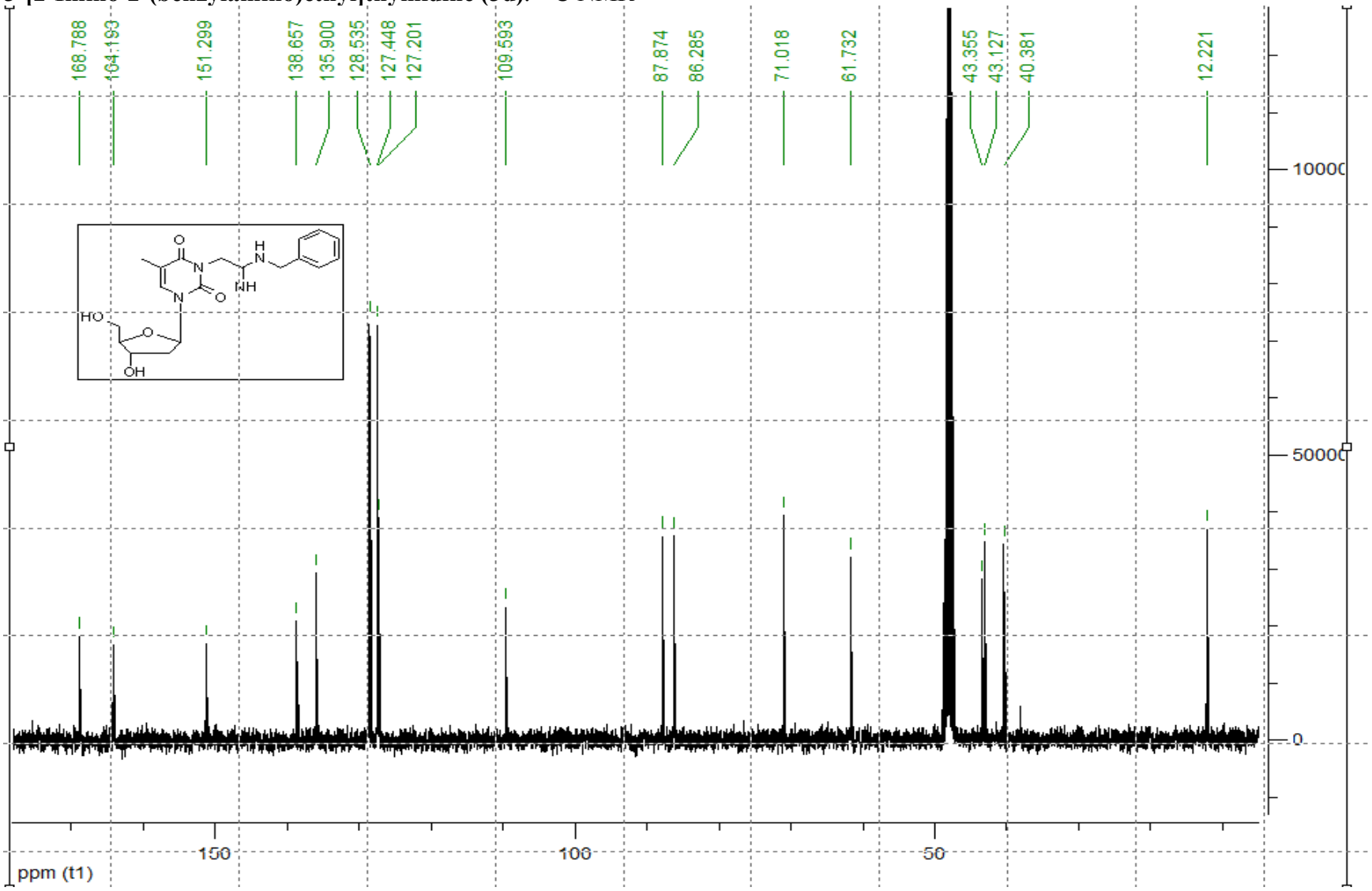
Analytical traces in Water:Methanol gradient



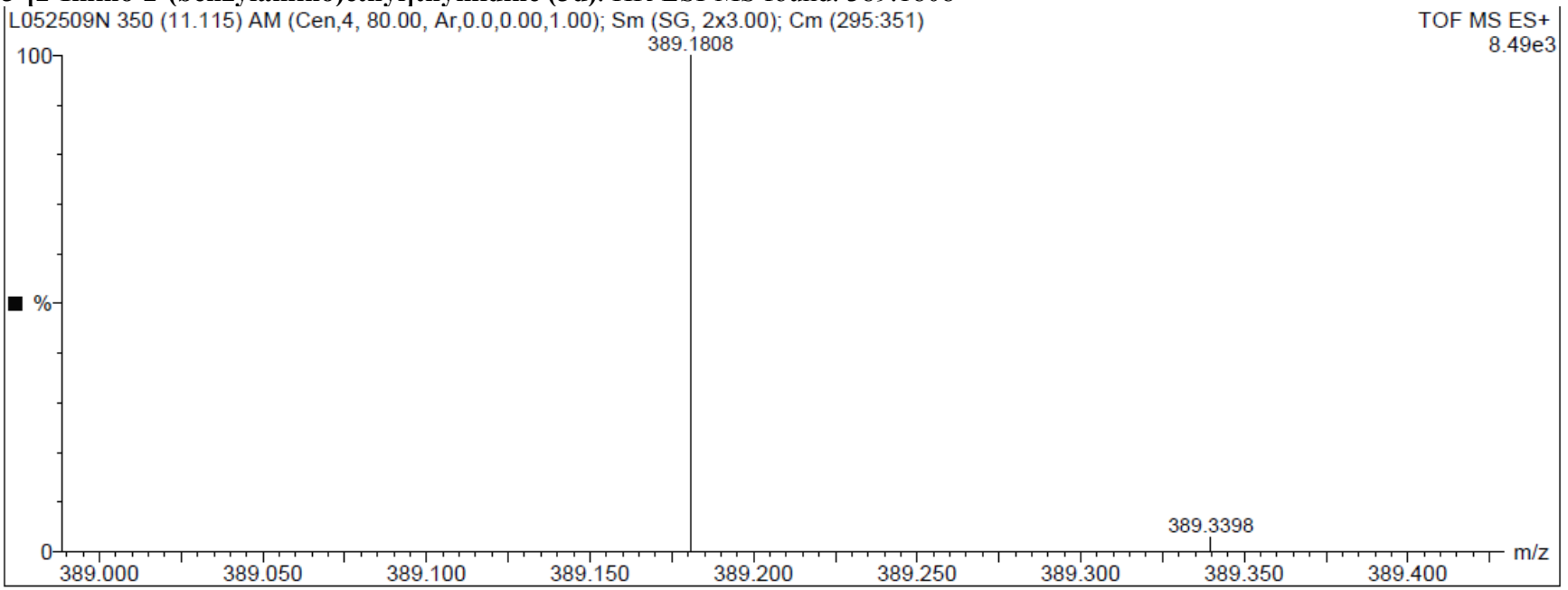
3-[2-Imino-2-(benzylamino)ethyl]thymidine (3d). ^{1}H NMR



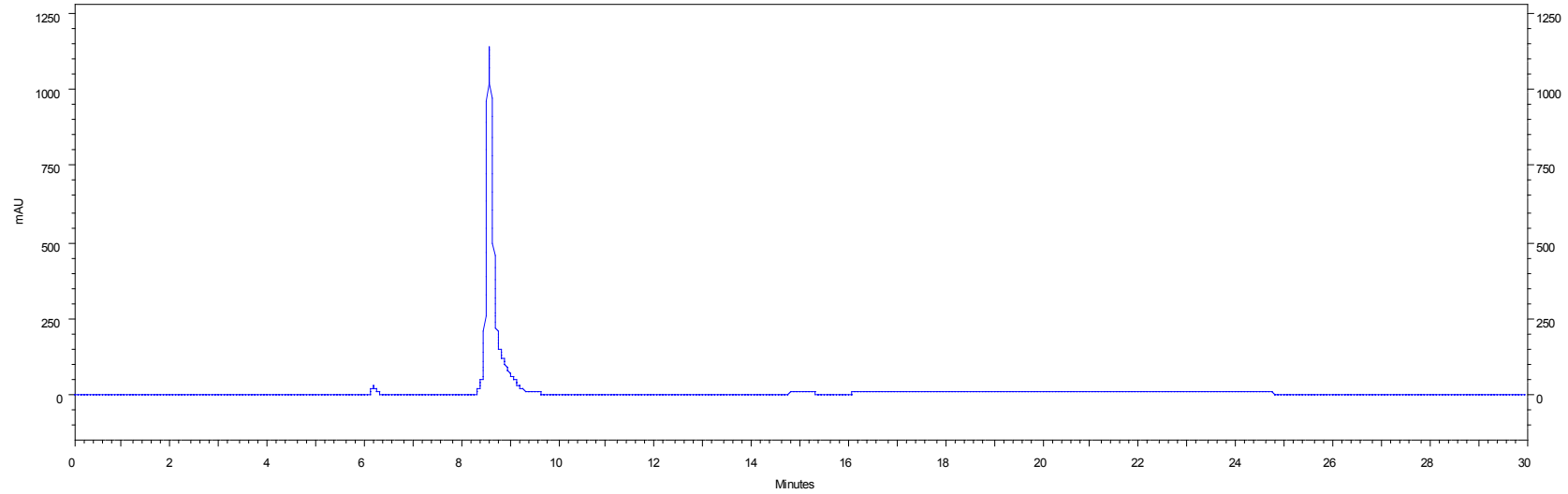
3-[2-Imino-2-(benzylamino)ethyl]thymidine (3d). ^{13}C NMR



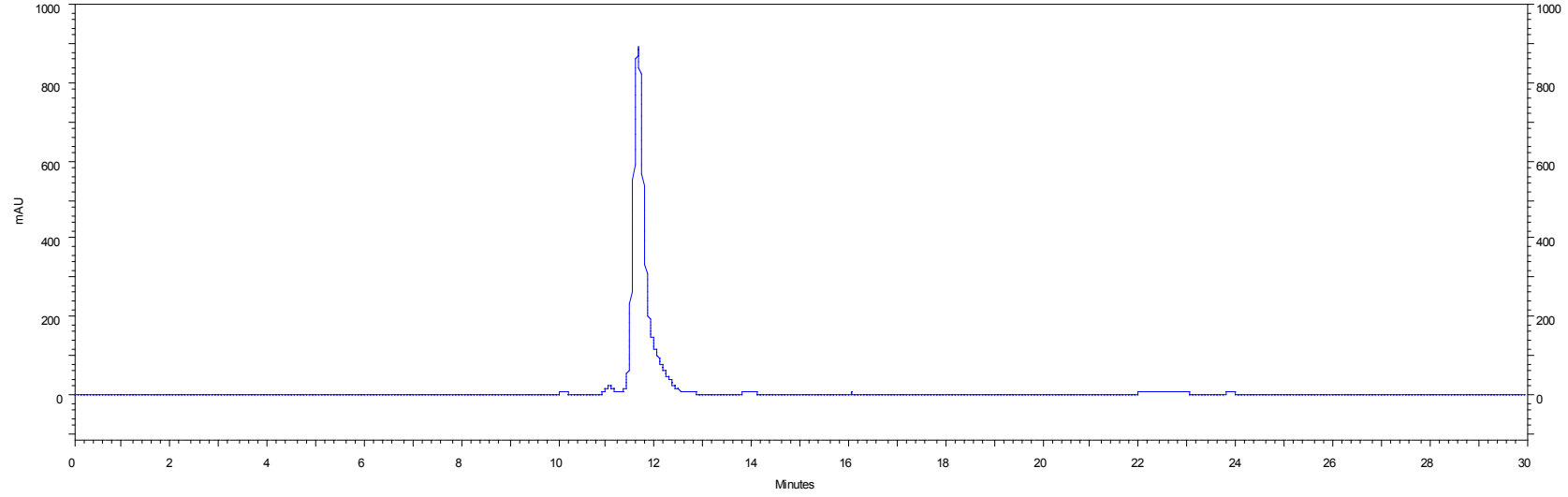
3-[2-Imino-2-(benzylamino)ethyl]thymidine (3d). HR-ESI-MS found: 389.1808



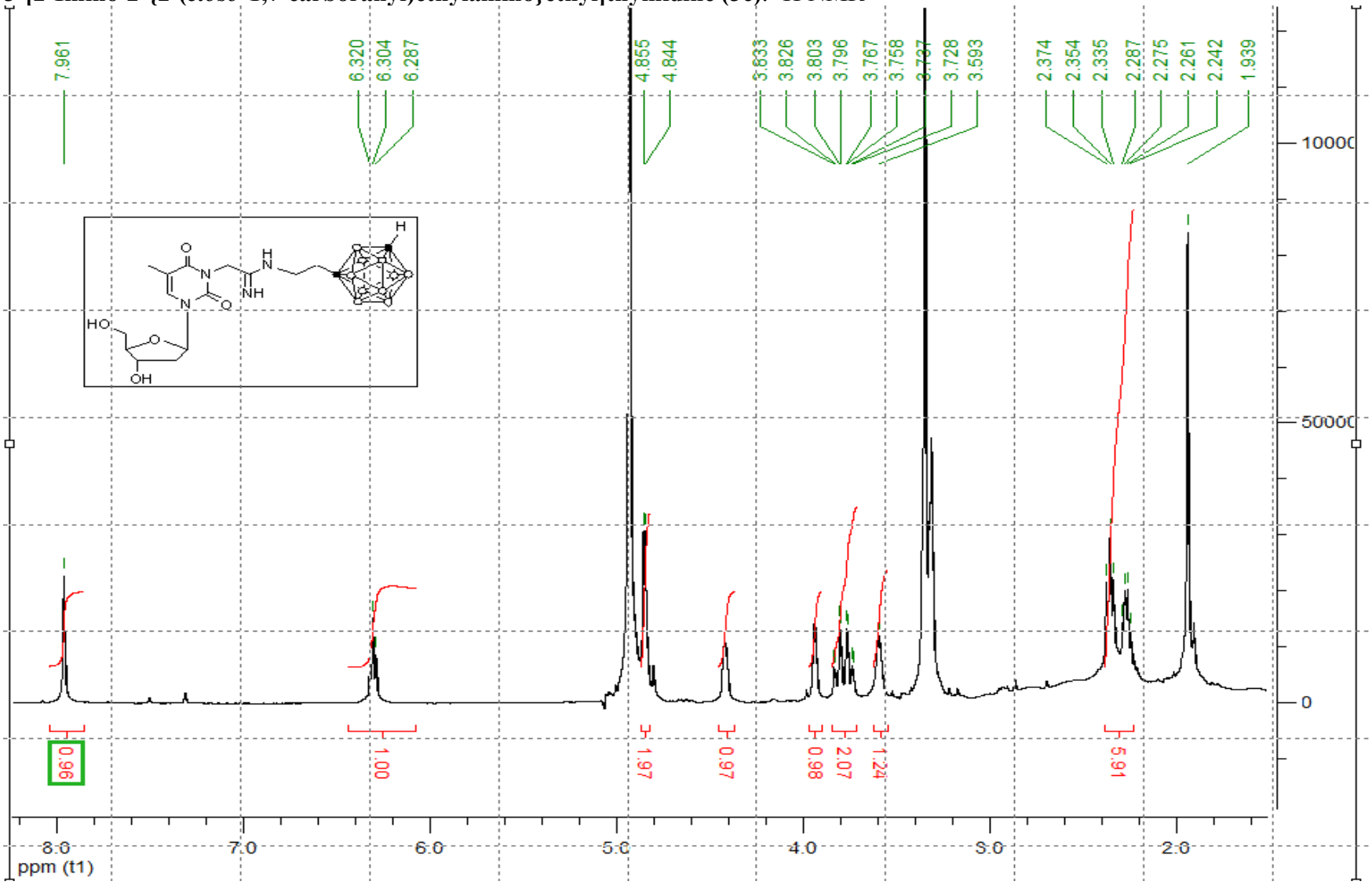
3-[2-Imino-2-(benzylamino)ethyl]thymidine (3d). Analytical traces in Water:Acetonitrile gradient



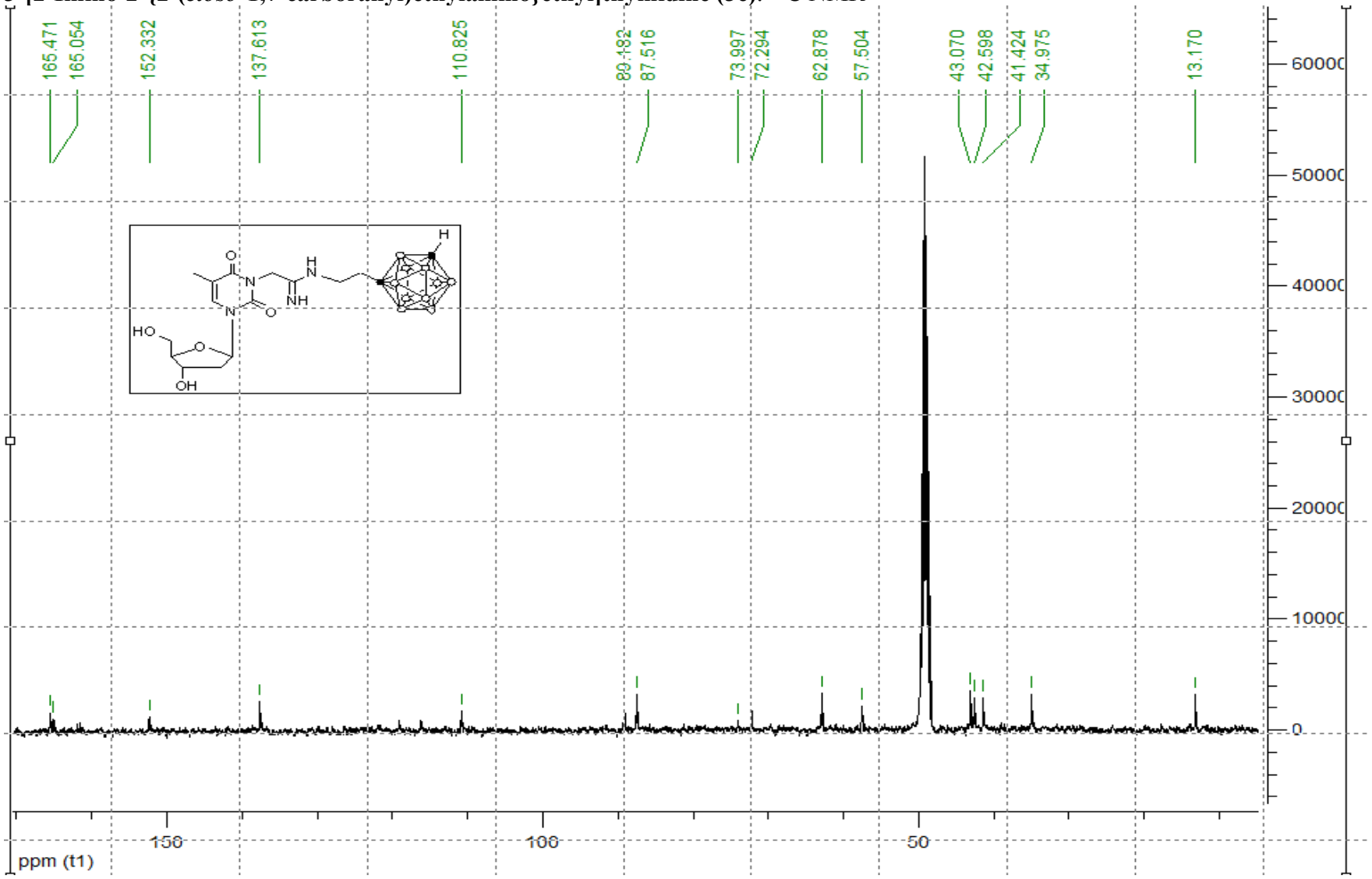
Analytical traces in Water:Methanol gradient



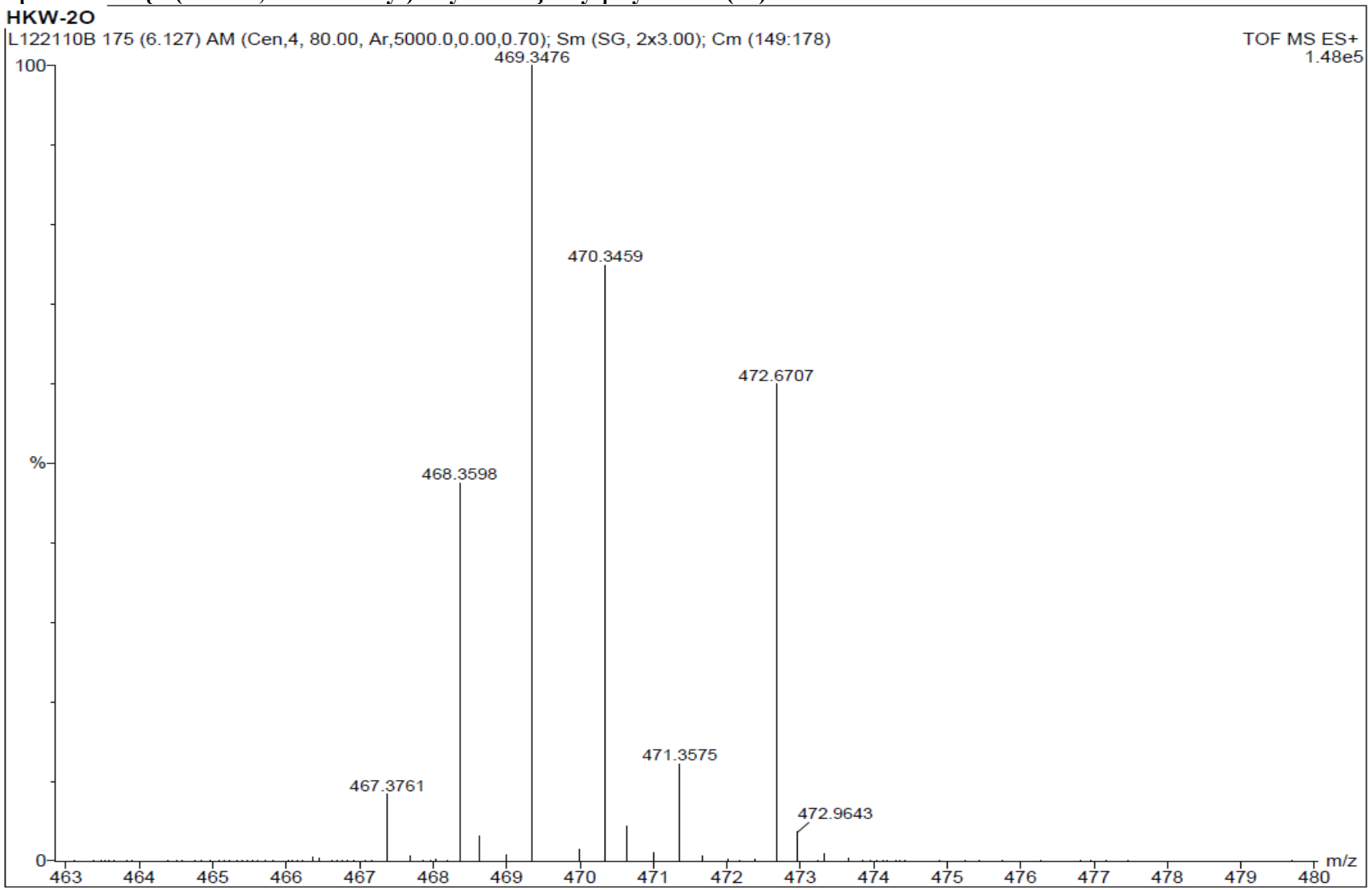
3-[2-Imino-2-{2-(*closo*-1,7-carboranyl)ethylamino}ethyl]thymidine (3e). ^{1}H NMR



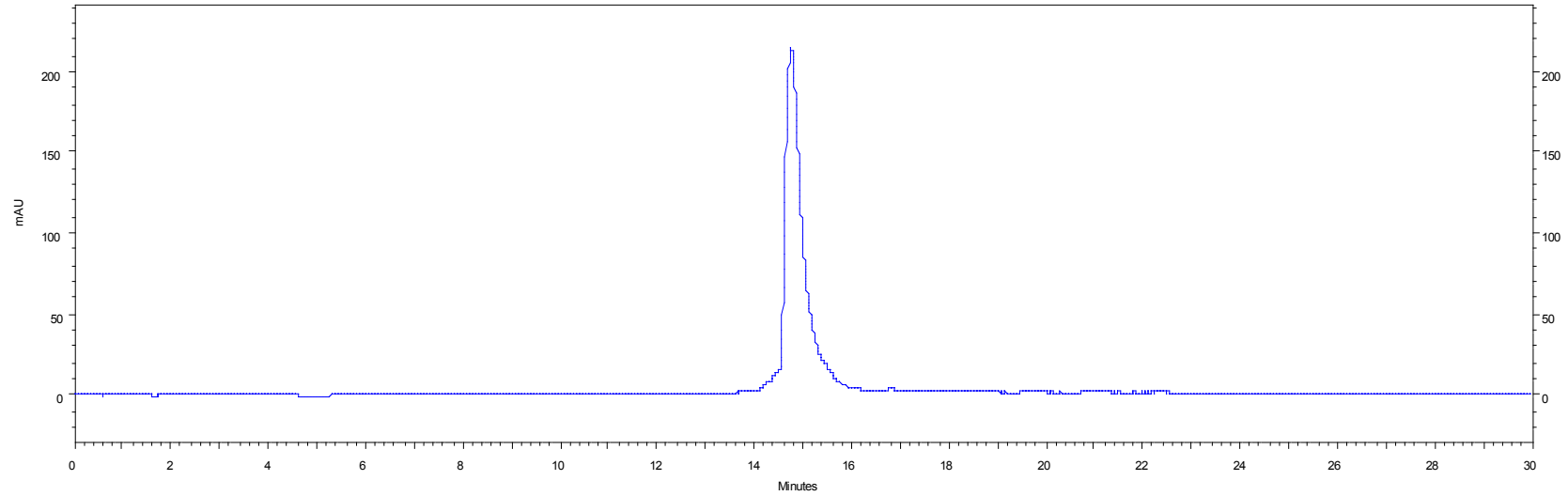
3-[2-Imino-2-{2-(*closo*-1,7-carboranyl)ethylamino}ethyl]thymidine (3e). ^{13}C NMR



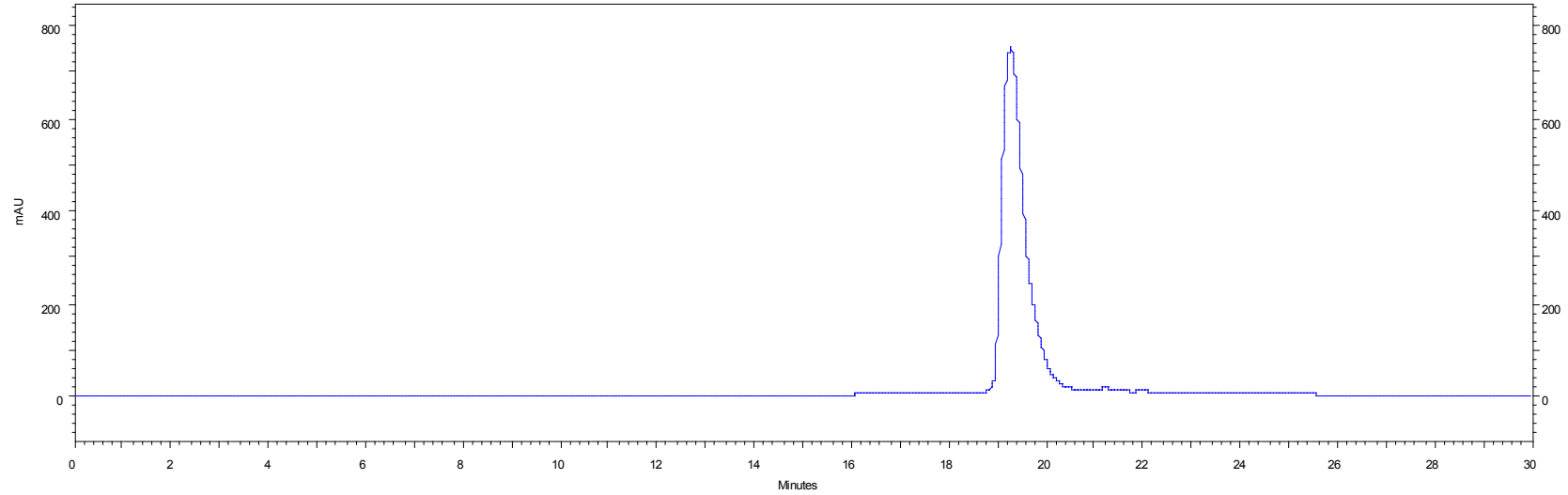
3-[2-Imino-2-{2-(*closo*-1,7-carboranyl)ethylamino}ethyl]thymidine (3e). HR-ESI-MS found: 469.3476.



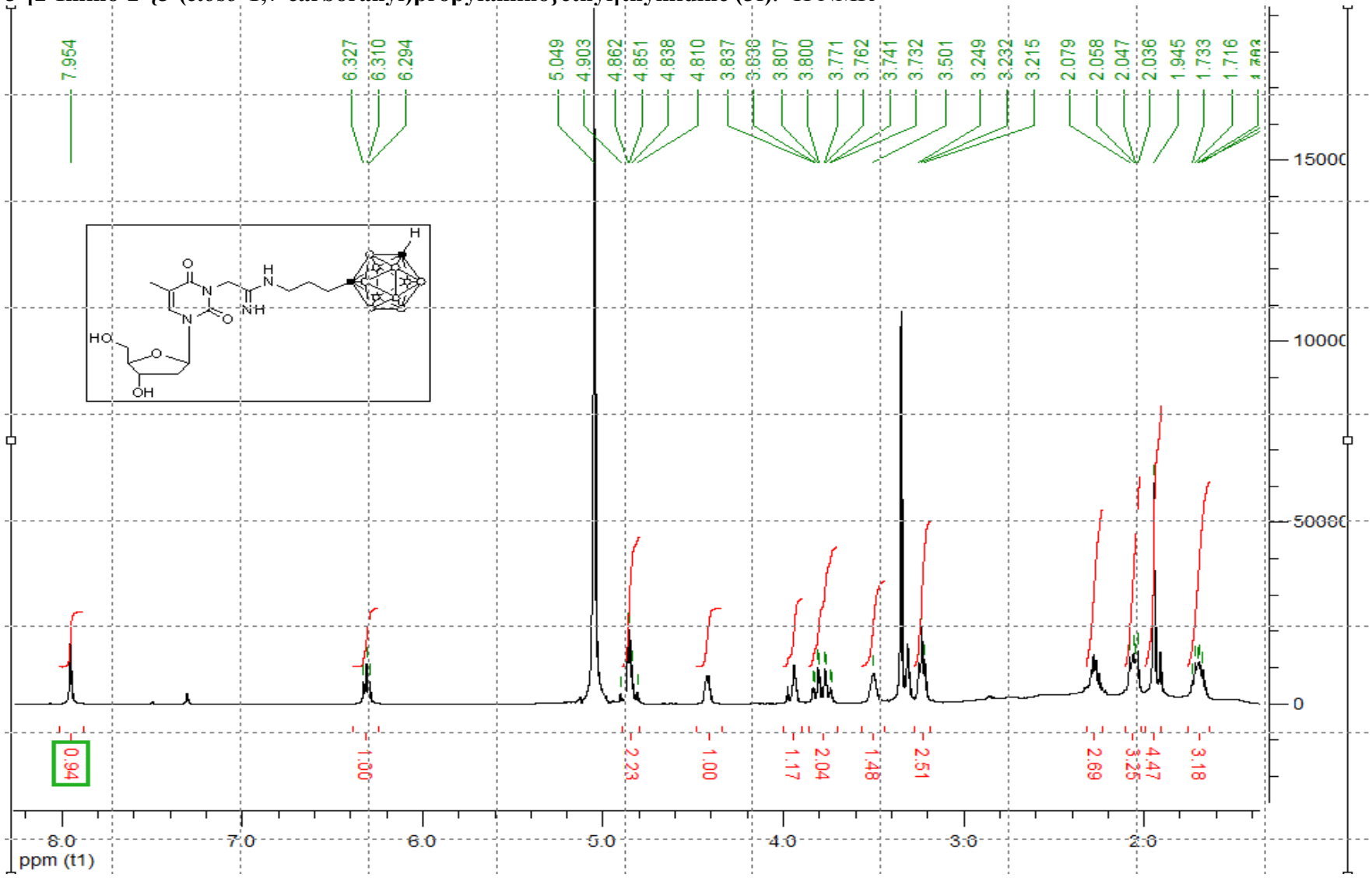
3-[2-Imino-2-{2-(*closo*-1,7-carboranyl)ethylamino}ethyl]thymidine (3e). Analytical traces in Water:Acetonitrile gradient



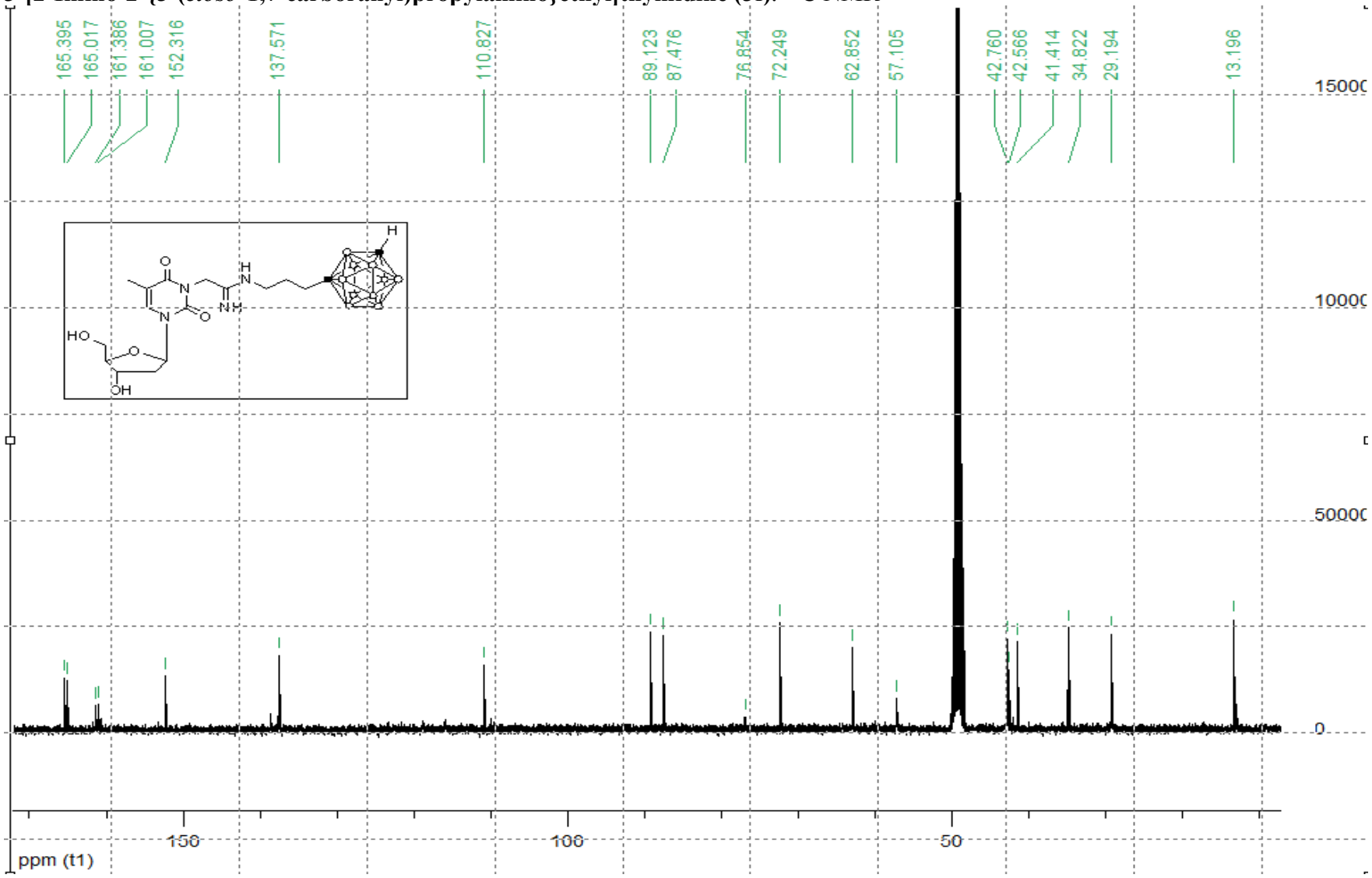
Analytical traces in Water:Methanol gradient



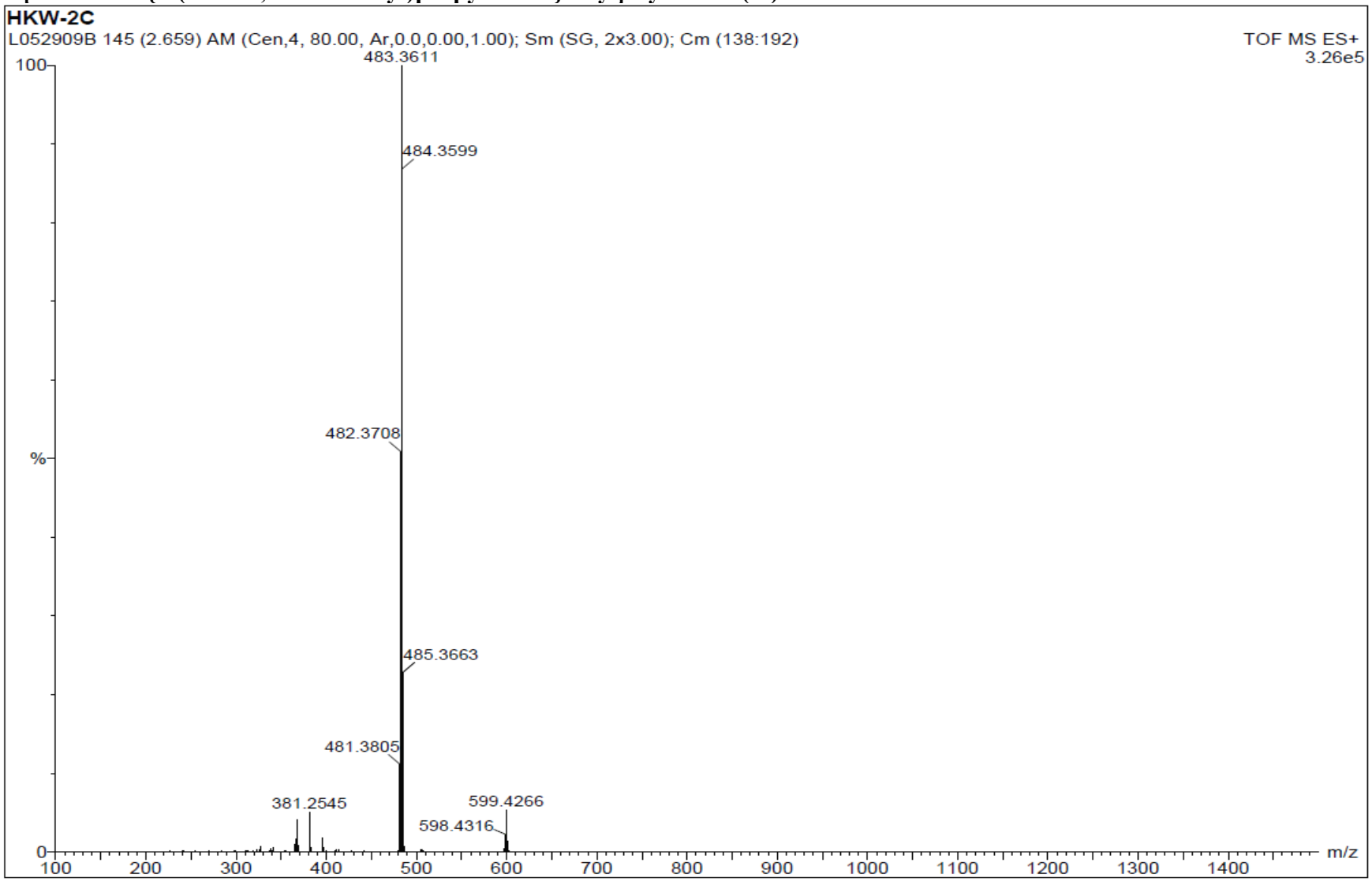
3-[2-Imino-2-{3-(*closo*-1,7-carboranyl)propylamino}ethyl]thymidine (3f). ^{1}H NMR



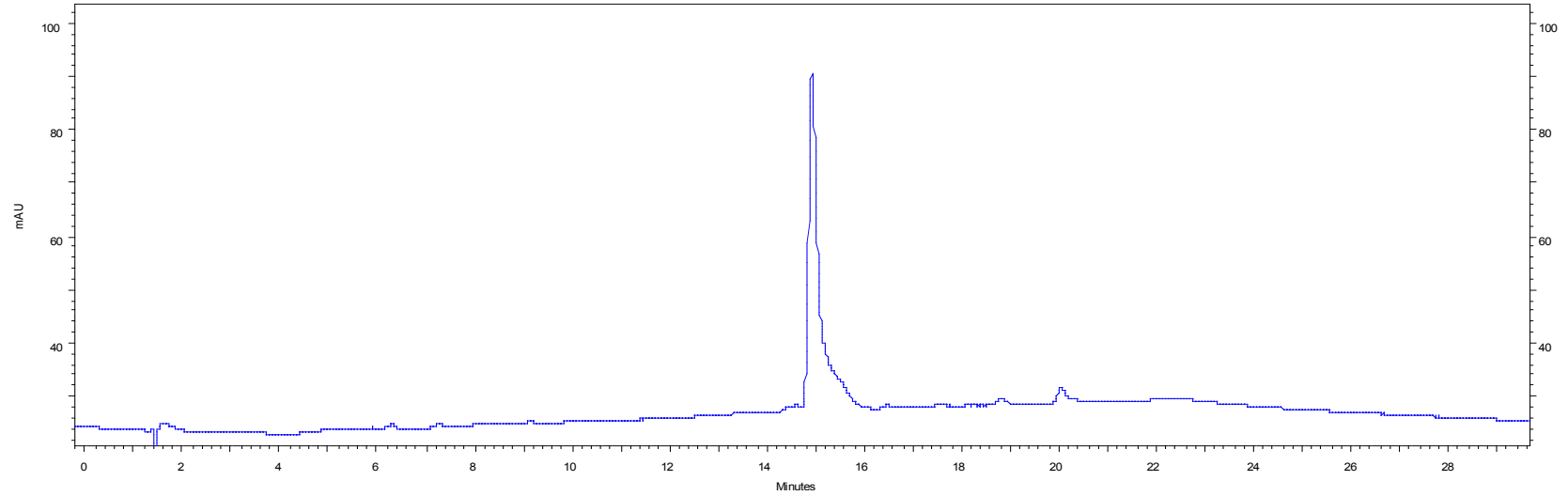
3-[2-Imino-2-{3-(*closo*-1,7-carboranyl)propylamino}ethyl]thymidine (3f). ^{13}C NMR



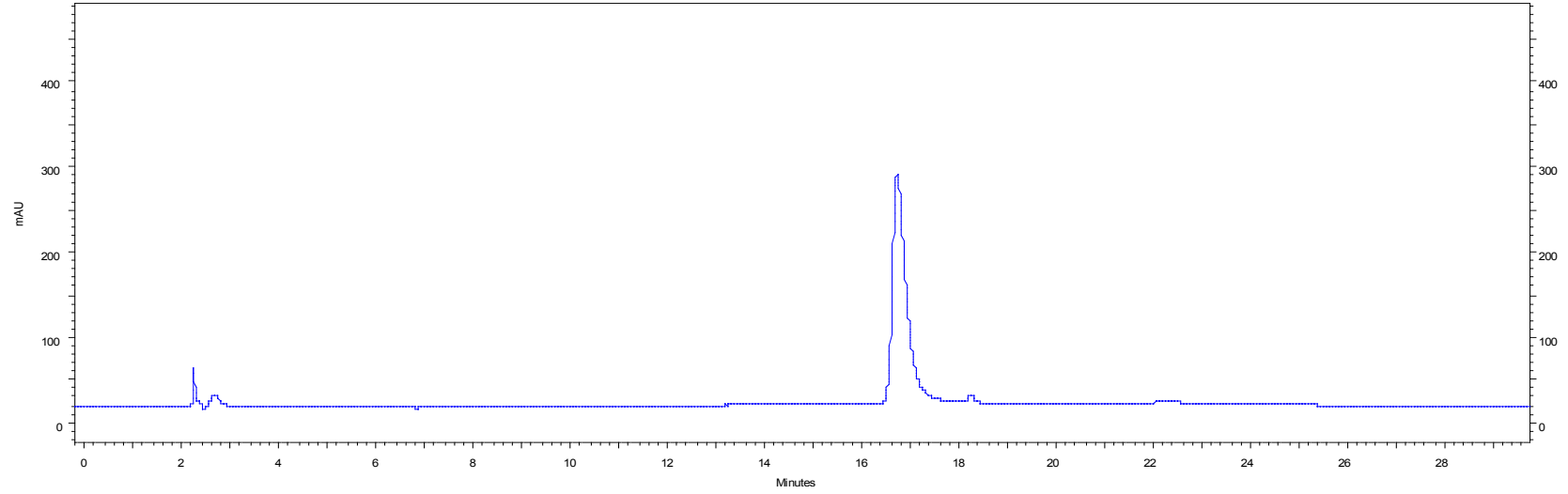
3-[2-Imino-2-{3-(*closo*-1,7-carboranyl)propylamino}ethyl]thymidine (3f). HR-ESI-MS found: 483.3611.



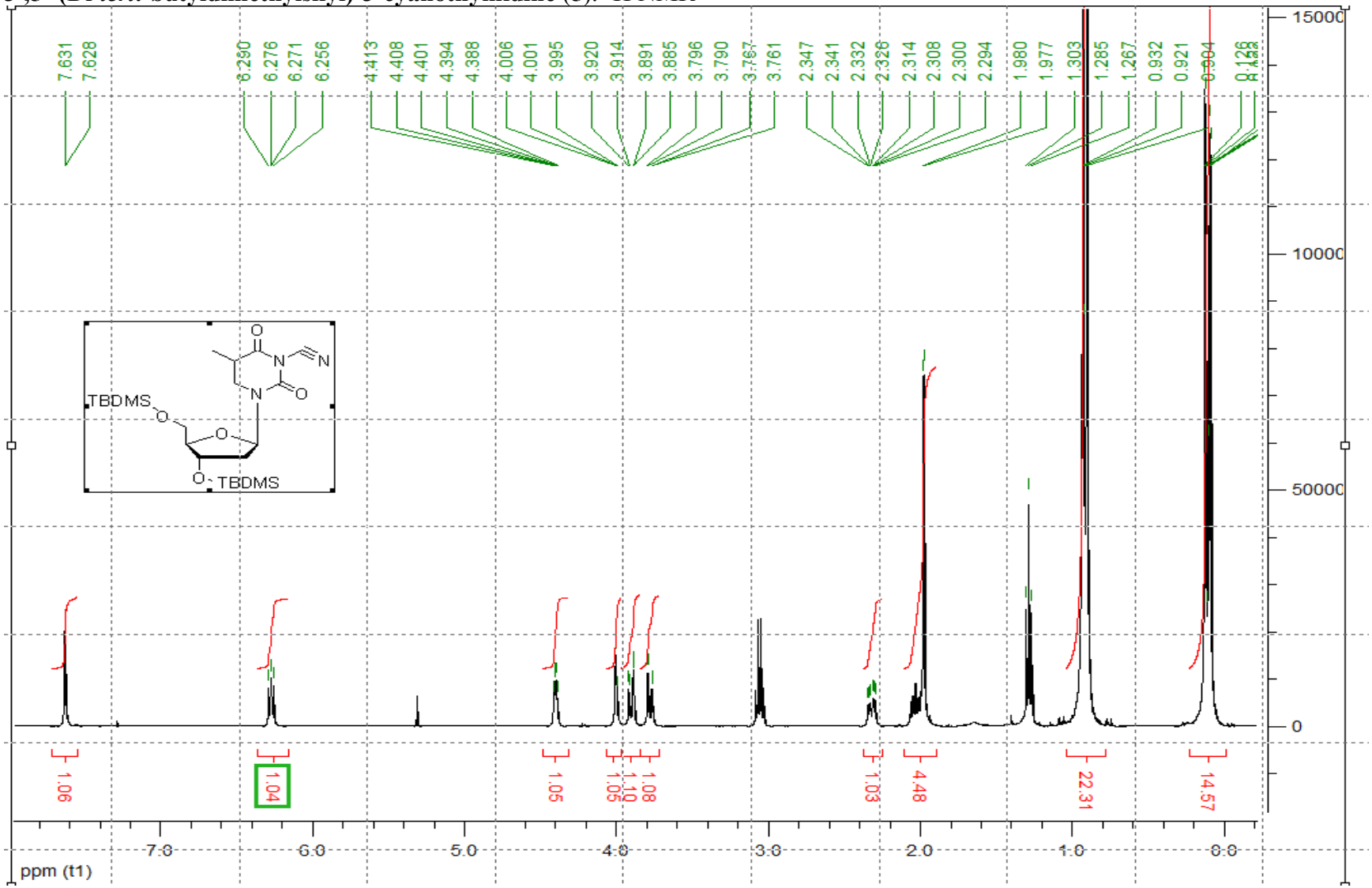
3-[2-Imino-2-{3-(*closo*-1,7-carboranyl)propylamino}ethyl]thymidine (3f). Analytical traces in Water:Acetonitrile gradient



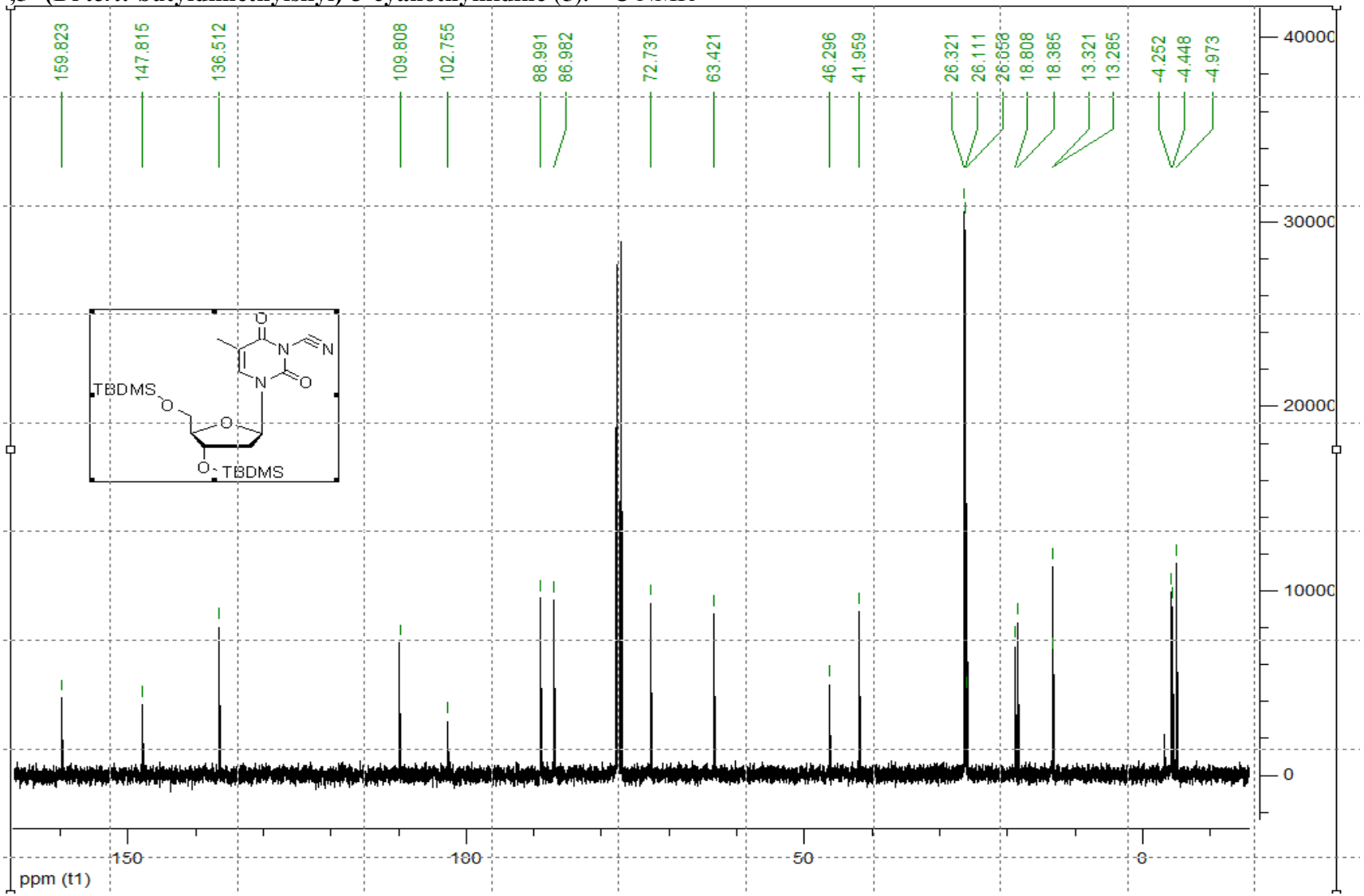
Analytical traces in Water:Methanol gradient



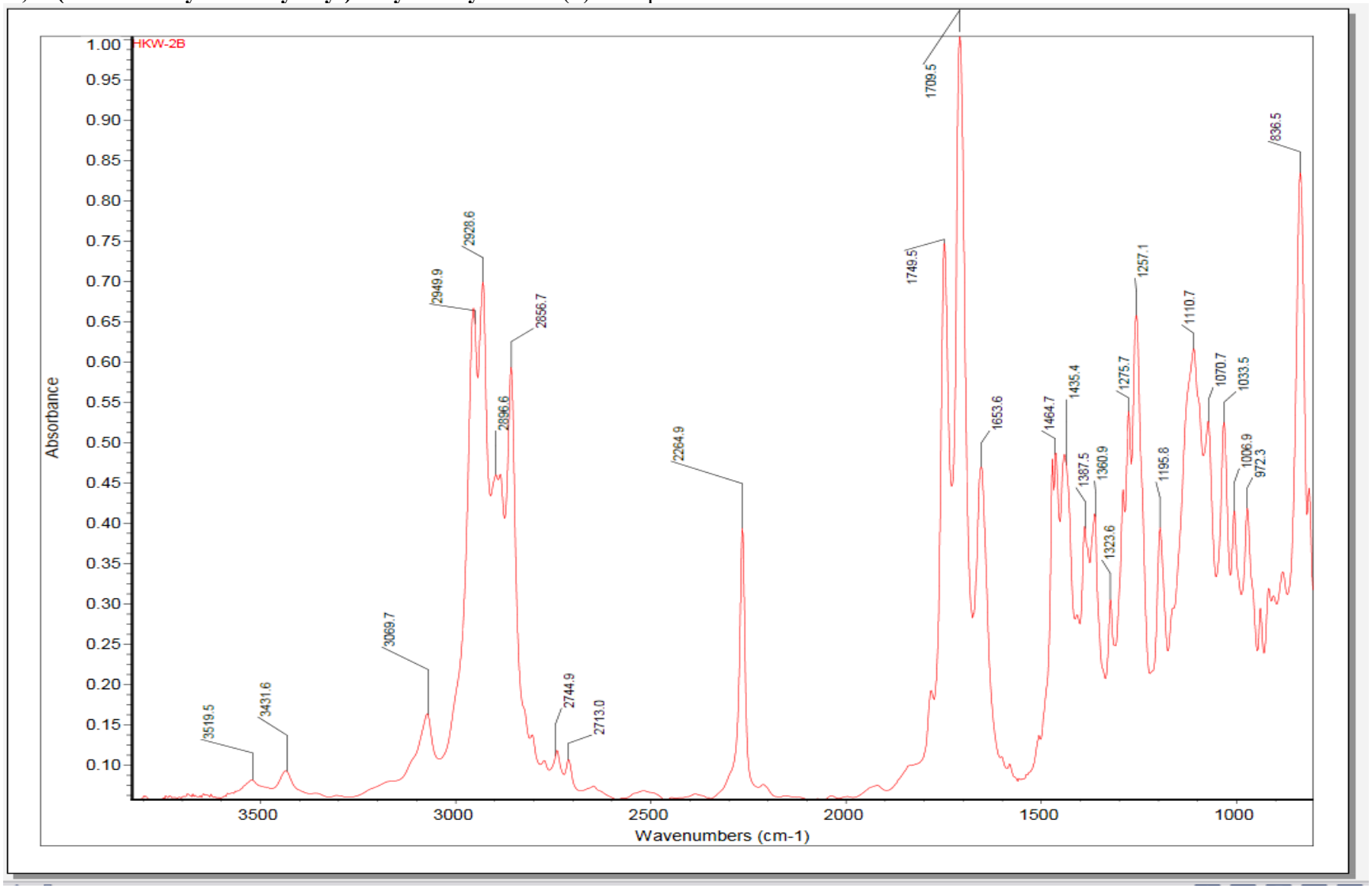
3',5'-(Di-*tert*.-butyldimethylsilyl)-3-cyanothymidine (5). ^{1}H NMR



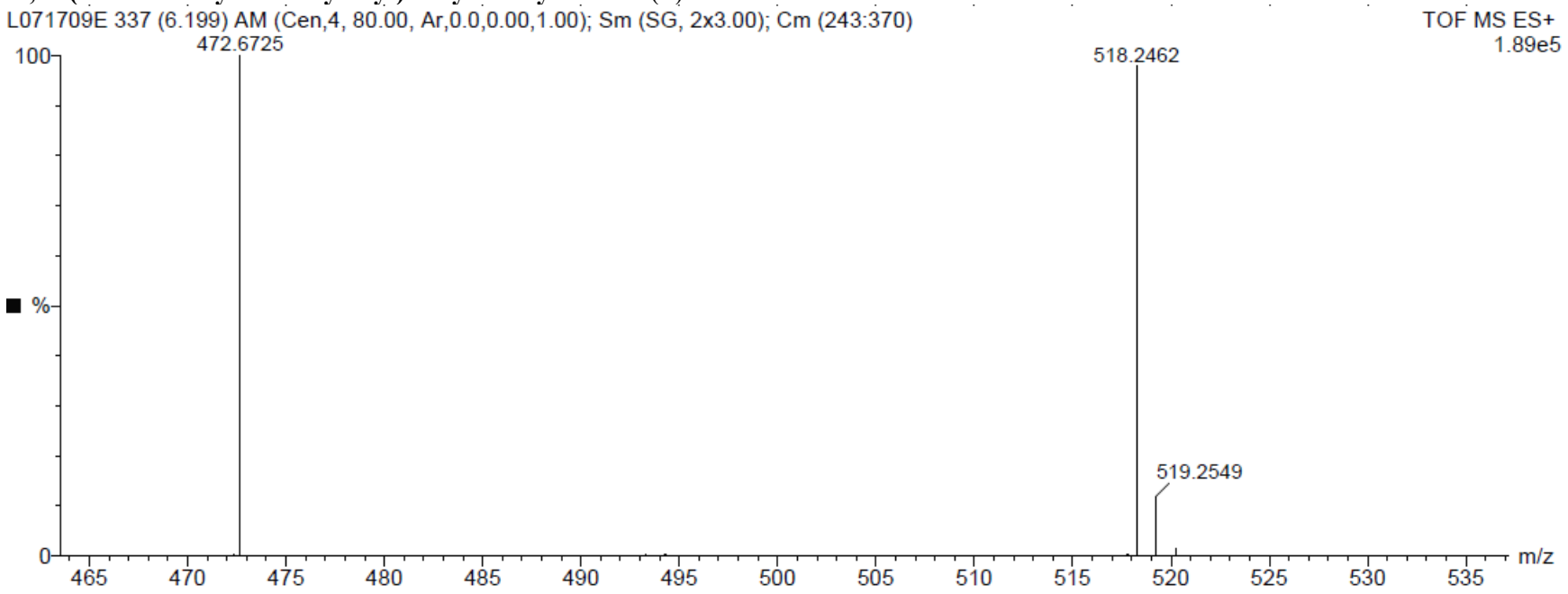
3',5'-(Di-*tert.*-butyldimethylsilyl)-3-cyanothymidine (5). ^{13}C NMR



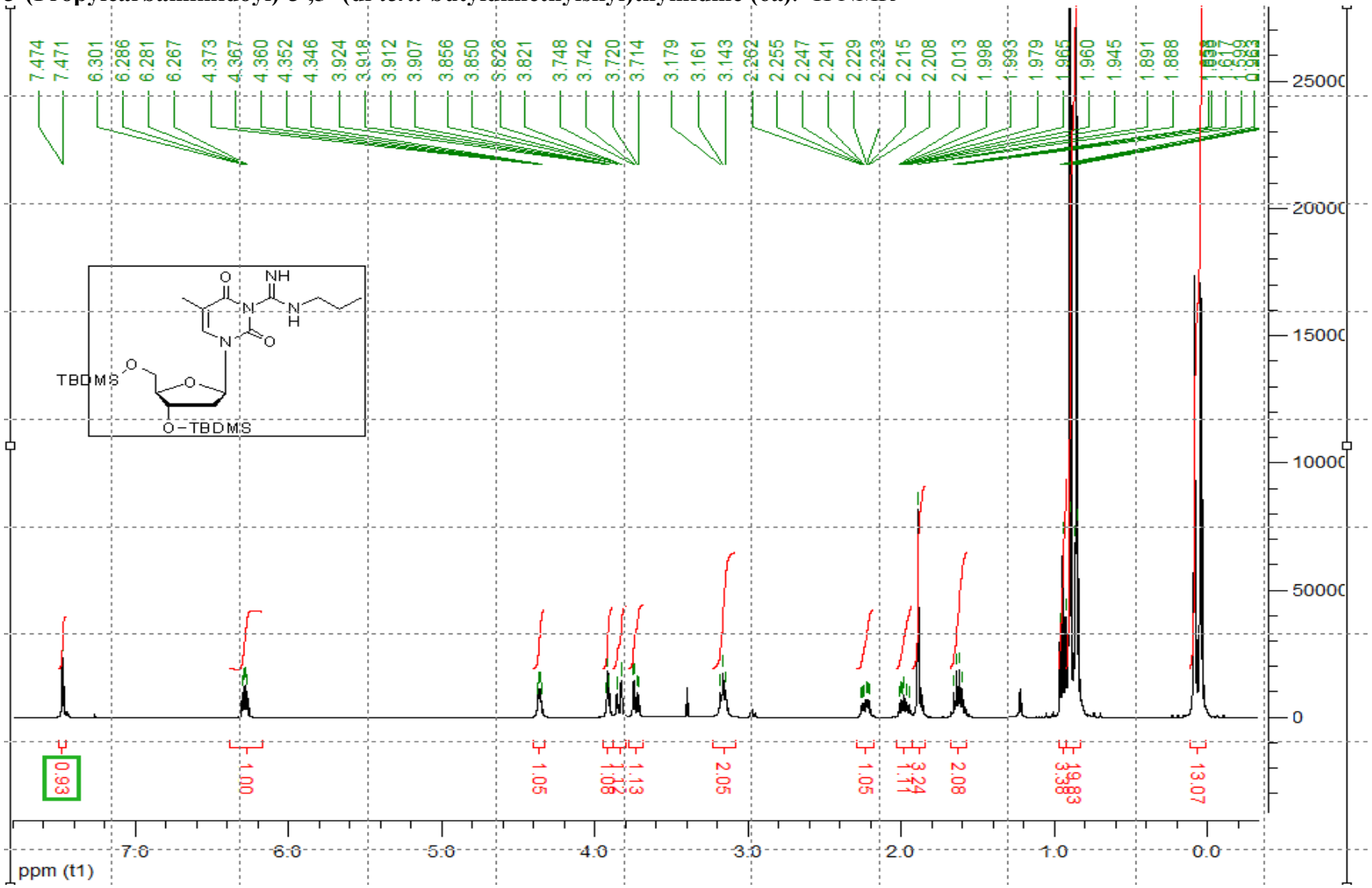
3',5'-(Di-*tert*.-butyldimethylsilyl)-3-cyanothymidine (**5**). IR-spectra



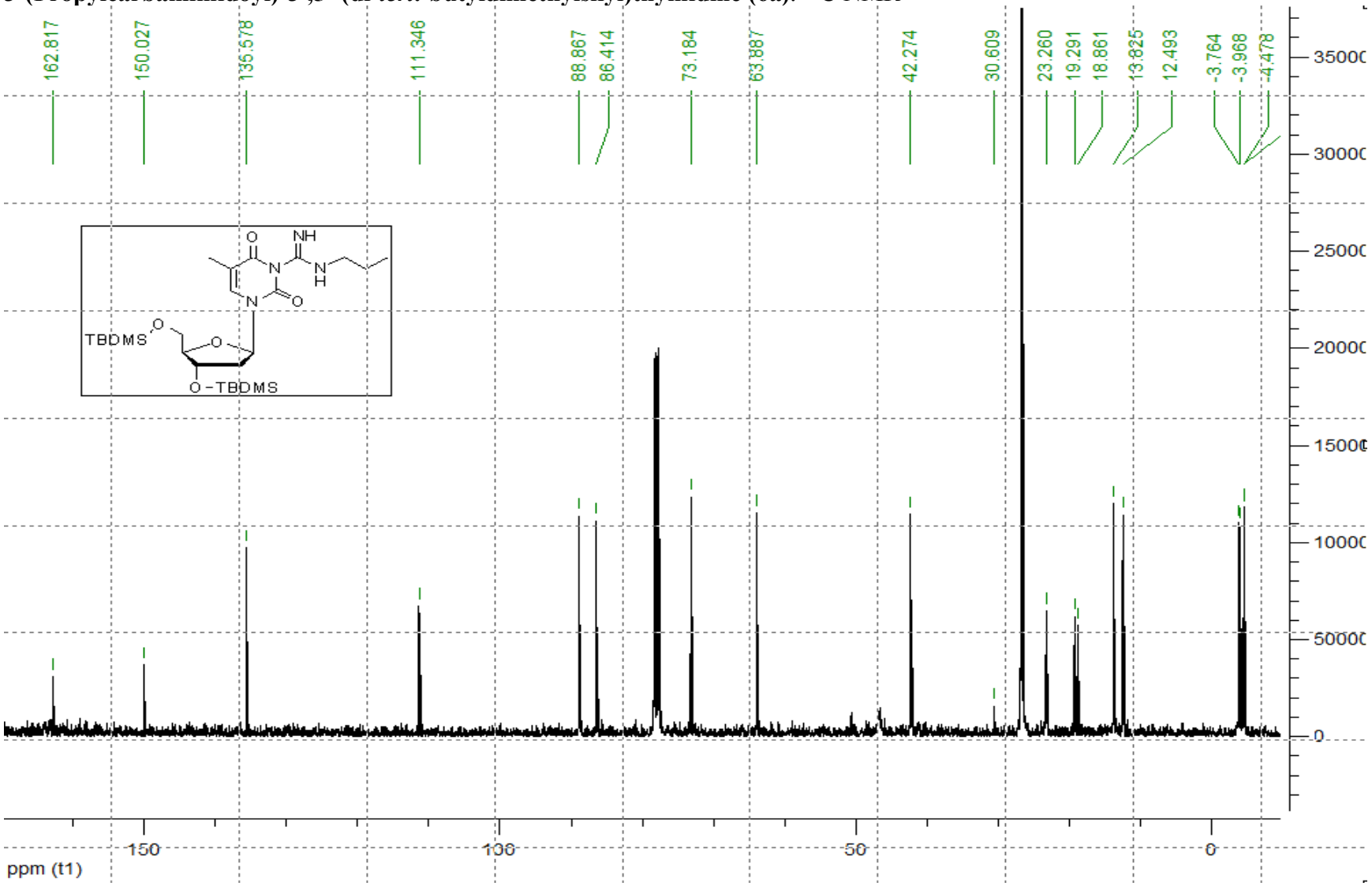
3',5'-(Di-*tert*.-butyldimethylsilyl)-3-cyanothymidine. (**5**). HR-ESI-MS: 518.2462.



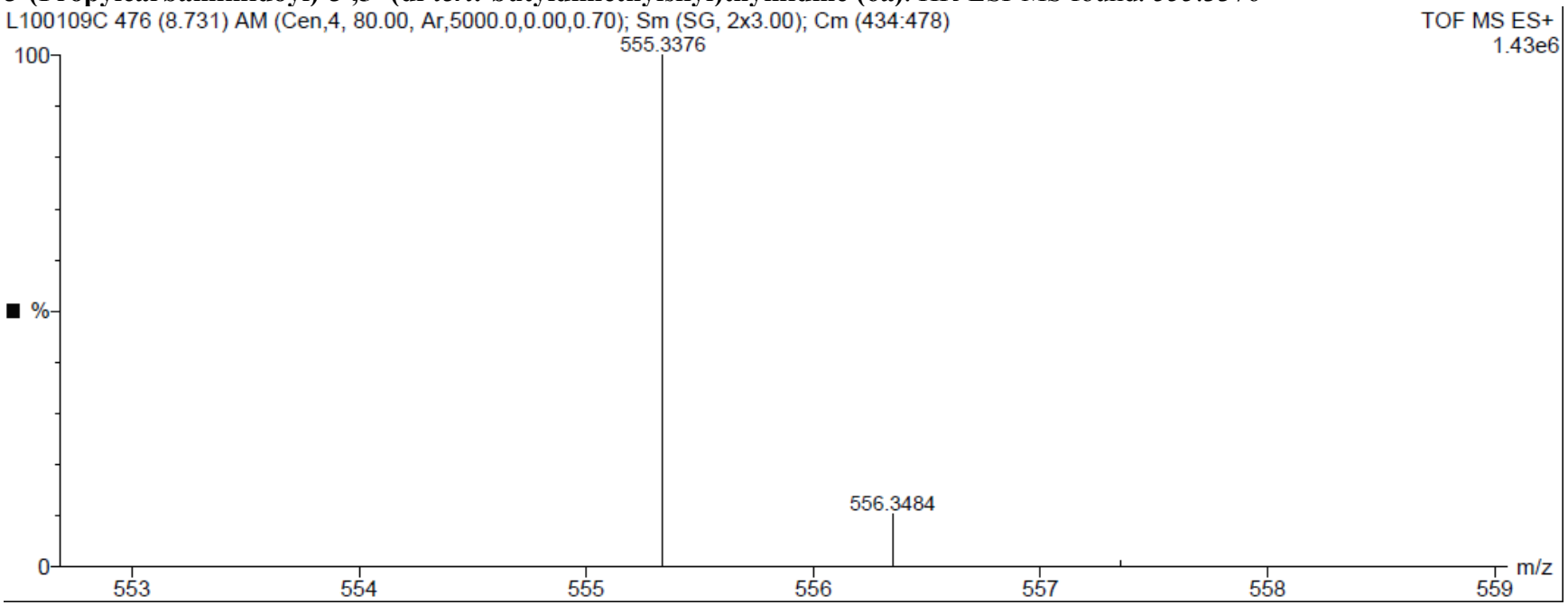
3-(Propylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6a). ^{1}H NMR



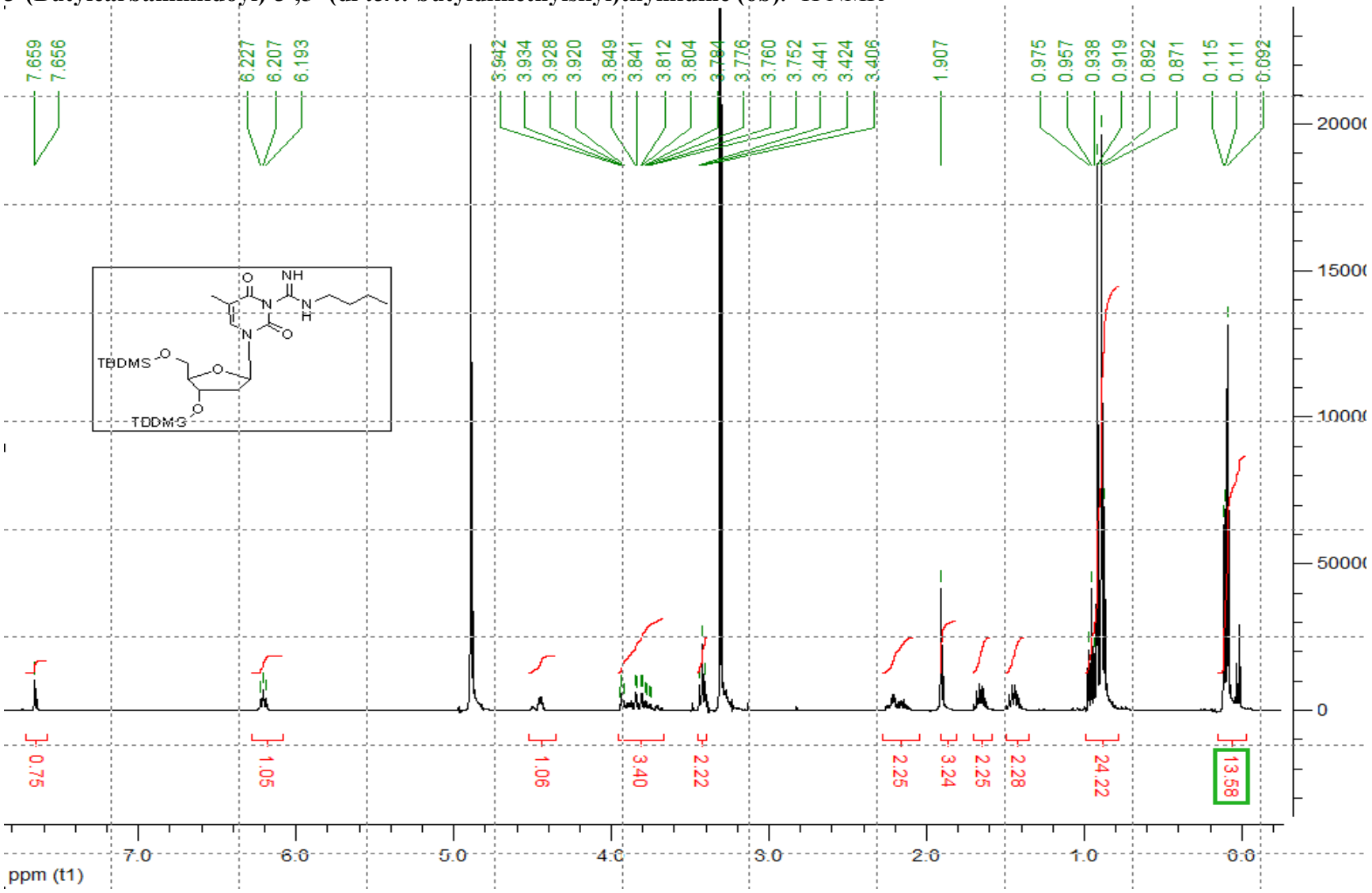
3-(Propylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6a). ^{13}C NMR



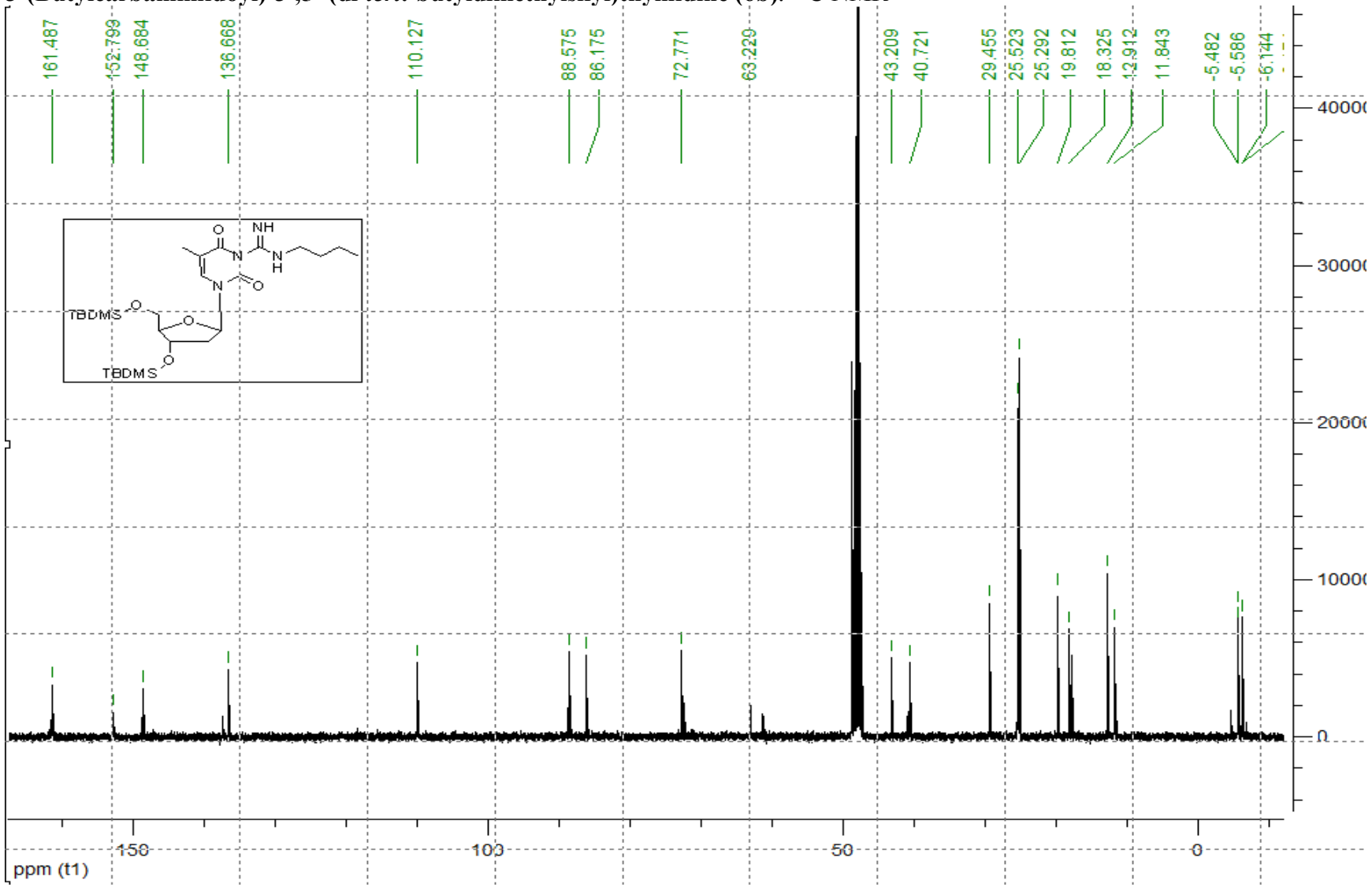
3-(Propylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6a). HR-ESI-MS found: 555.3376



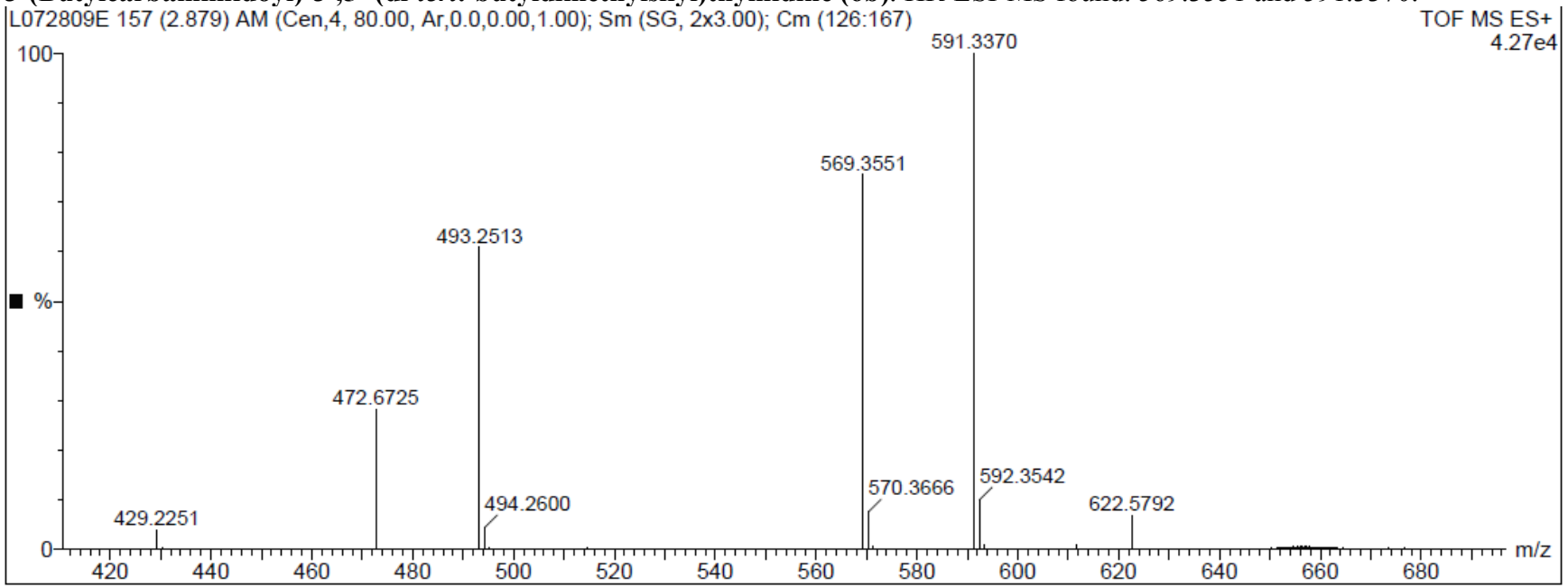
3-(Butylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6b). ^{1}H NMR



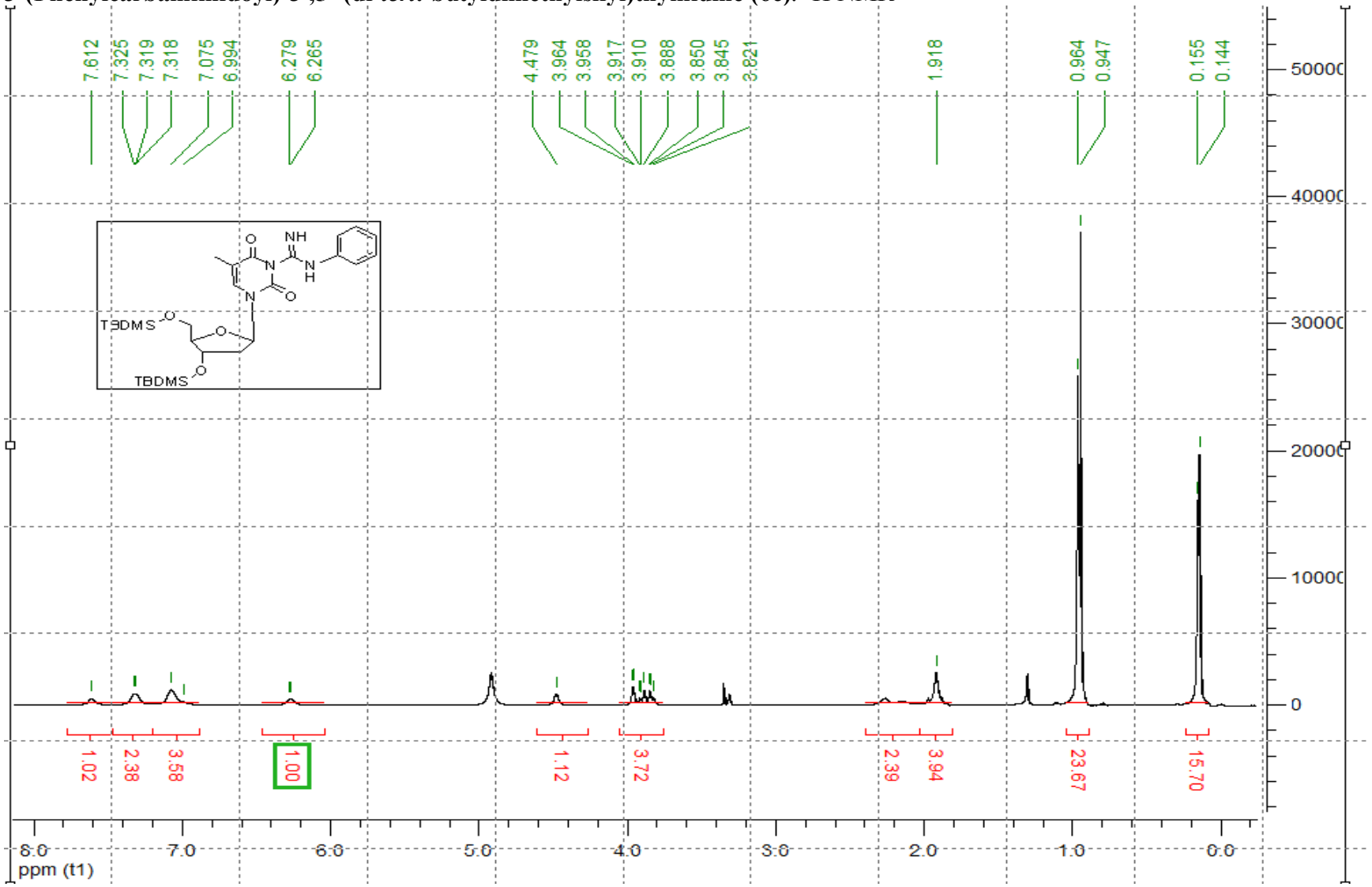
3-(Butylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6b). ^{13}C NMR



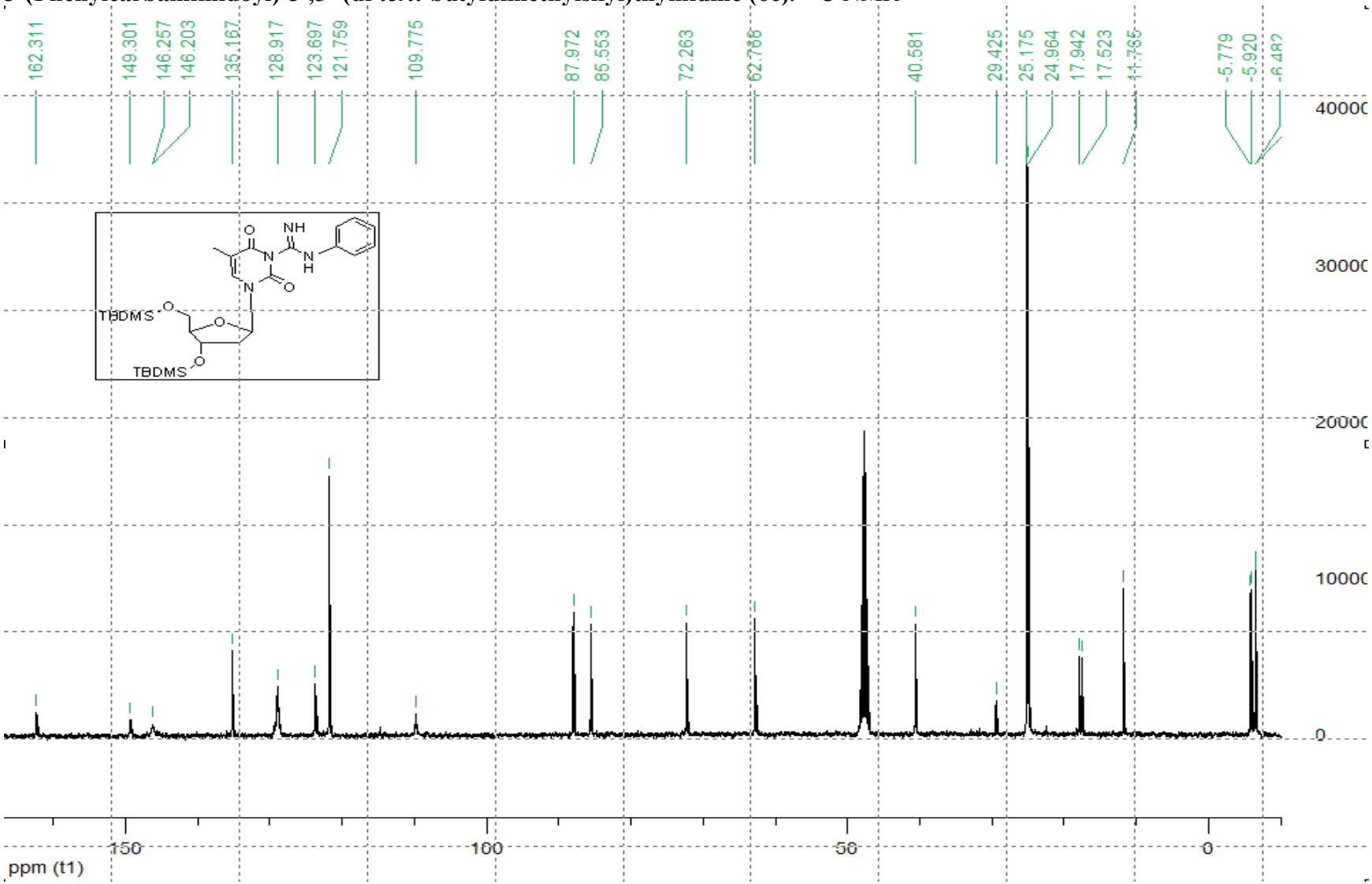
3-(Butylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6b). HR-ESI-MS found: 569.3551 and 591.3370.



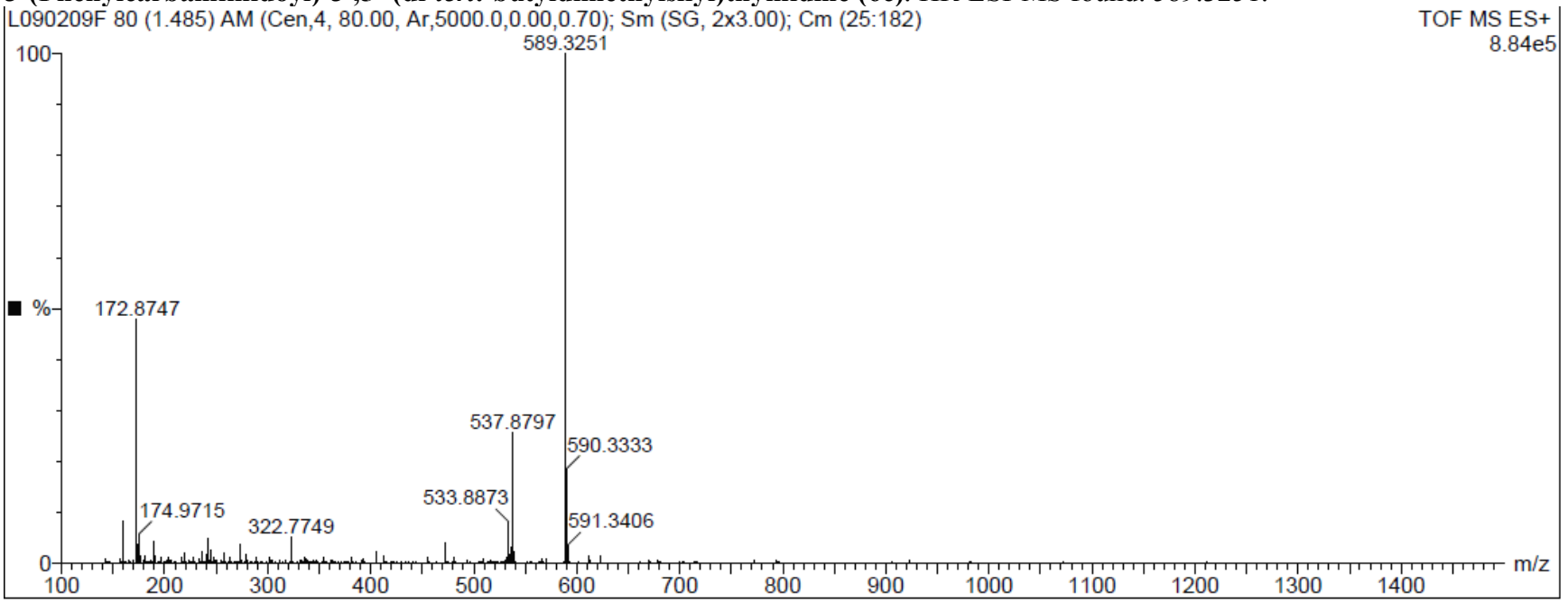
3-(Phenylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6c). ^{1}H NMR



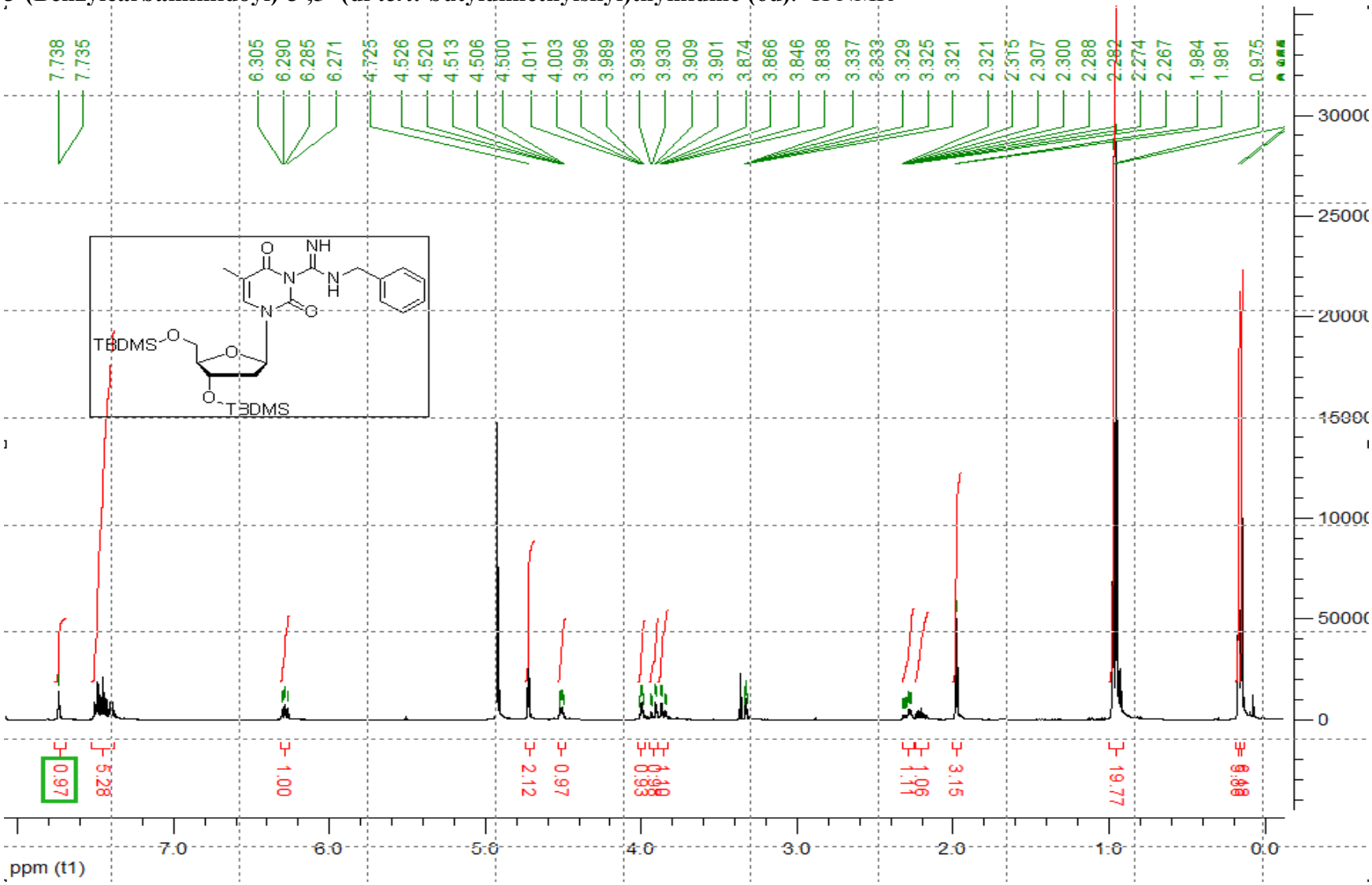
3-(Phenylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6c). ^{13}C NMR



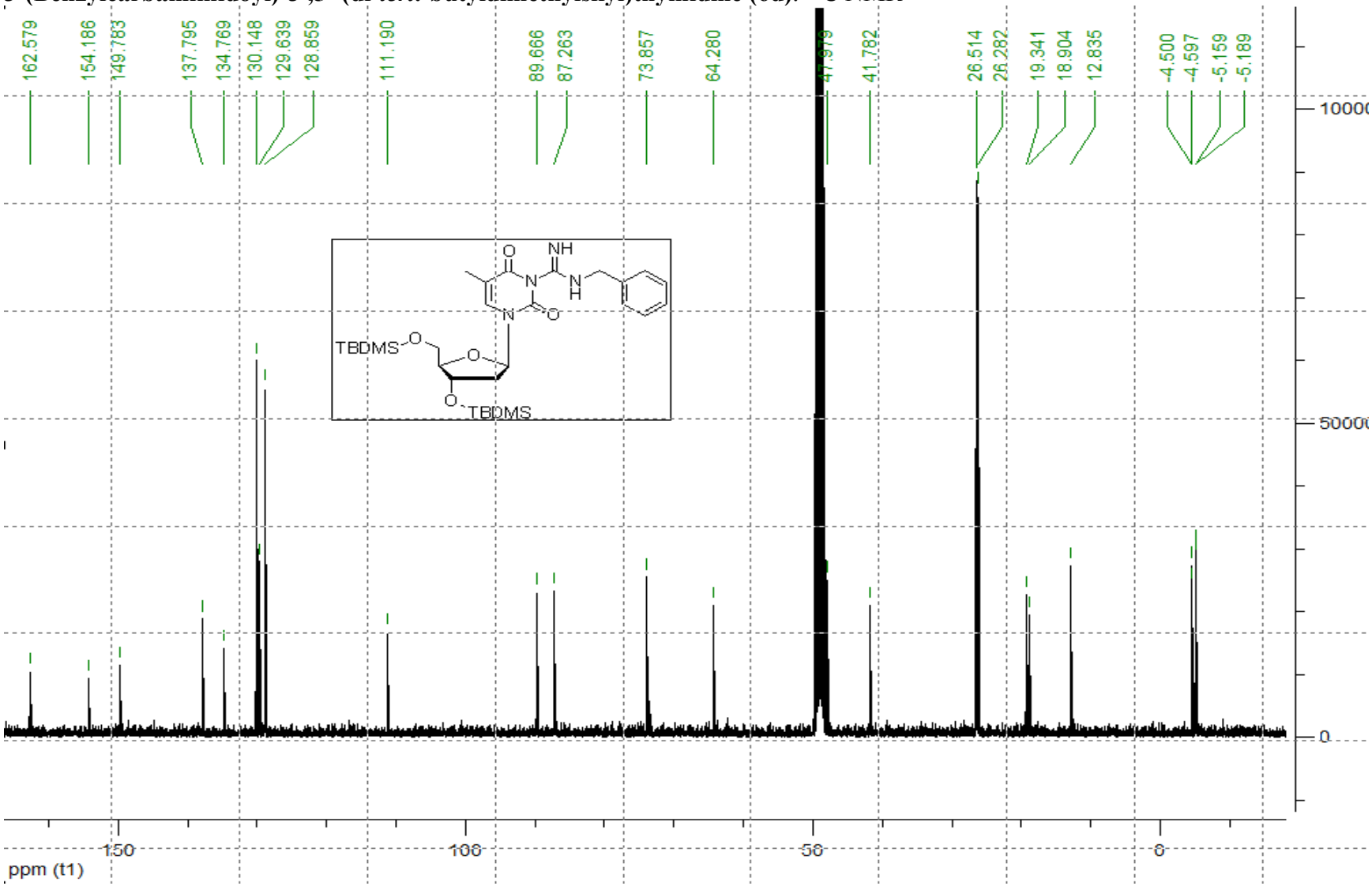
3-(Phenylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6c). HR-ESI-MS found: 589.3251.



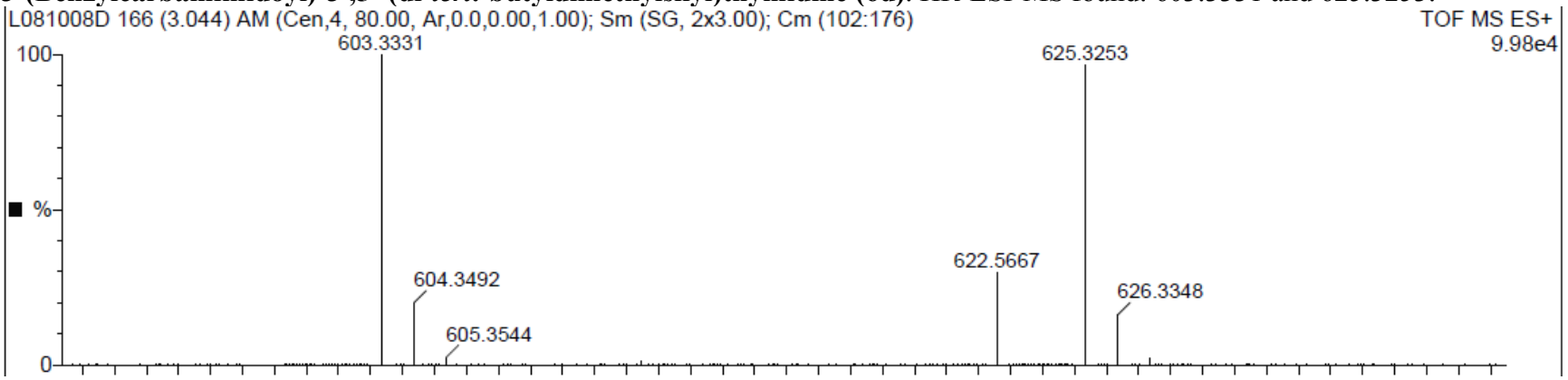
3-(Benzylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6d). ^{1}H NMR



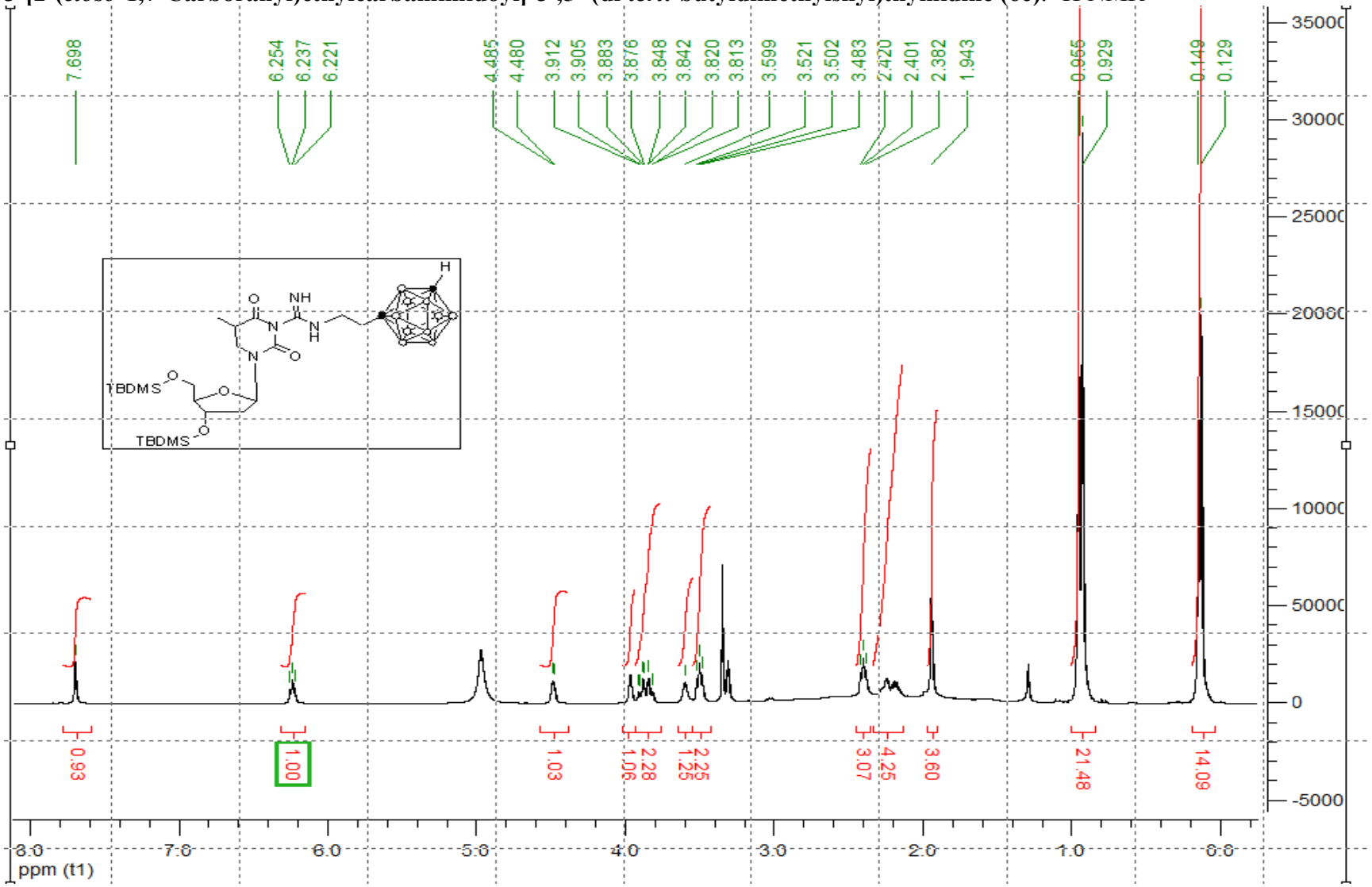
3-(Benzylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6d). ^{13}C NMR



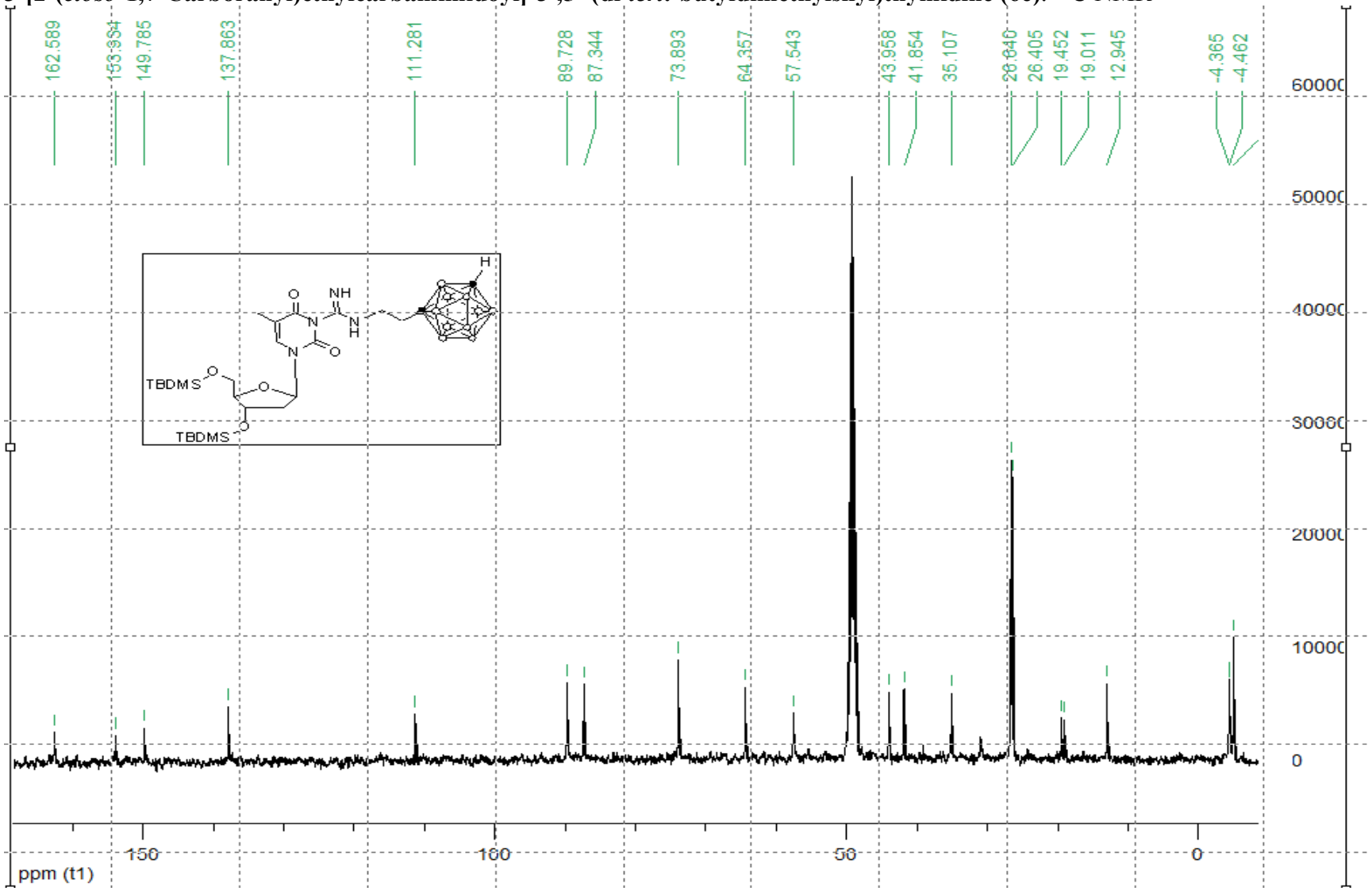
3-(Benzylcarbamimidoyl)-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6d). HR-ESI-MS found: 603.3331 and 625.3253.



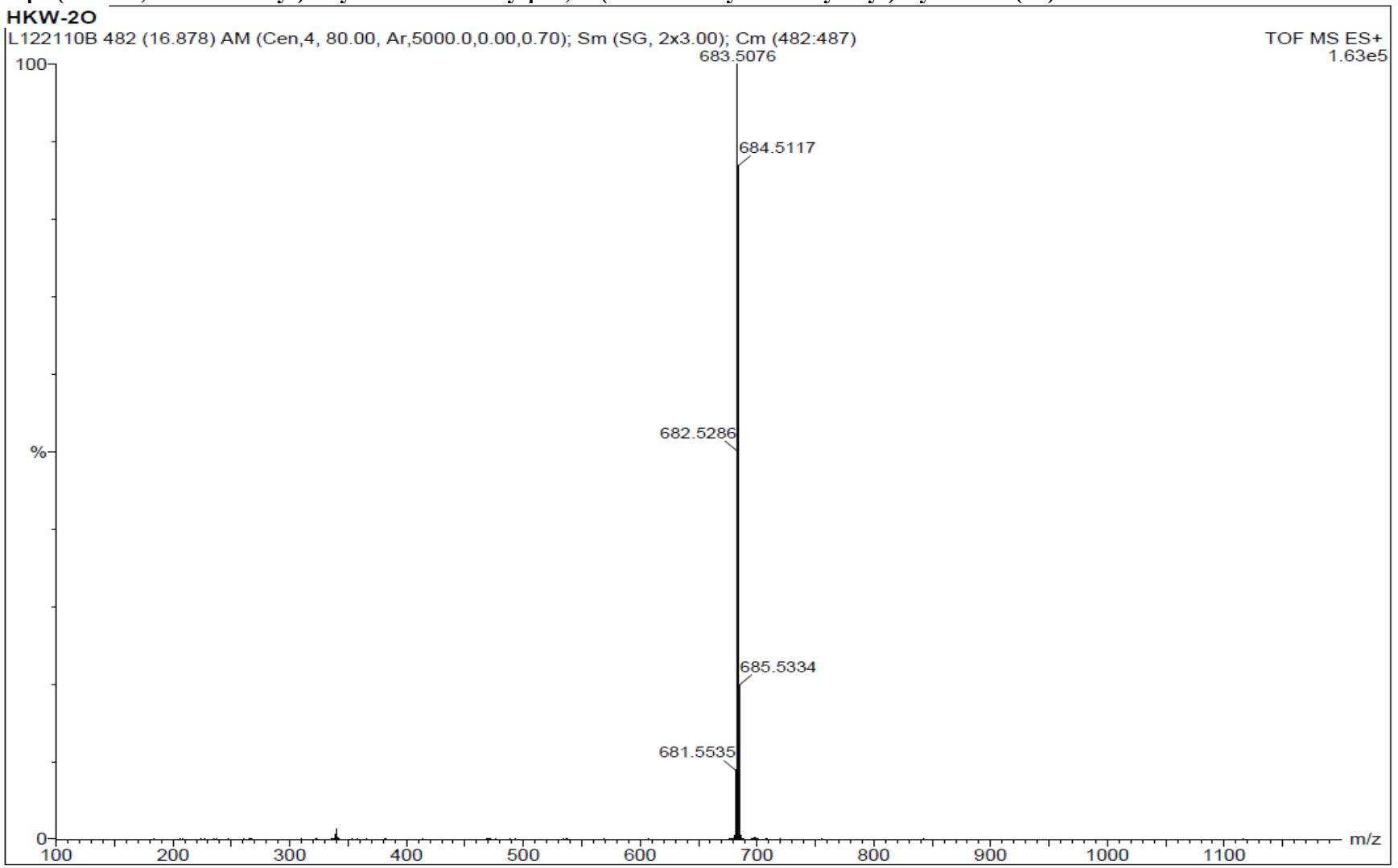
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6e). ^{1}H NMR



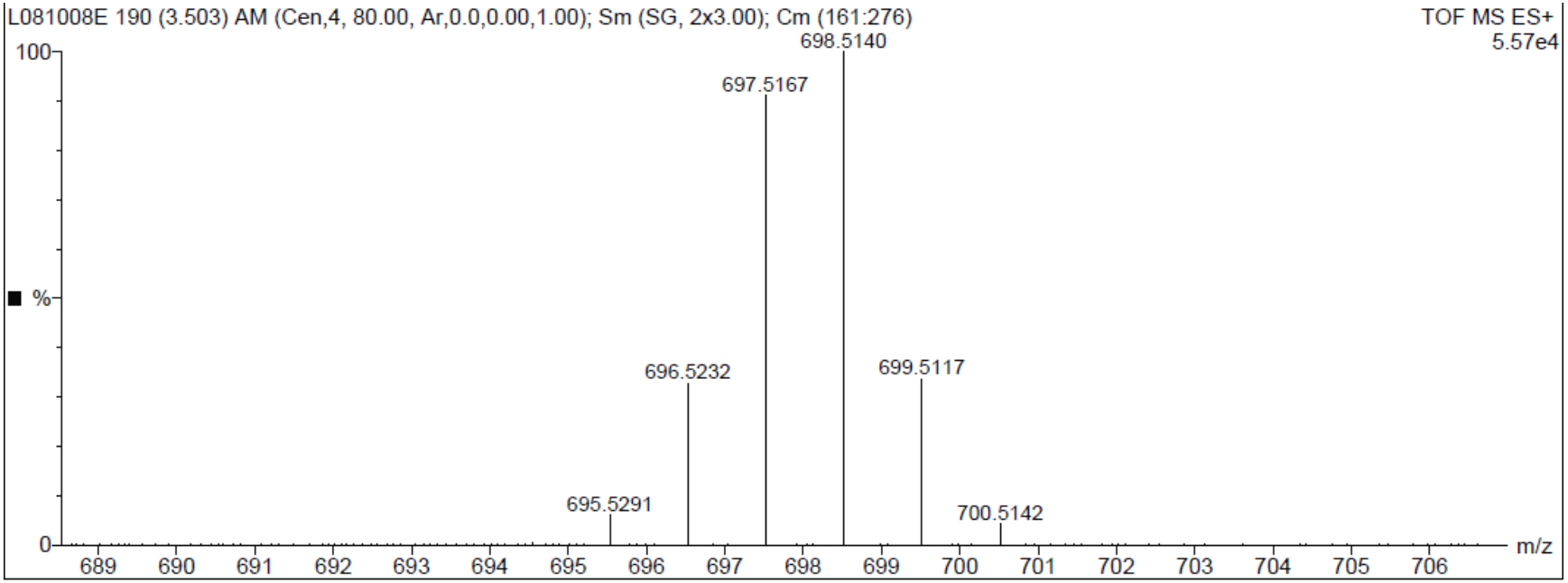
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6e). ^{13}C NMR



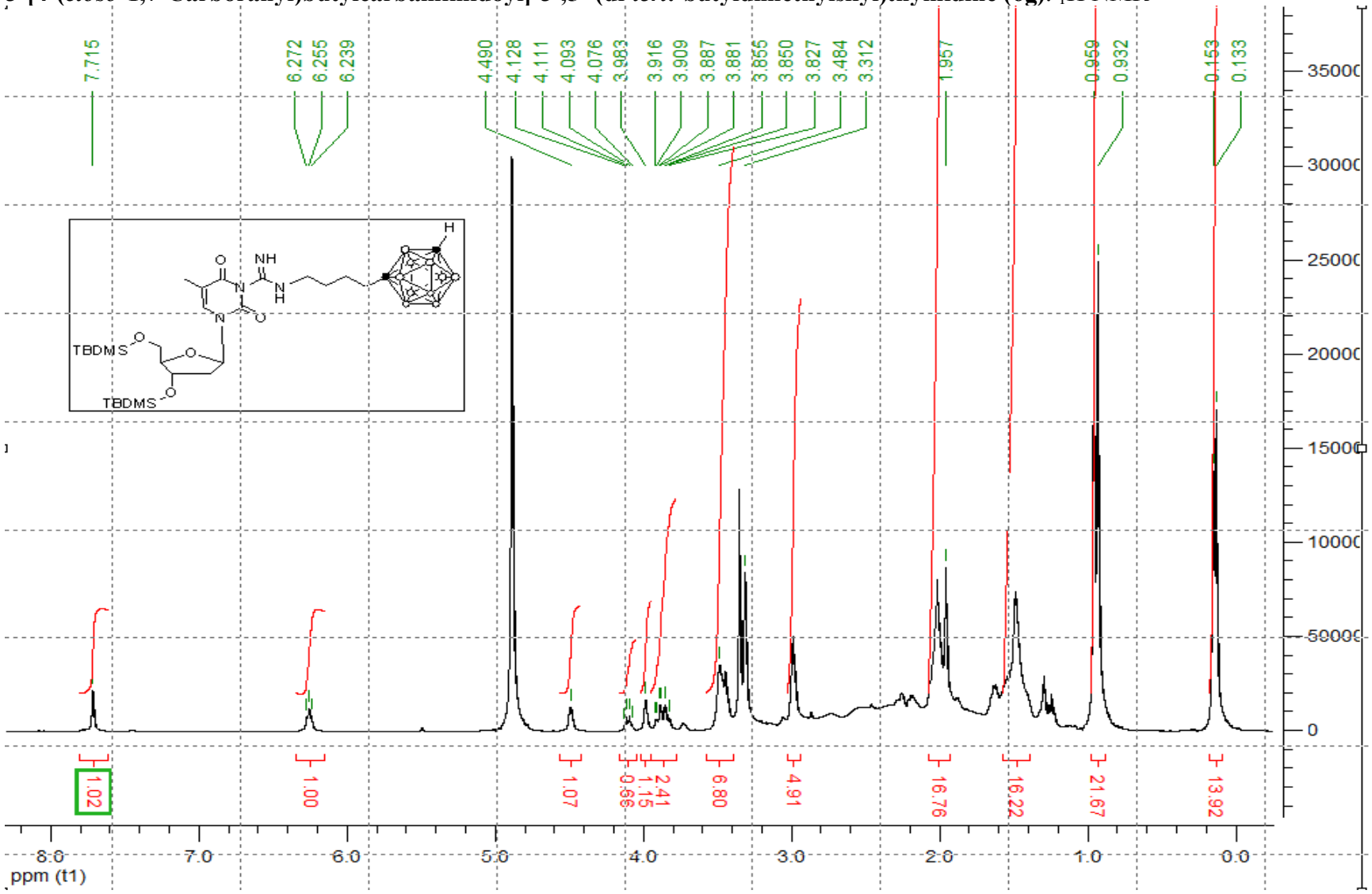
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6e). HR-ESI-MS found: 683.5076.



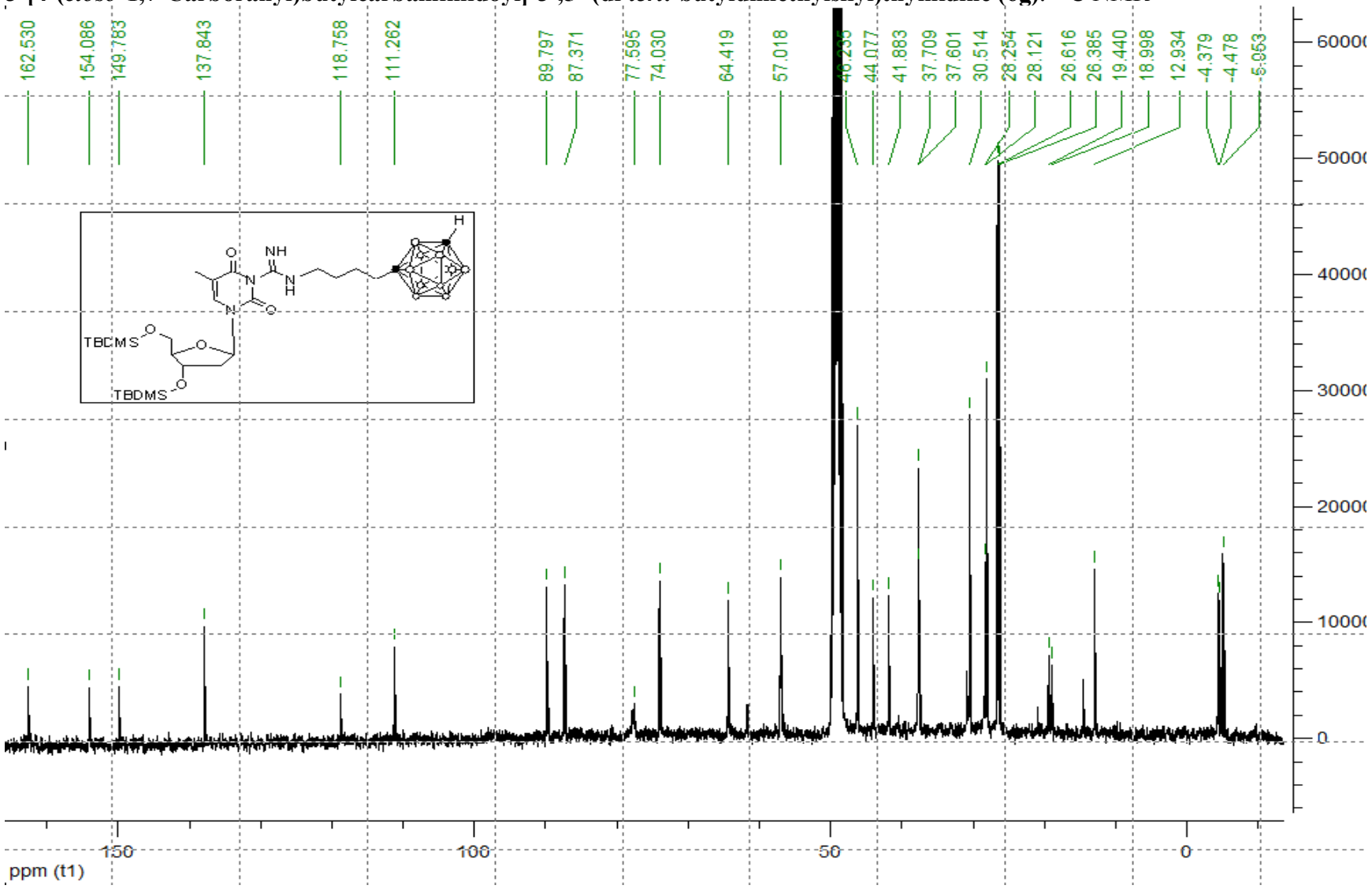
3-[3-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6f). HR-ESI-MS found: 697.5167.



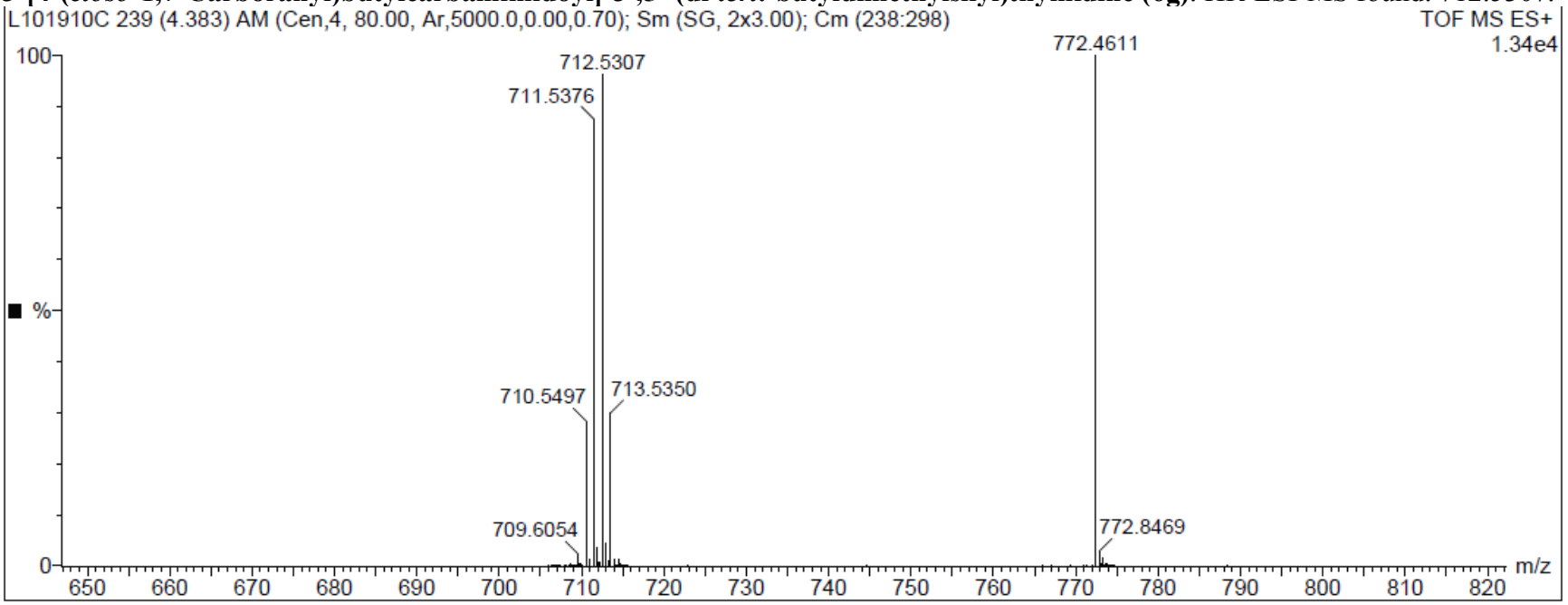
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6g). ^{1}H NMR



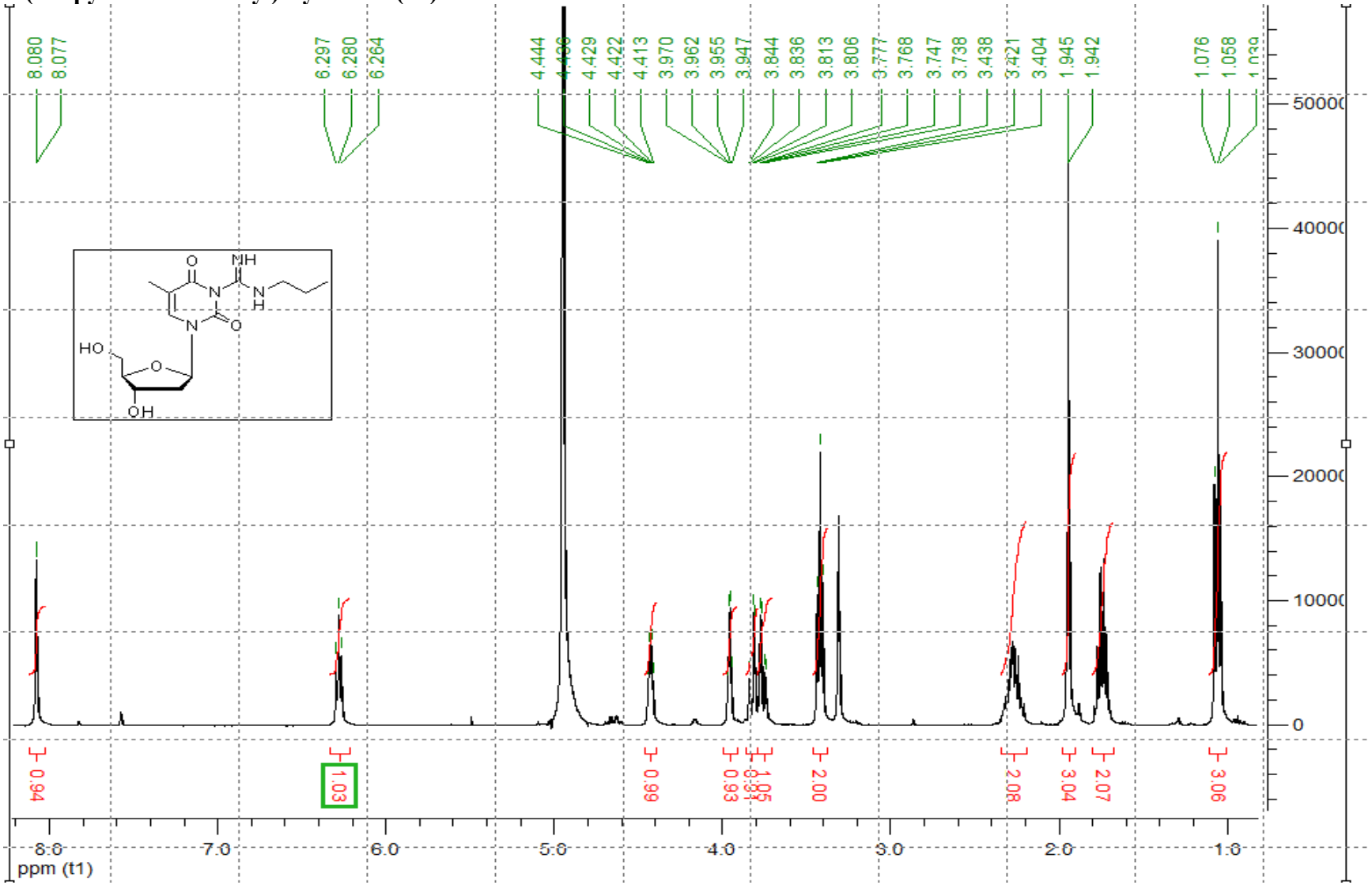
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6g). ^{13}C NMR



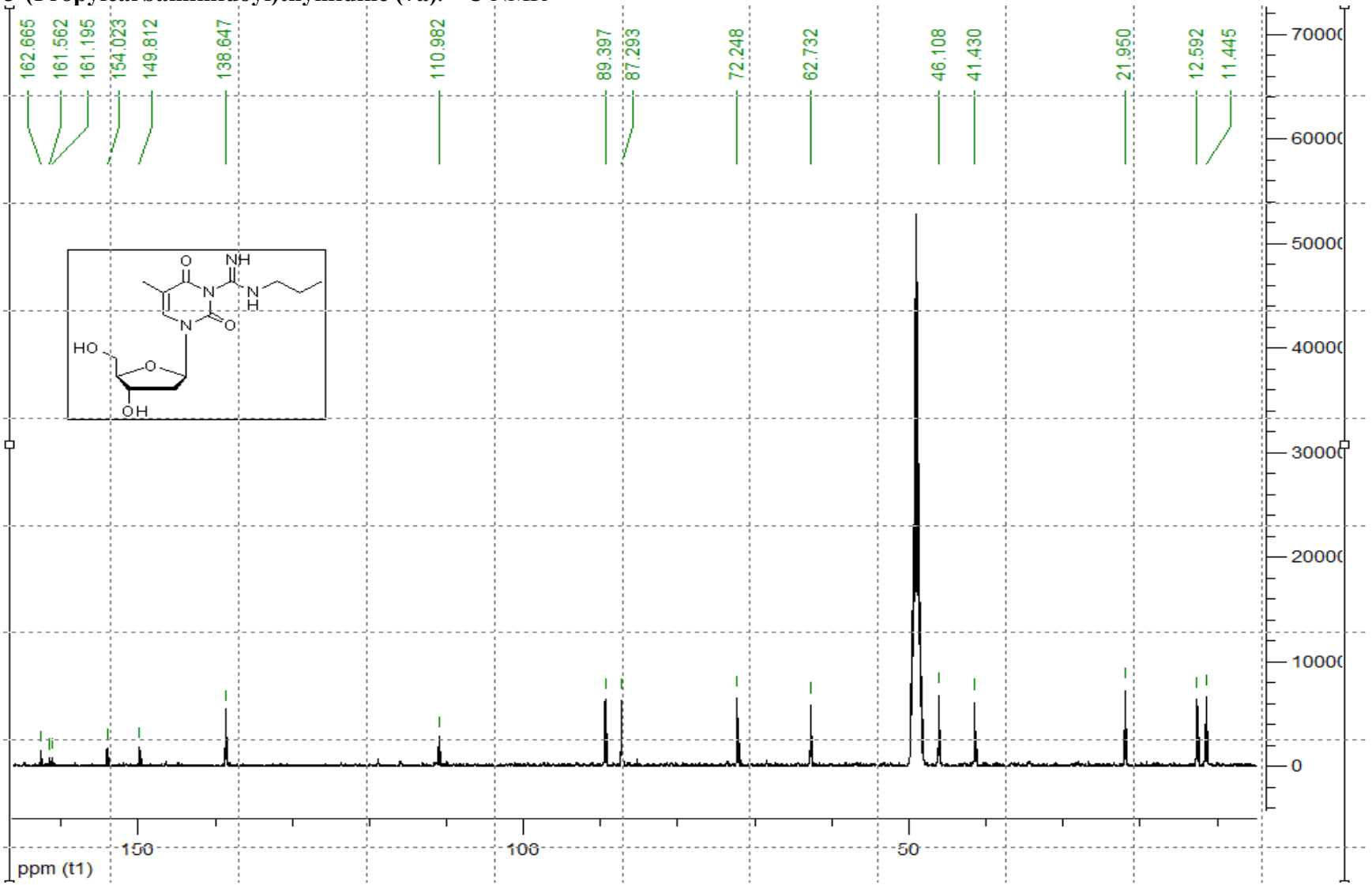
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]-3',5'-(di-*tert*.-butyldimethylsilyl)thymidine (6g). HR-ESI-MS found: 712.5307.



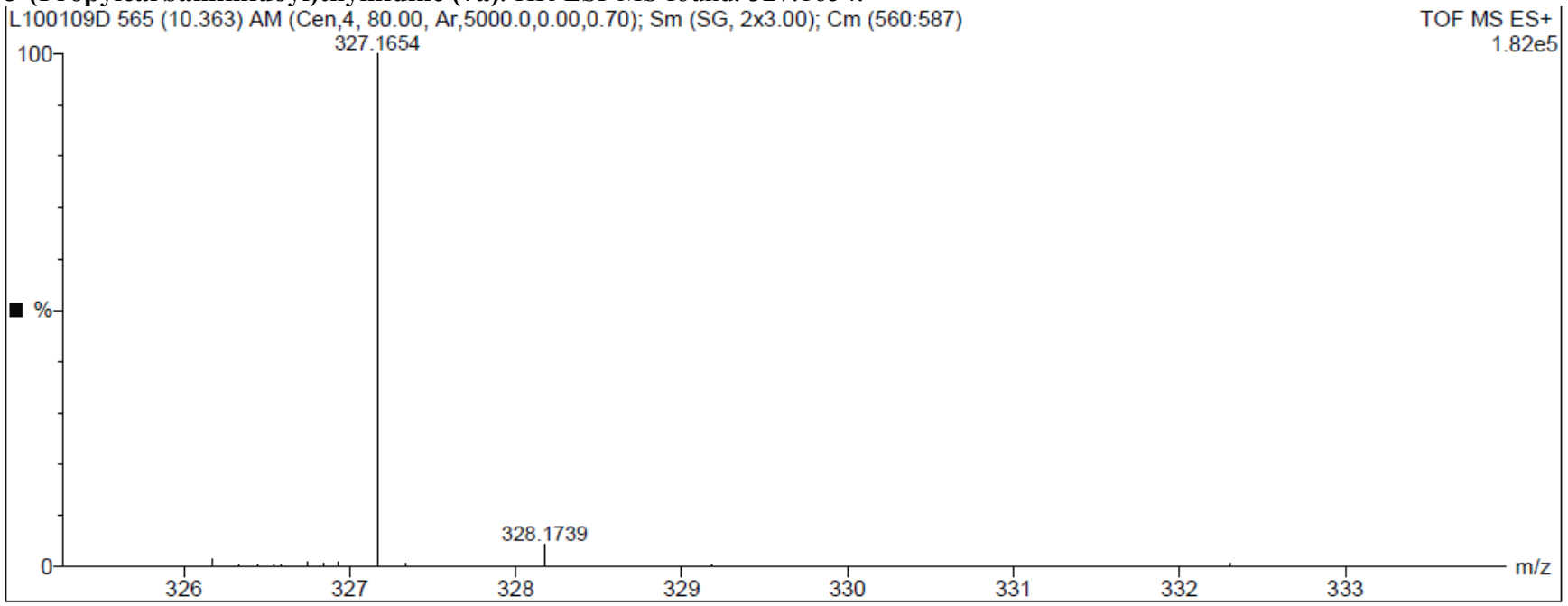
3-(Propylcarbamimidoyl)thymidine (7a). ^{1}H NMR



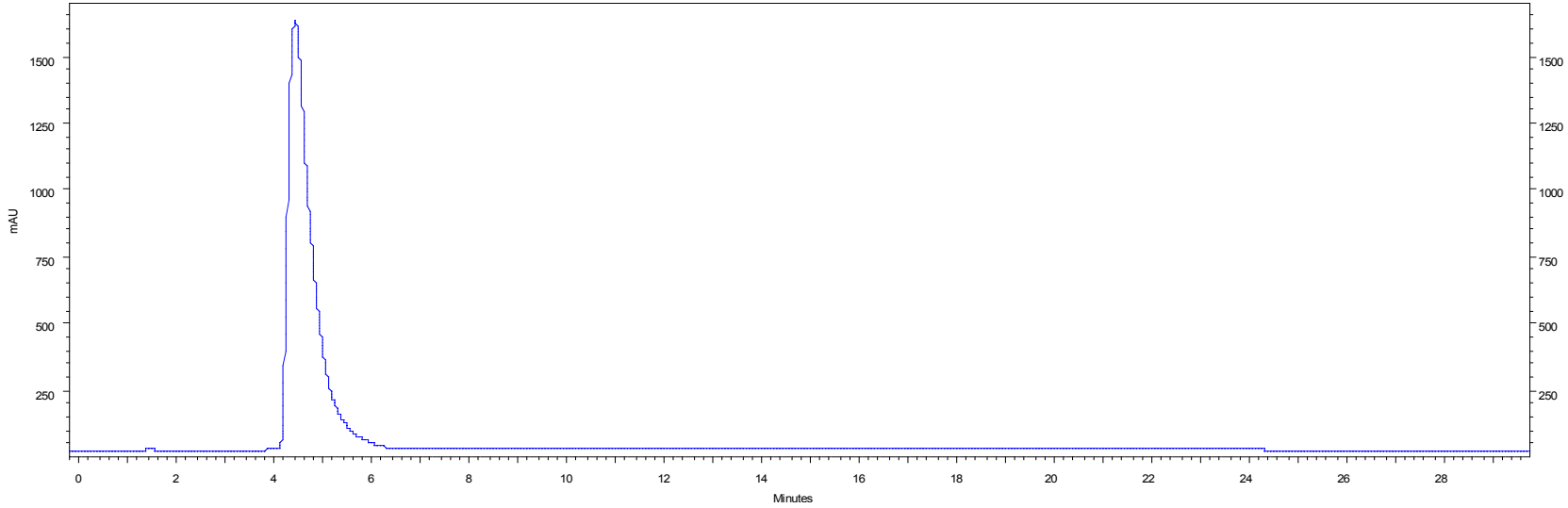
3-(Propylcarbamimidoyl)thymidine (7a). ^{13}C NMR



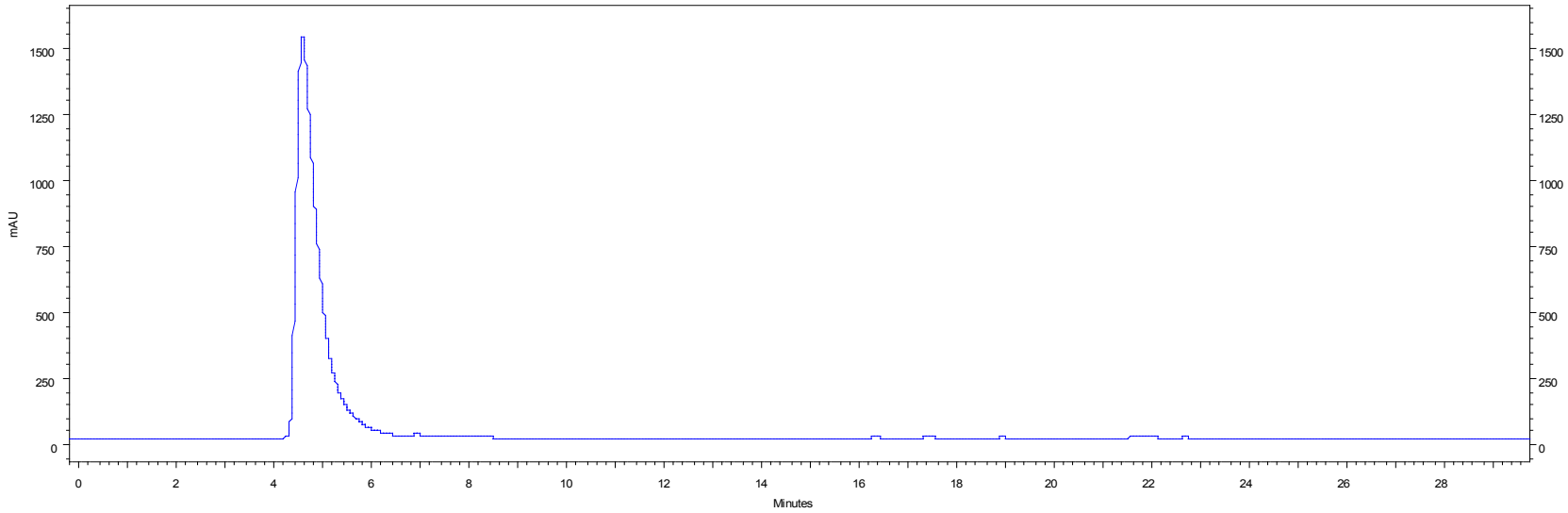
3-(Propylcarbamimidoyl)thymidine (7a). HR-ESI-MS found: 327.1654.



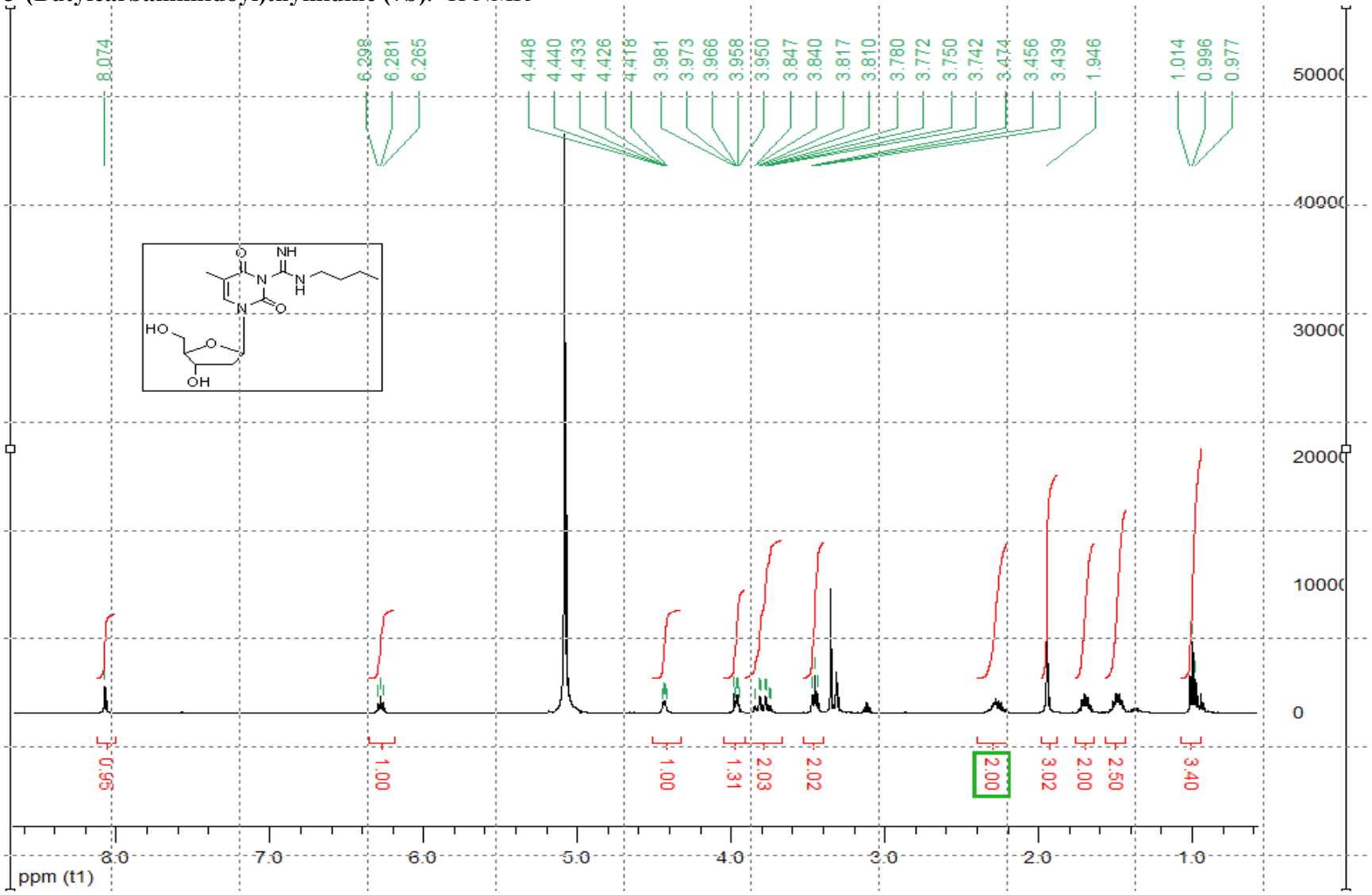
3-(Propylcarbamimidoyl)thymidine (7a). Analytical traces in Water:Acetonitrile gradient



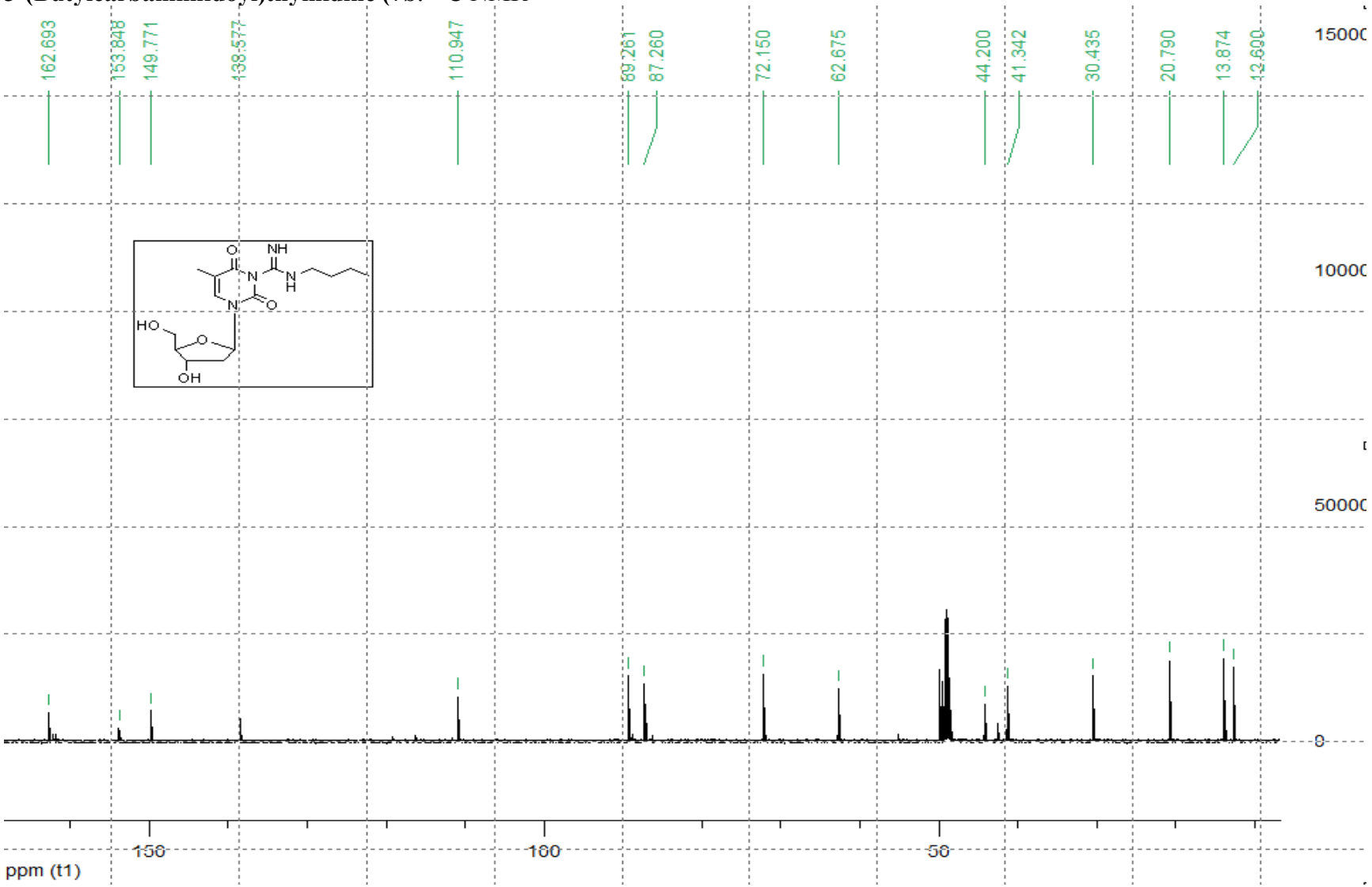
Analytical traces in Water:Methanol gradient



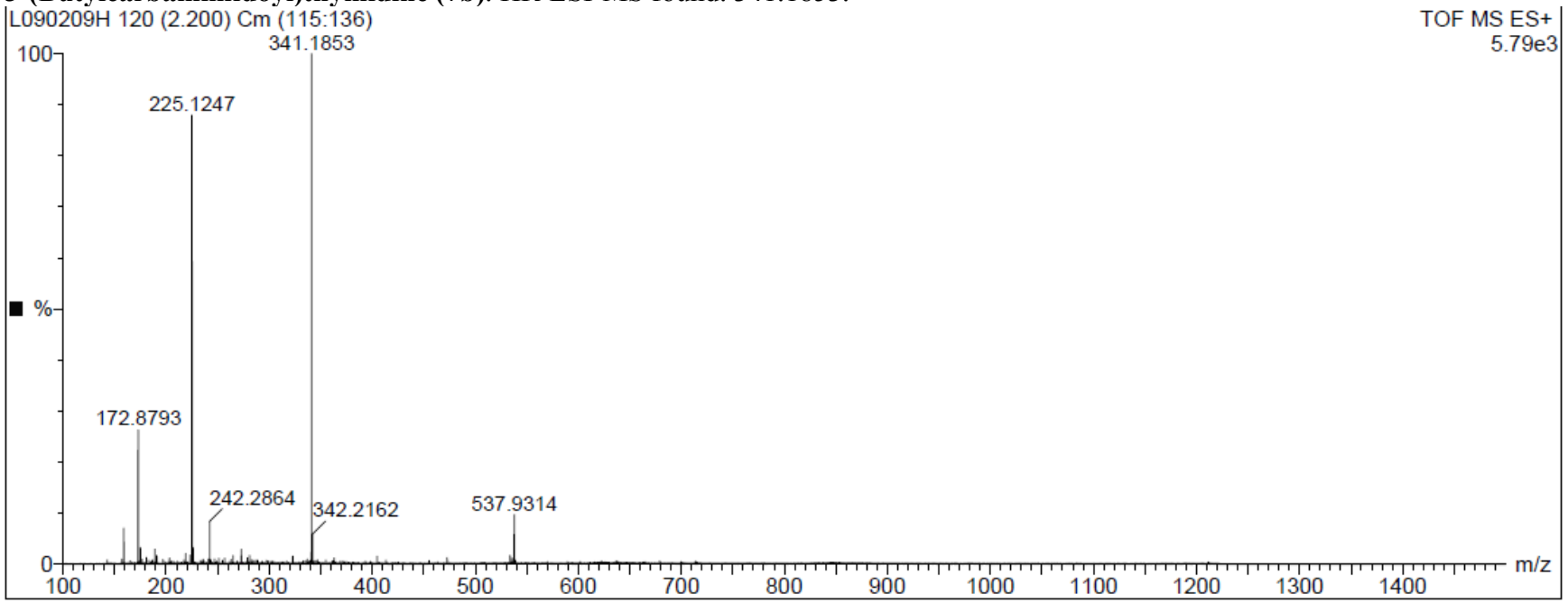
3-(Butylcarbamimidoyl)thymidine (7b). ^{1}H NMR



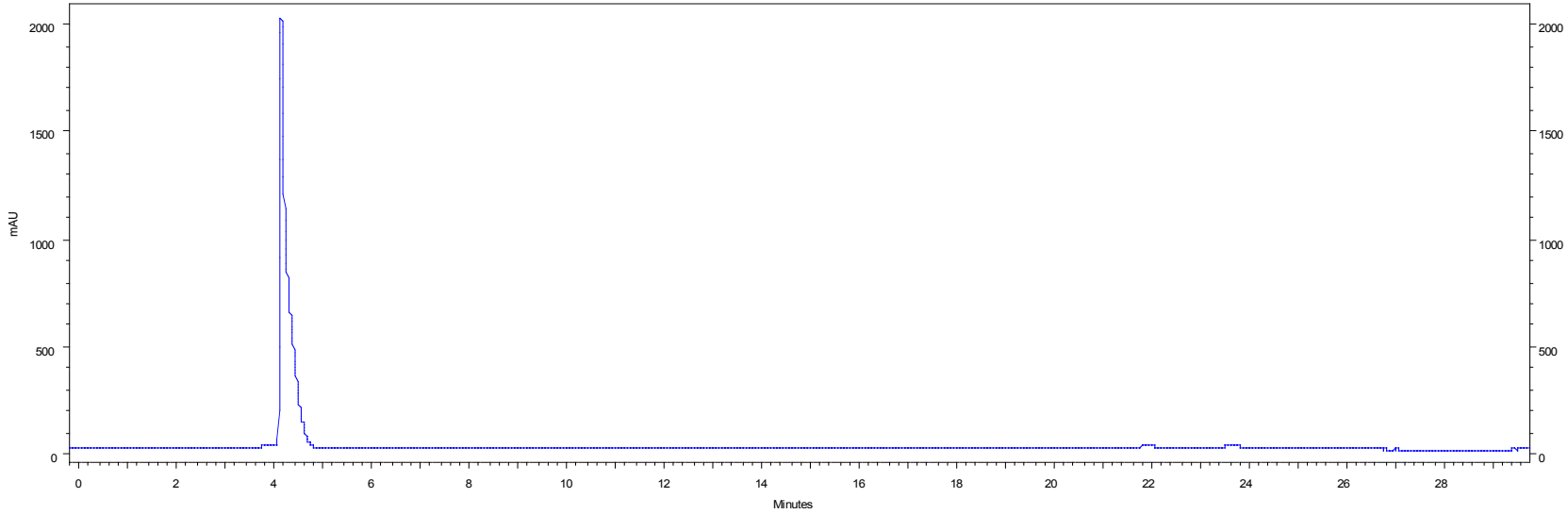
3-(Butylcarbamimidoyl)thymidine (7b. ^{13}C NMR



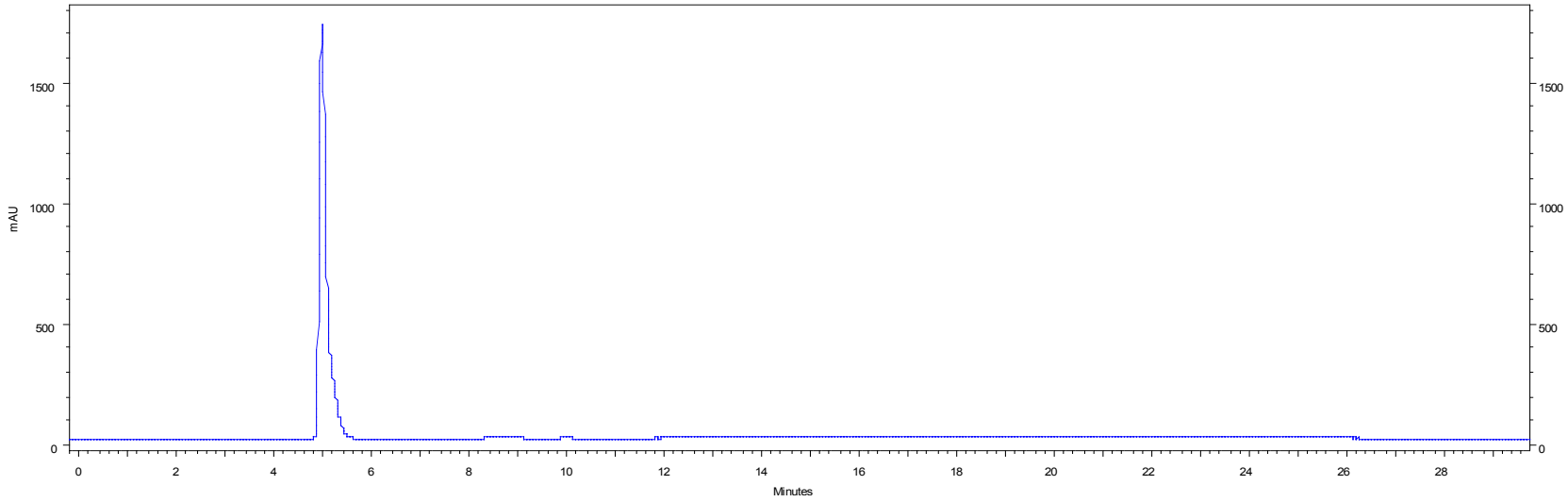
3-(Butylcarbamimidoyl)thymidine (7b). HR-ESI-MS found: 341.1853.



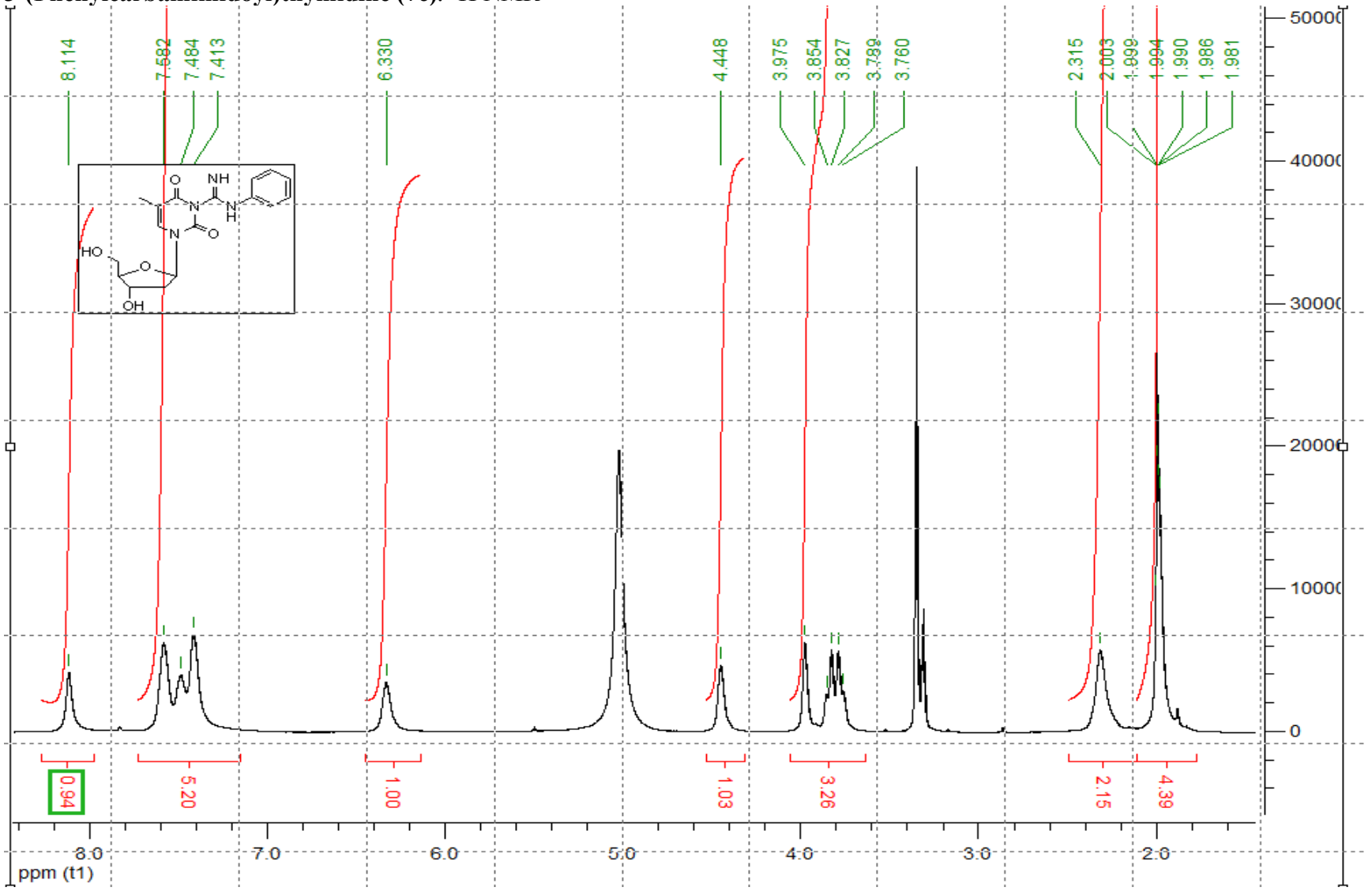
3-(Butylcarbamimidoyl)thymidine (7b). Analytical traces in Water:Acetonitrile gradient



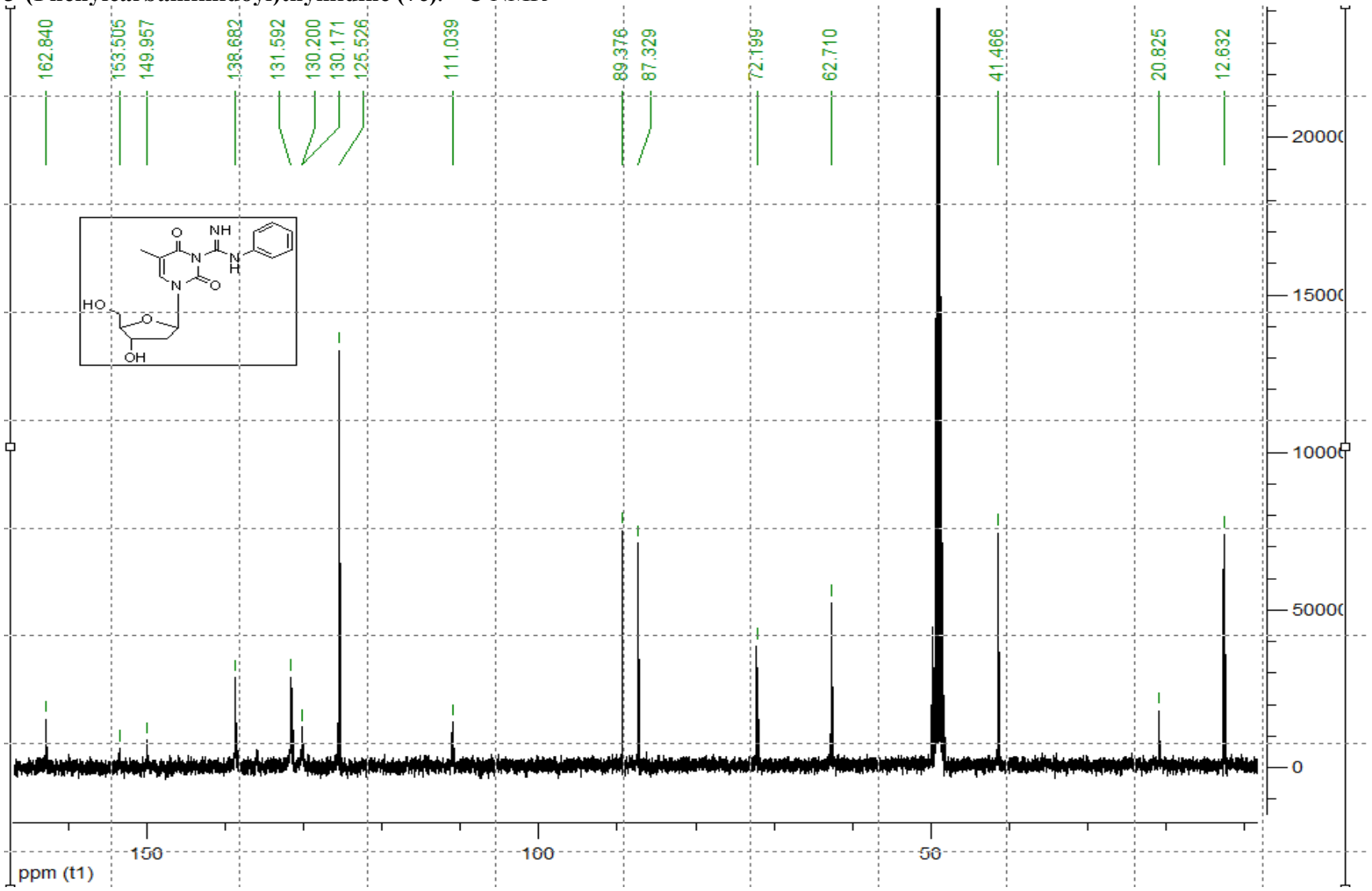
Analytical traces in Water:Methanol gradient



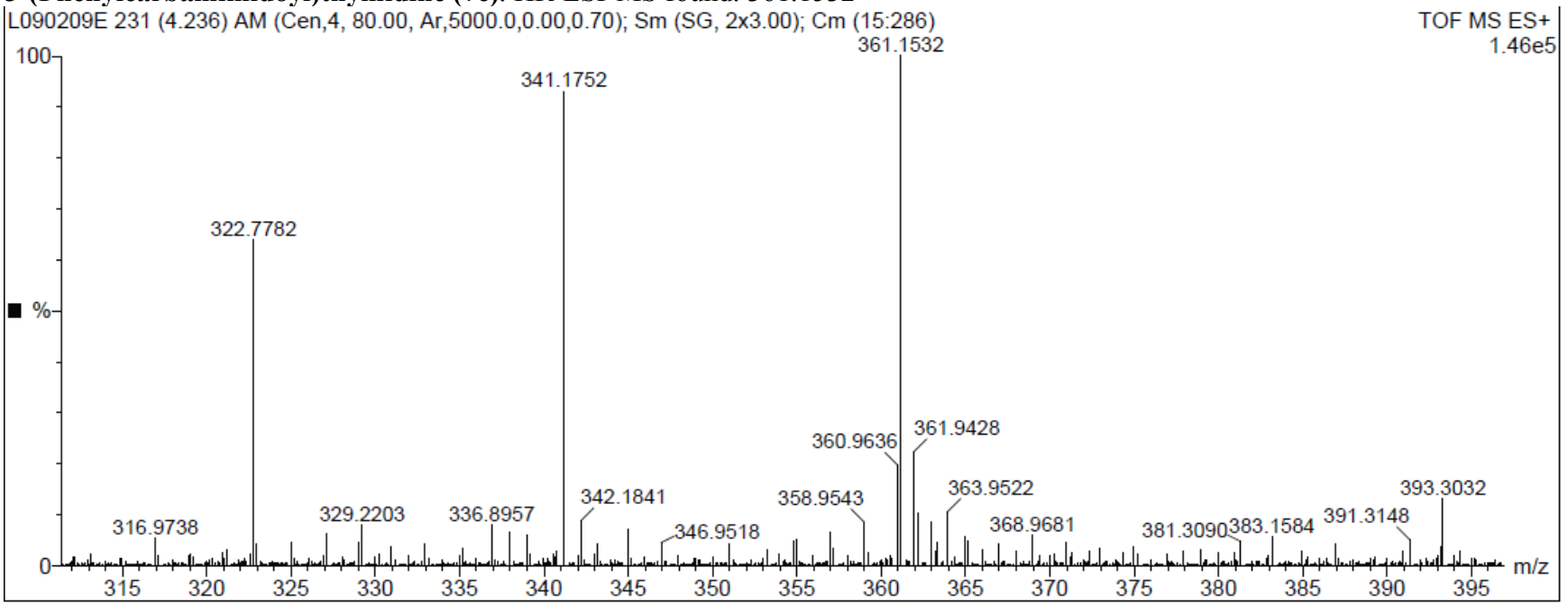
3-(Phenylcarbamimidoyl)thymidine (7c). ^{1}H NMR



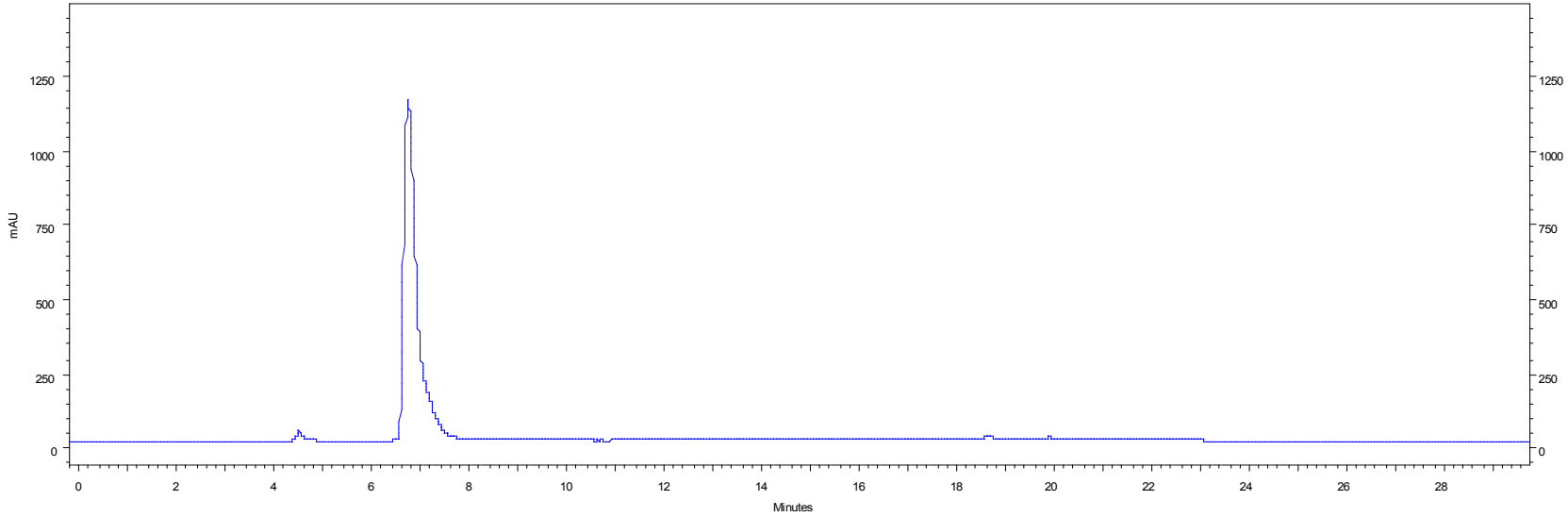
3-(Phenylcarbamimidoyl)thymidine (7c). ^{13}C NMR



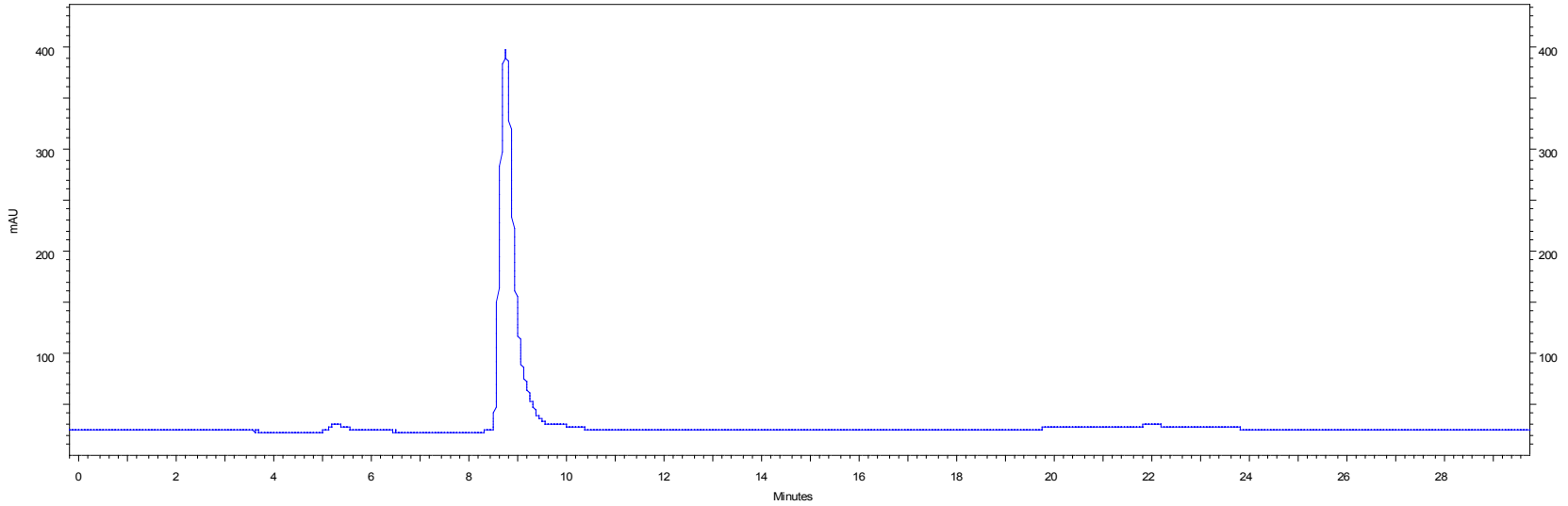
3-(Phenylcarbamimidoyl)thymidine (7c). HR-ESI-MS found: 361.1532



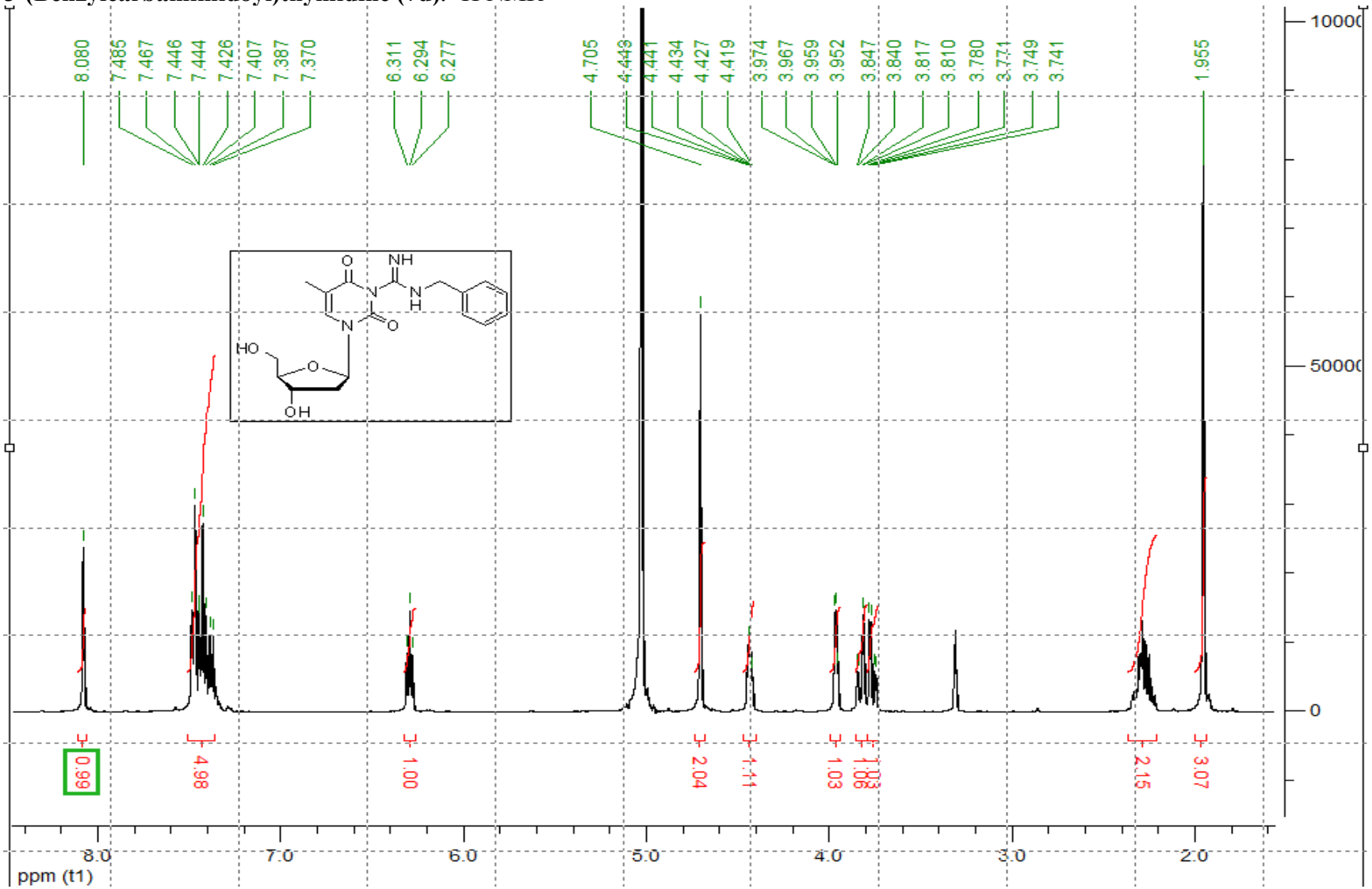
3-(Phenylcarbamimidoyl)thymidine (7c). Analytical traces in Water:Acetonitrile gradient



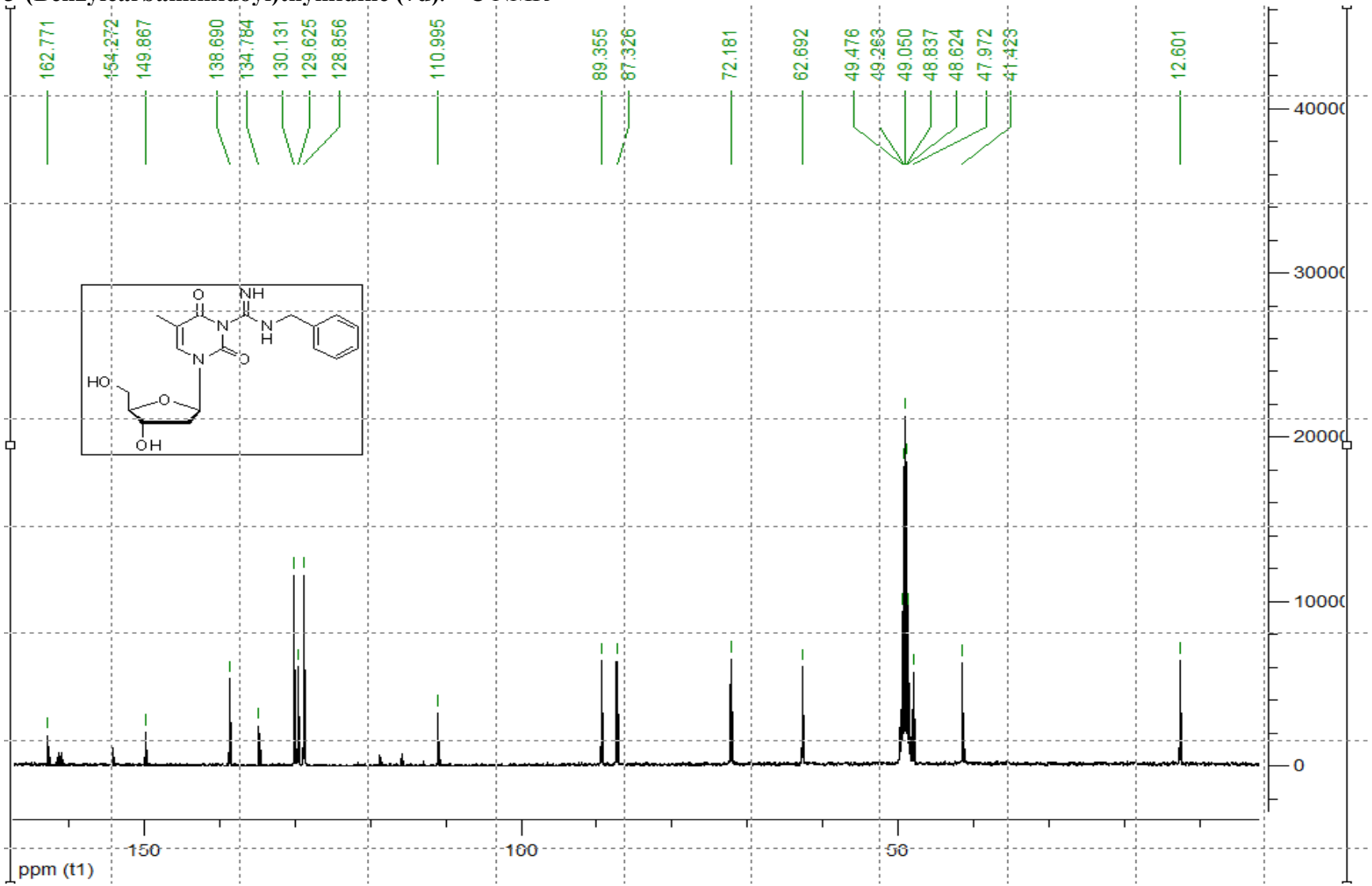
Analytical traces in Water:Methanol gradient



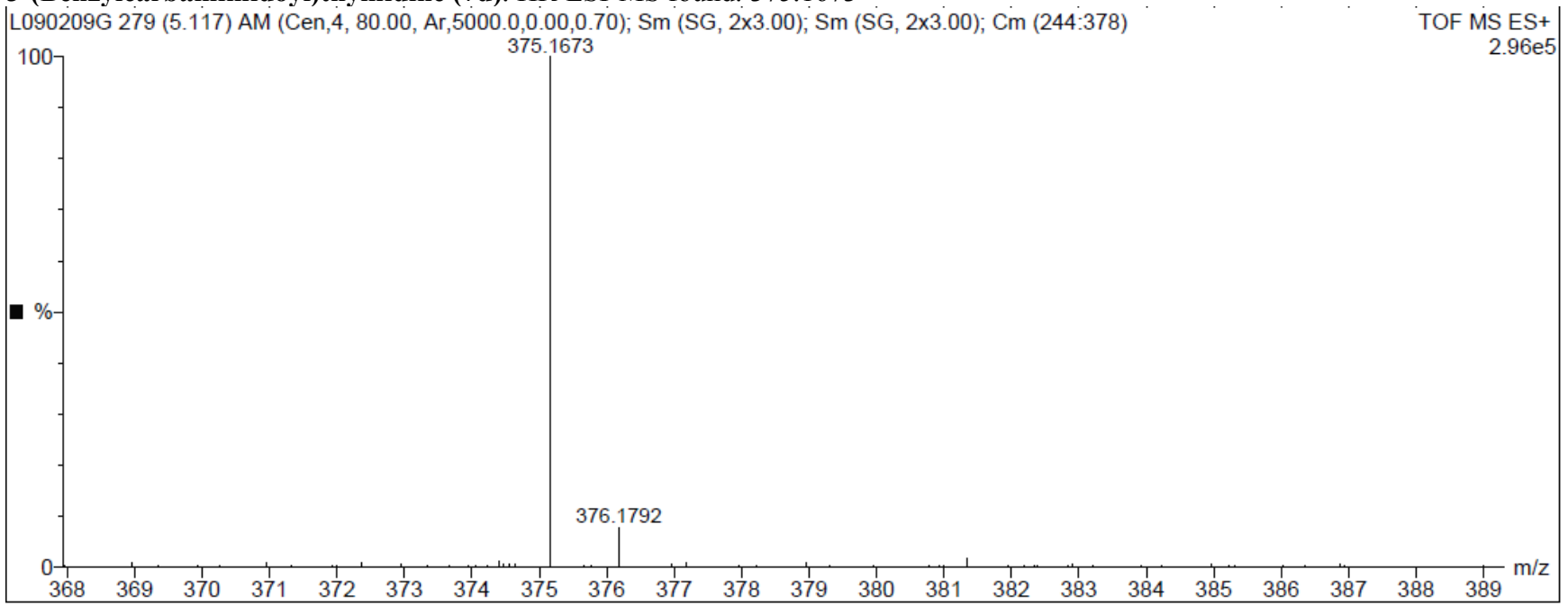
3-(Benzylcarbamimidoyl)thymidine (7d). ^{1}H NMR



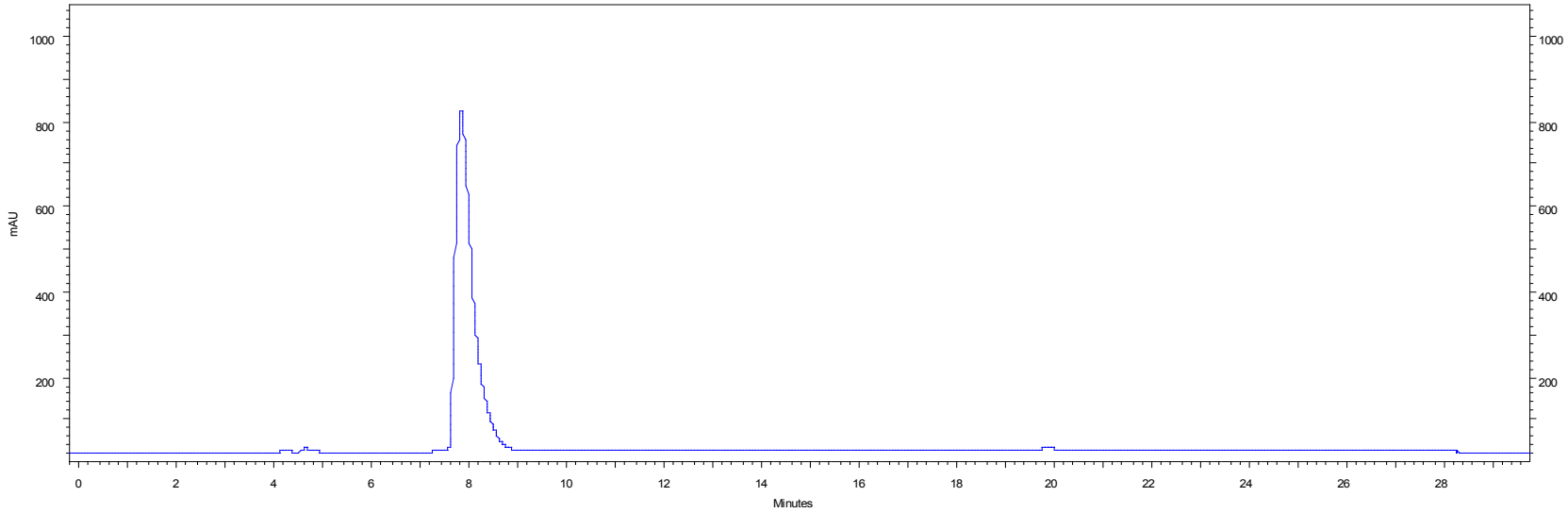
3-(Benzylcarbamimidoyl)thymidine (7d). ^{13}C NMR



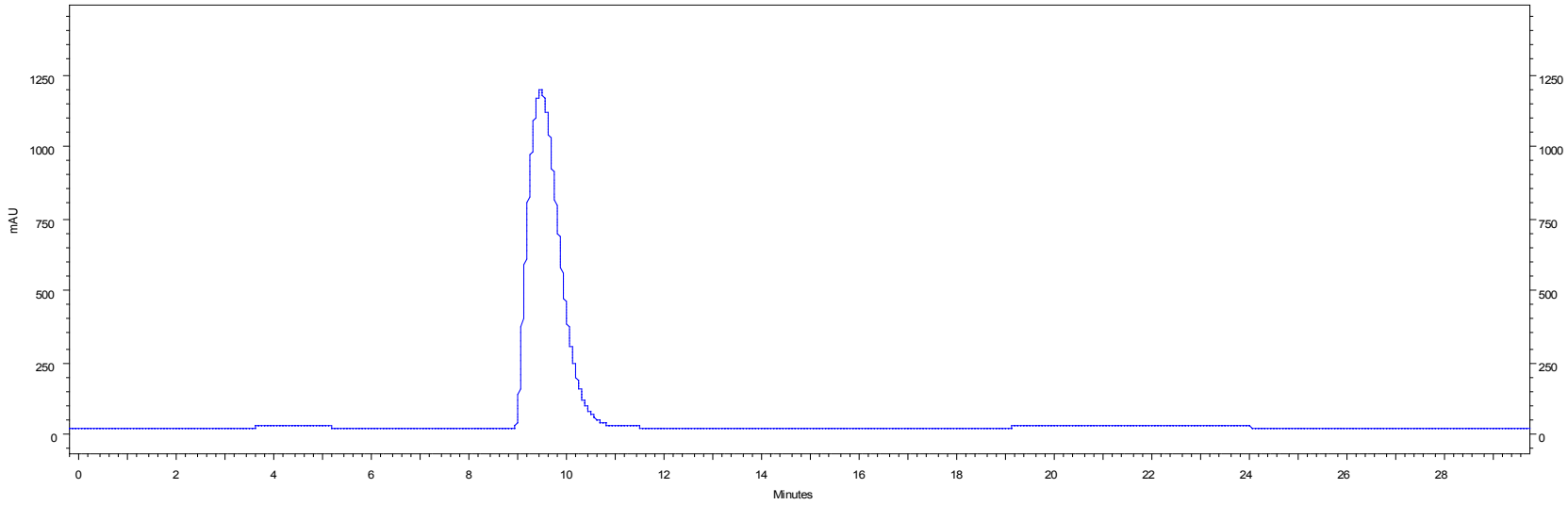
3-(Benzylcarbamimidoyl)thymidine (7d). HR-ESI-MS found: 375.1673



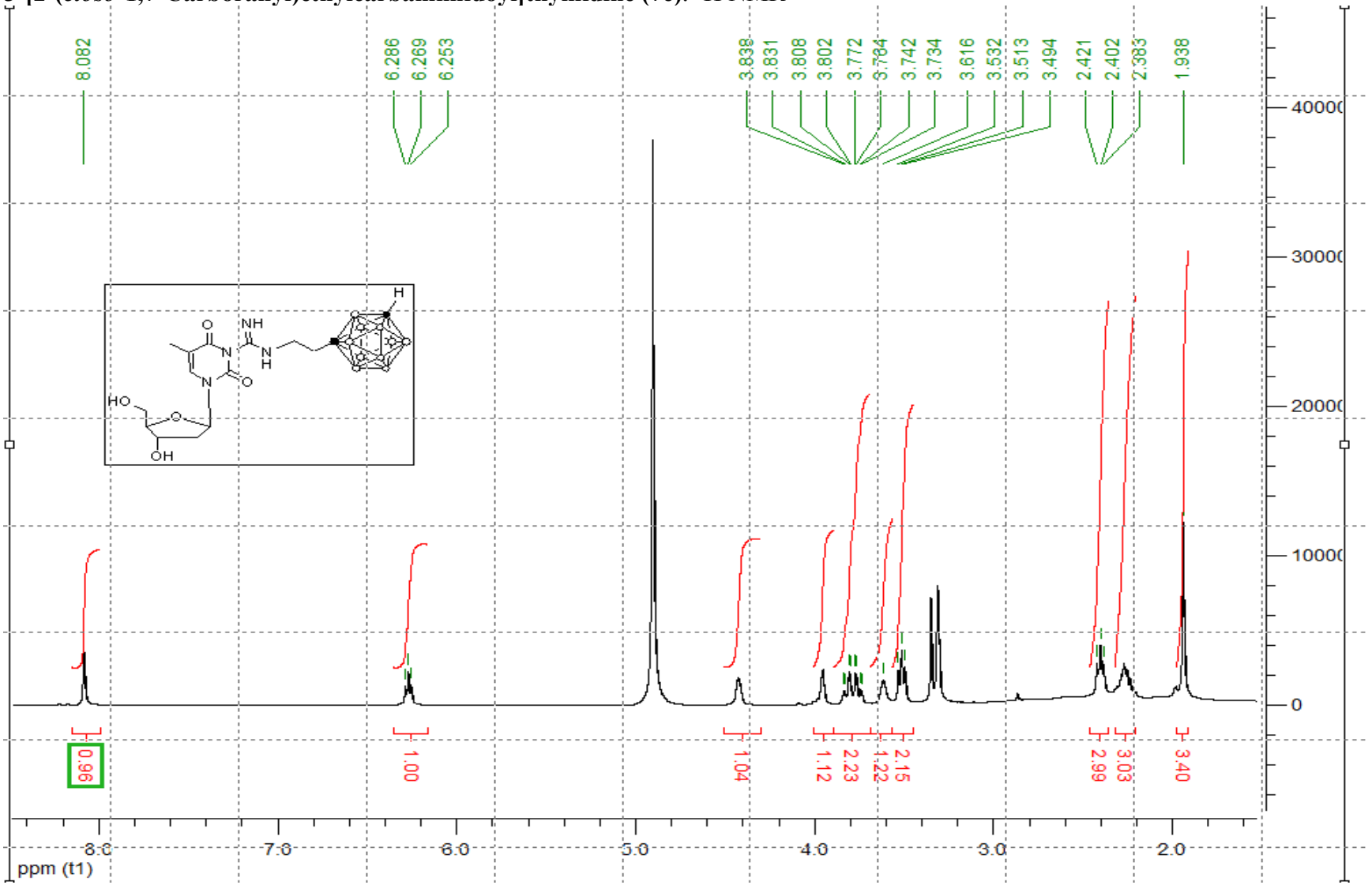
3-(Benzylcarbamimidoyl)thymidine (7d). Analytical traces in Water:Acetonitrile gradient



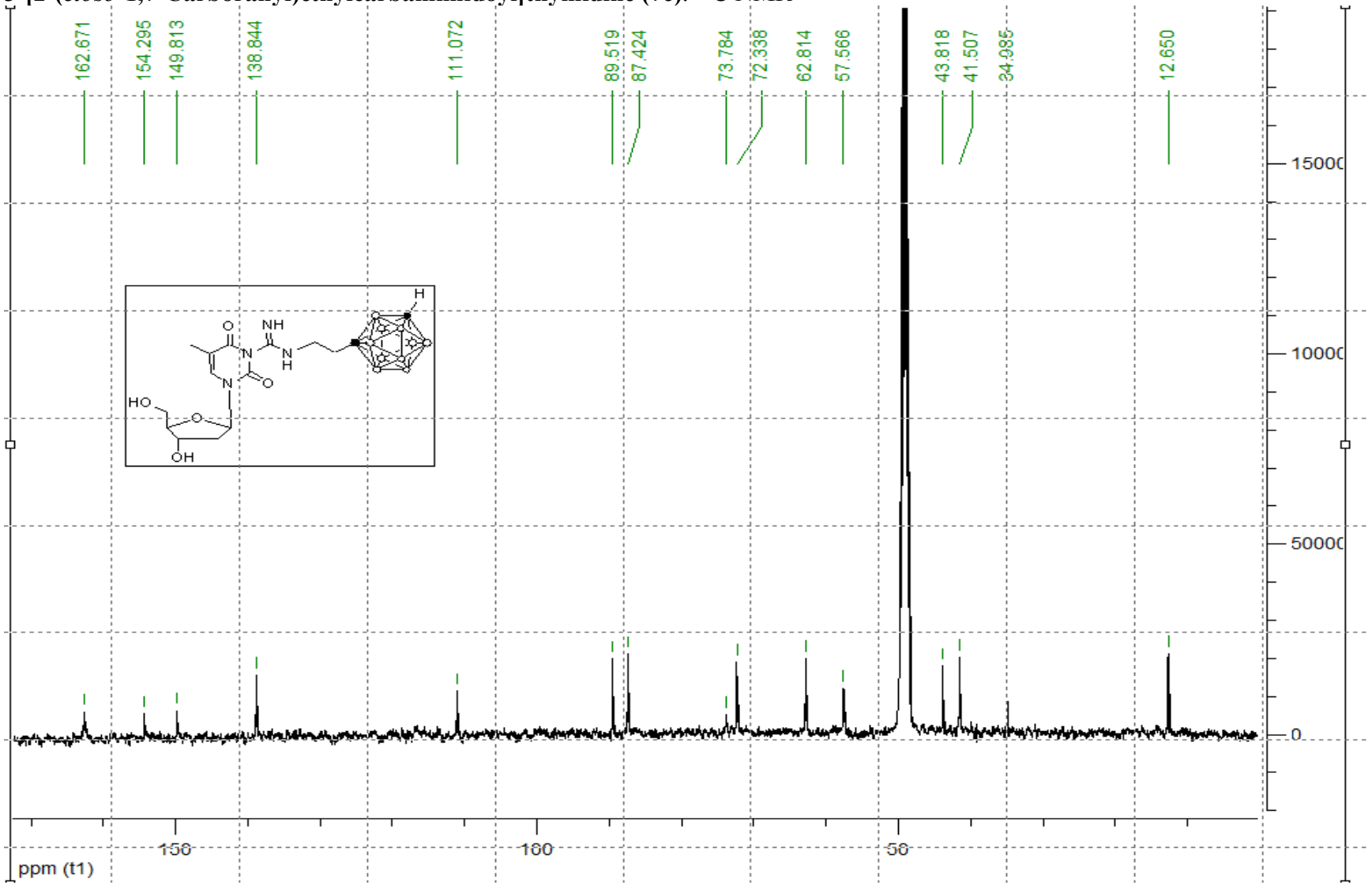
Analytical traces in Water:Methanol gradient



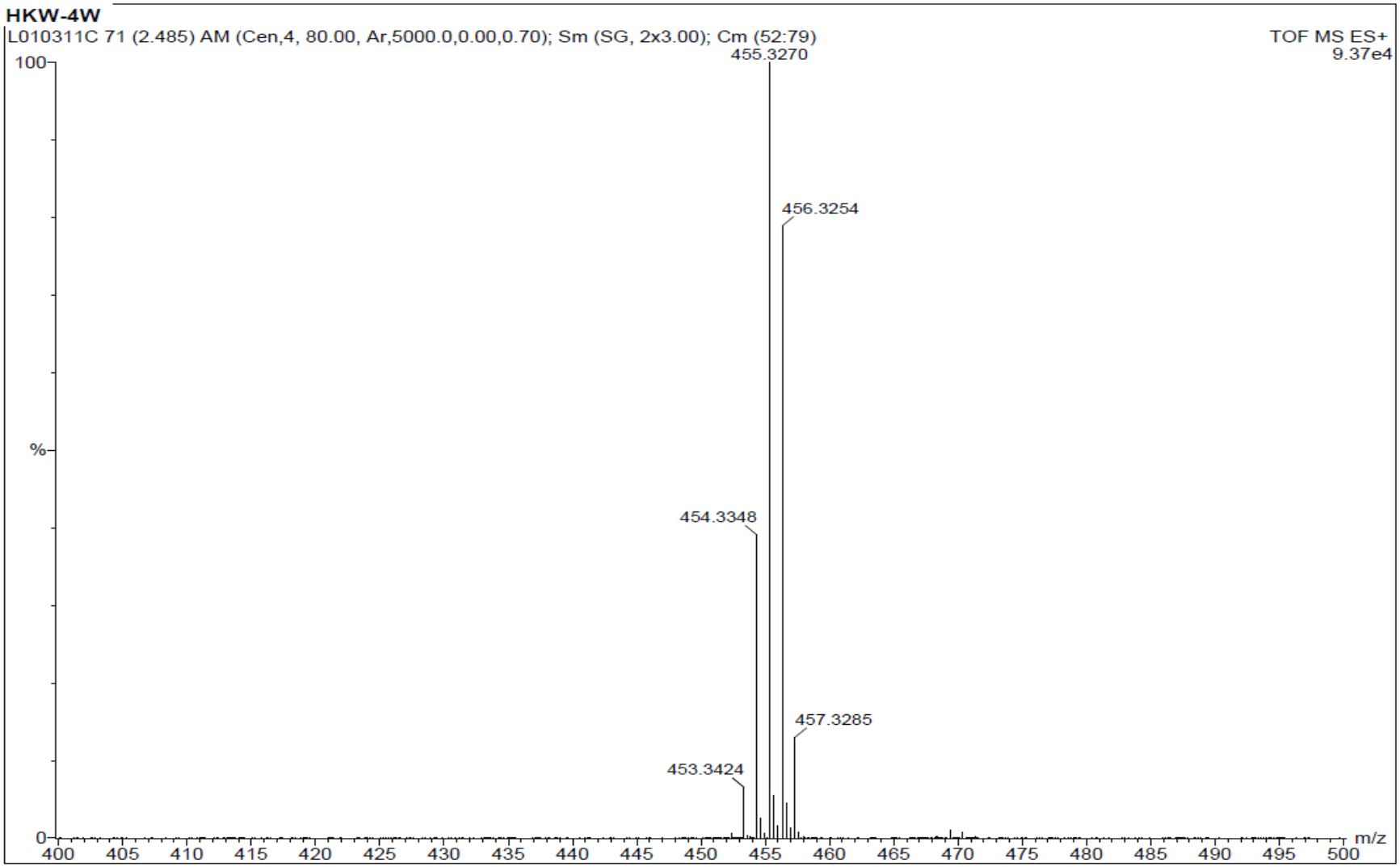
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]thymidine (7e). ^{1}H NMR



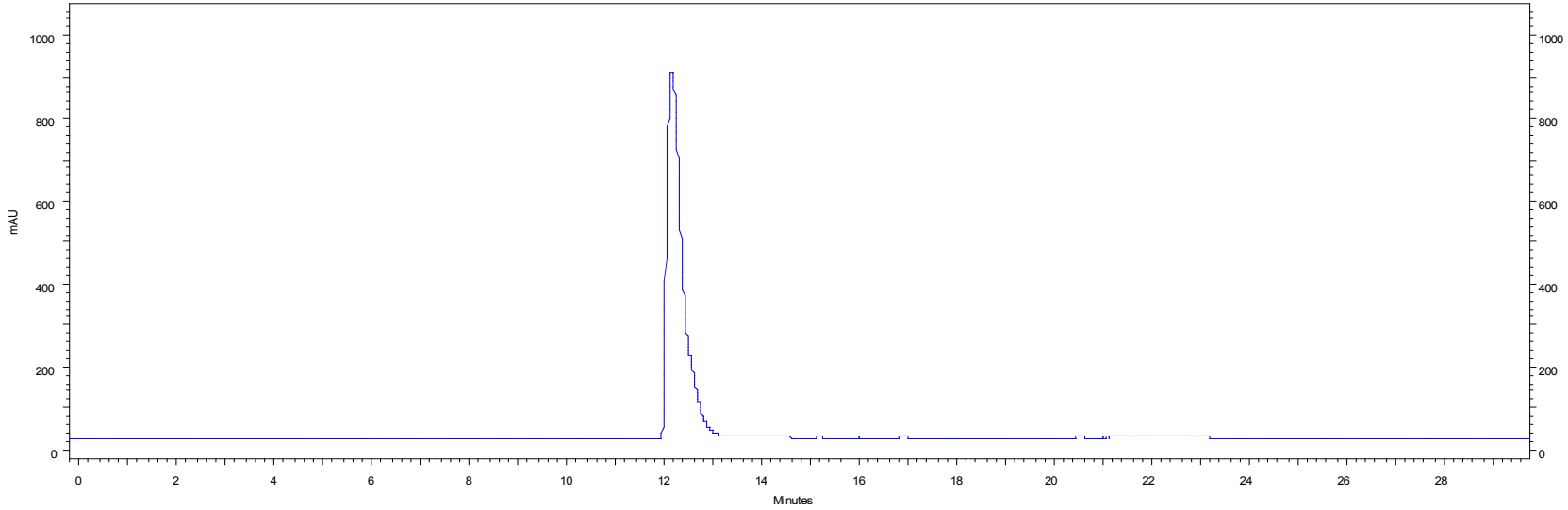
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]thymidine (7e). ^{13}C NMR



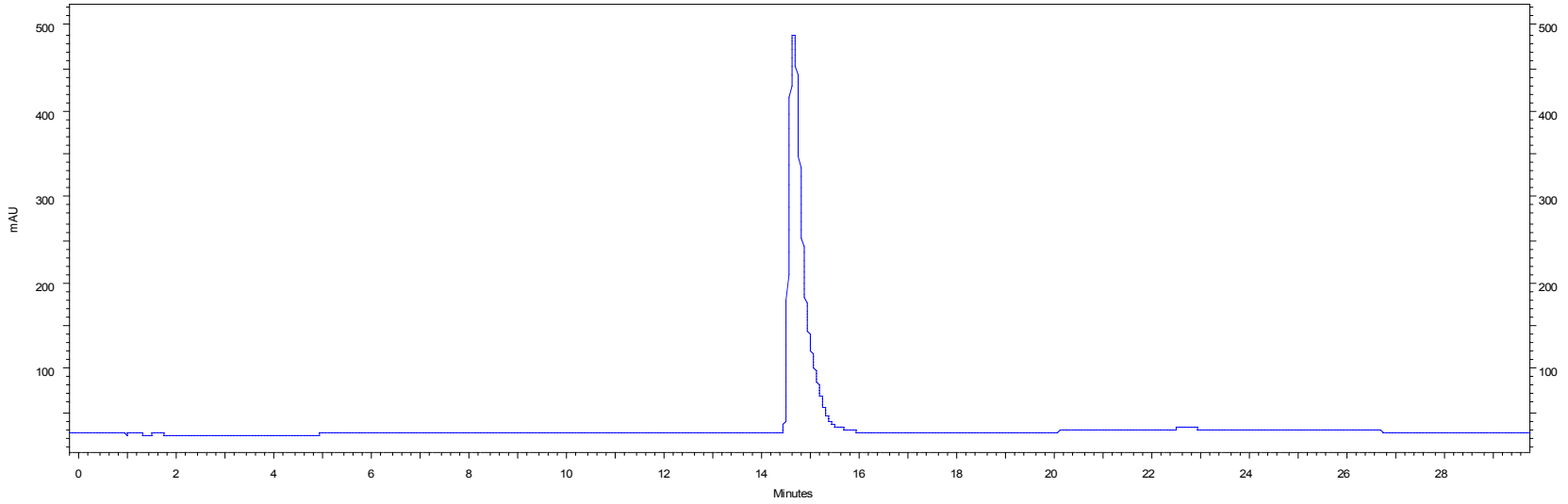
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]thymidine (7e). HR-ESI-MS found: 455.3270



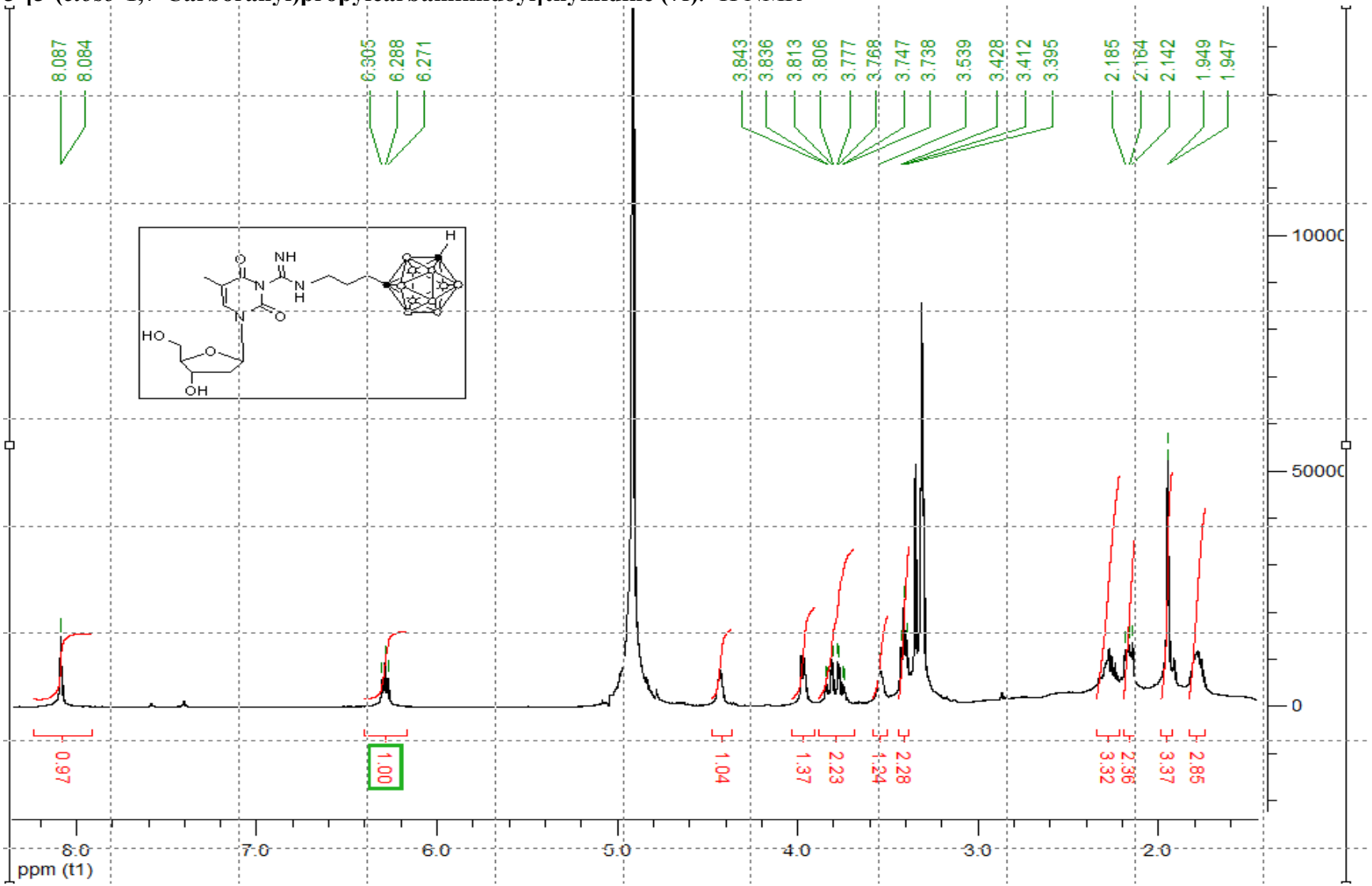
3-[2-(*closo*-1,7-Carboranyl)ethylcarbamimidoyl]thymidine (7e). Analytical traces in Water:Acetonitrile gradient



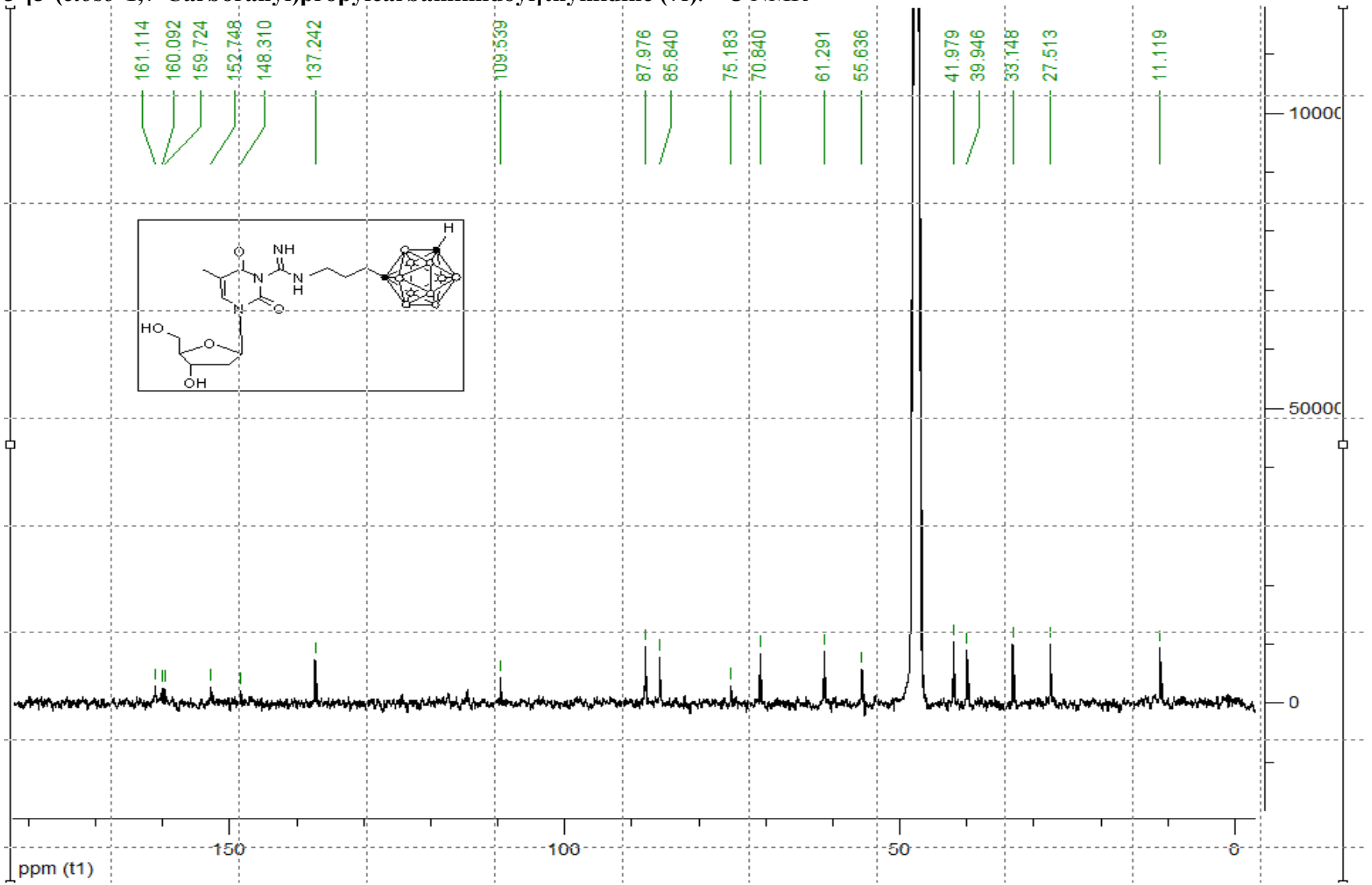
Analytical traces in Water:Methanol gradient



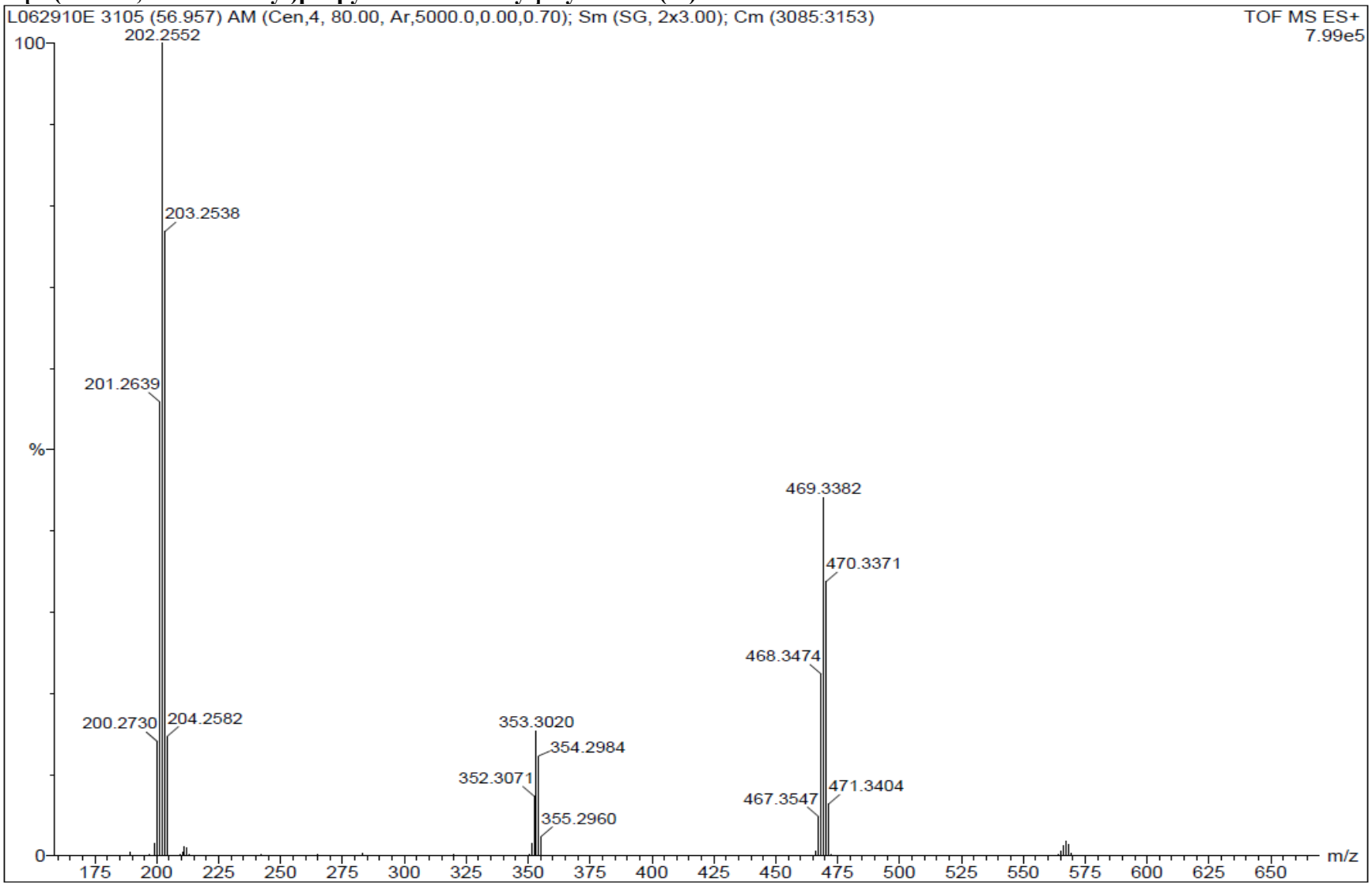
3-[3-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]thymidine (7f). ^{1}H NMR



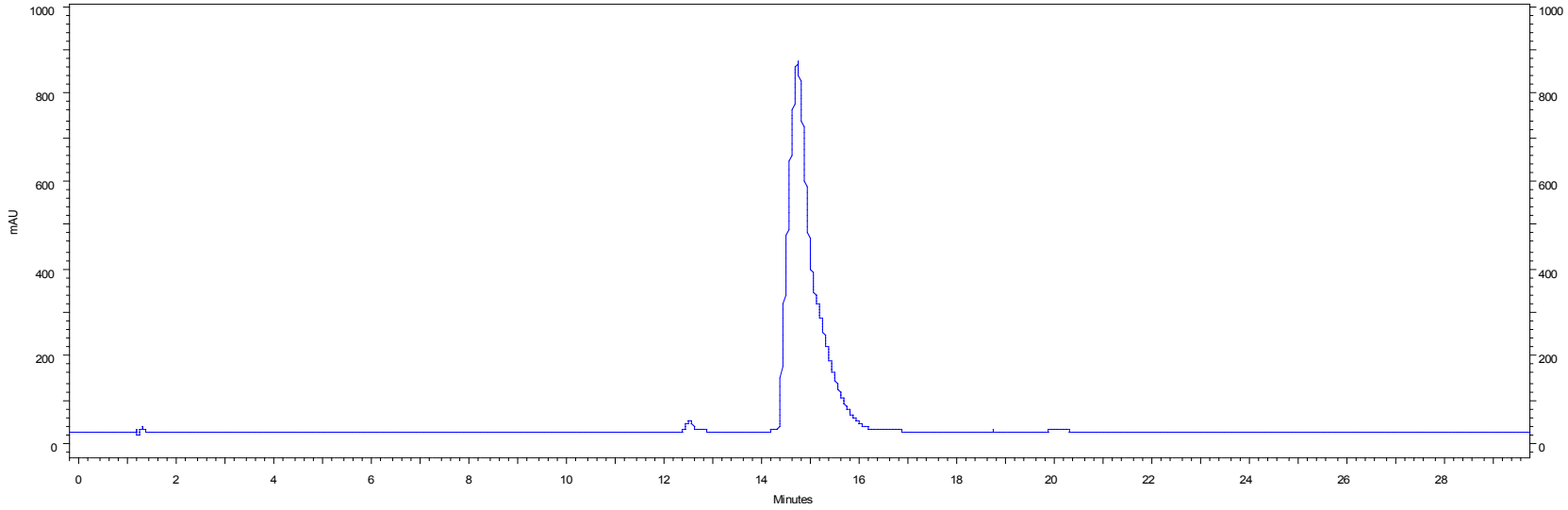
3-[3-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]thymidine (7f). ^{13}C NMR



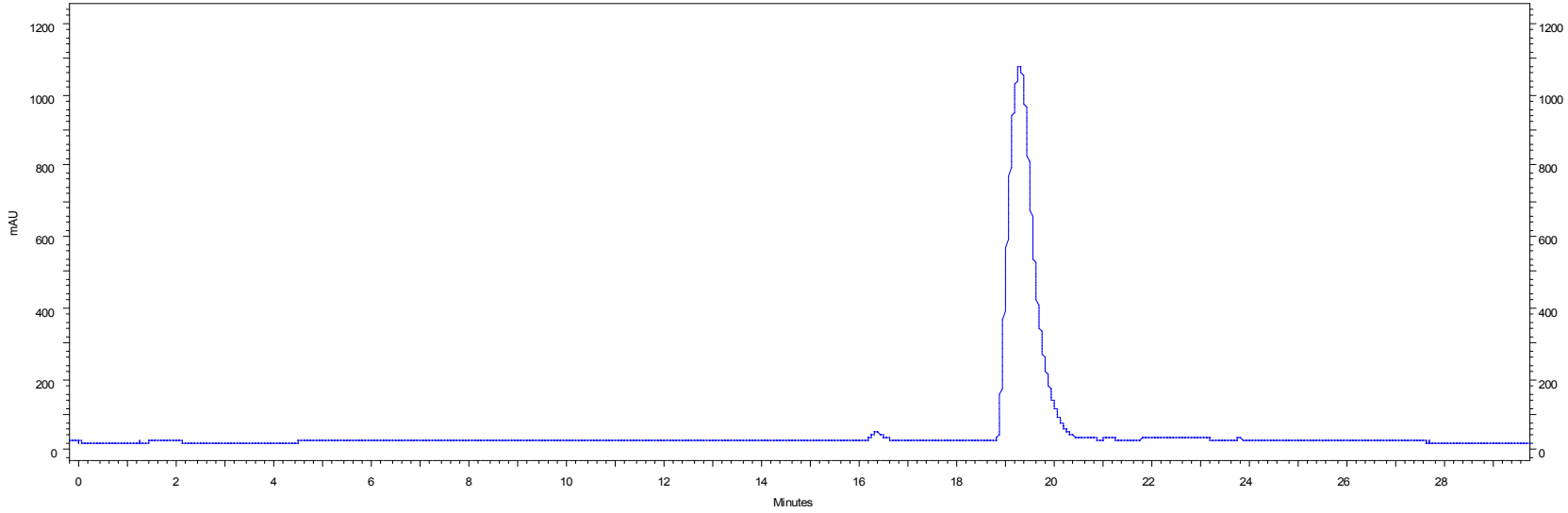
3-[3-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]thymidine (7f). HR-ESI-MS found: 469.3382.



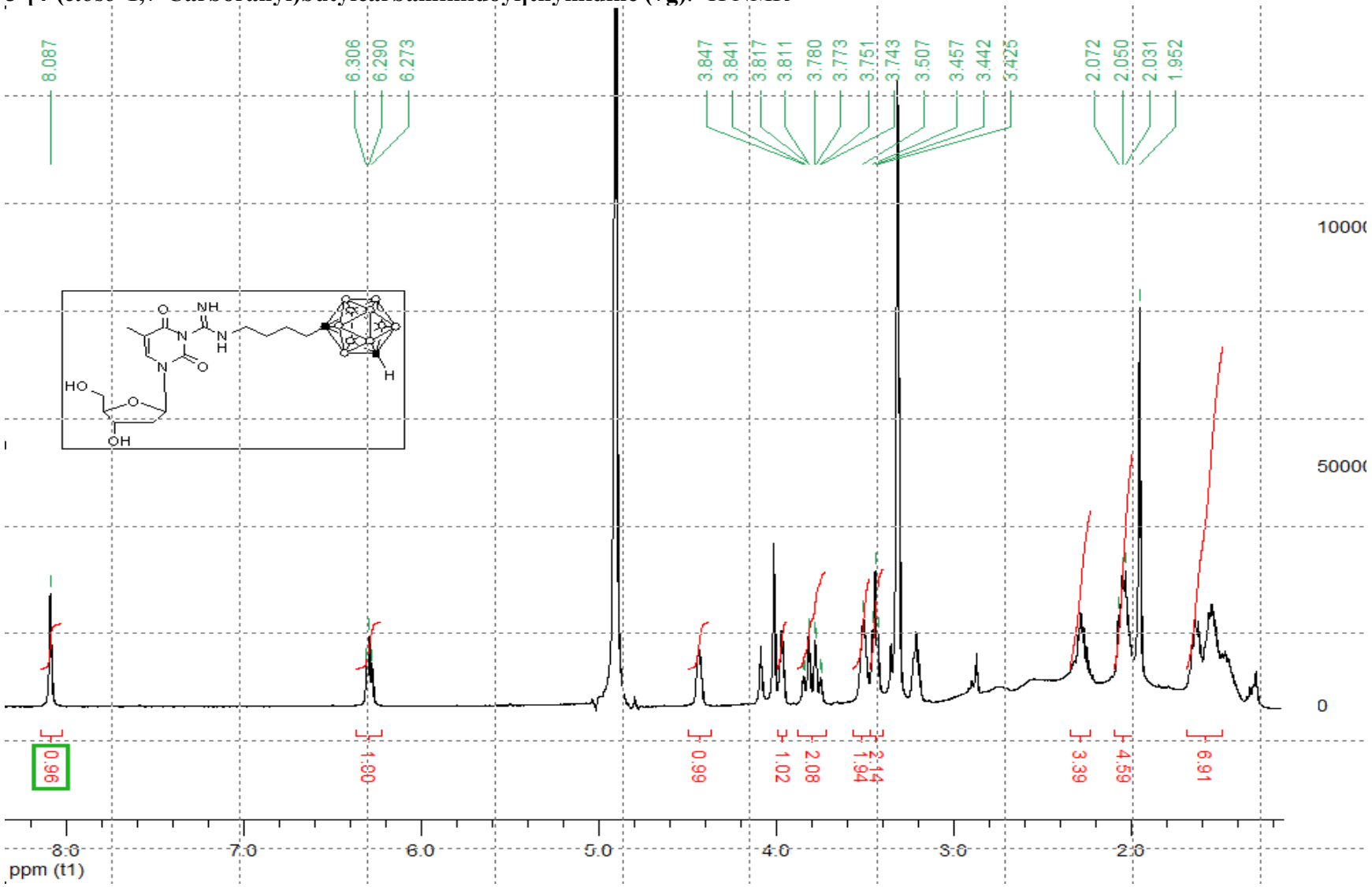
3-[3-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]thymidine (7f). Analytical traces in Water:Acetonitrile gradient



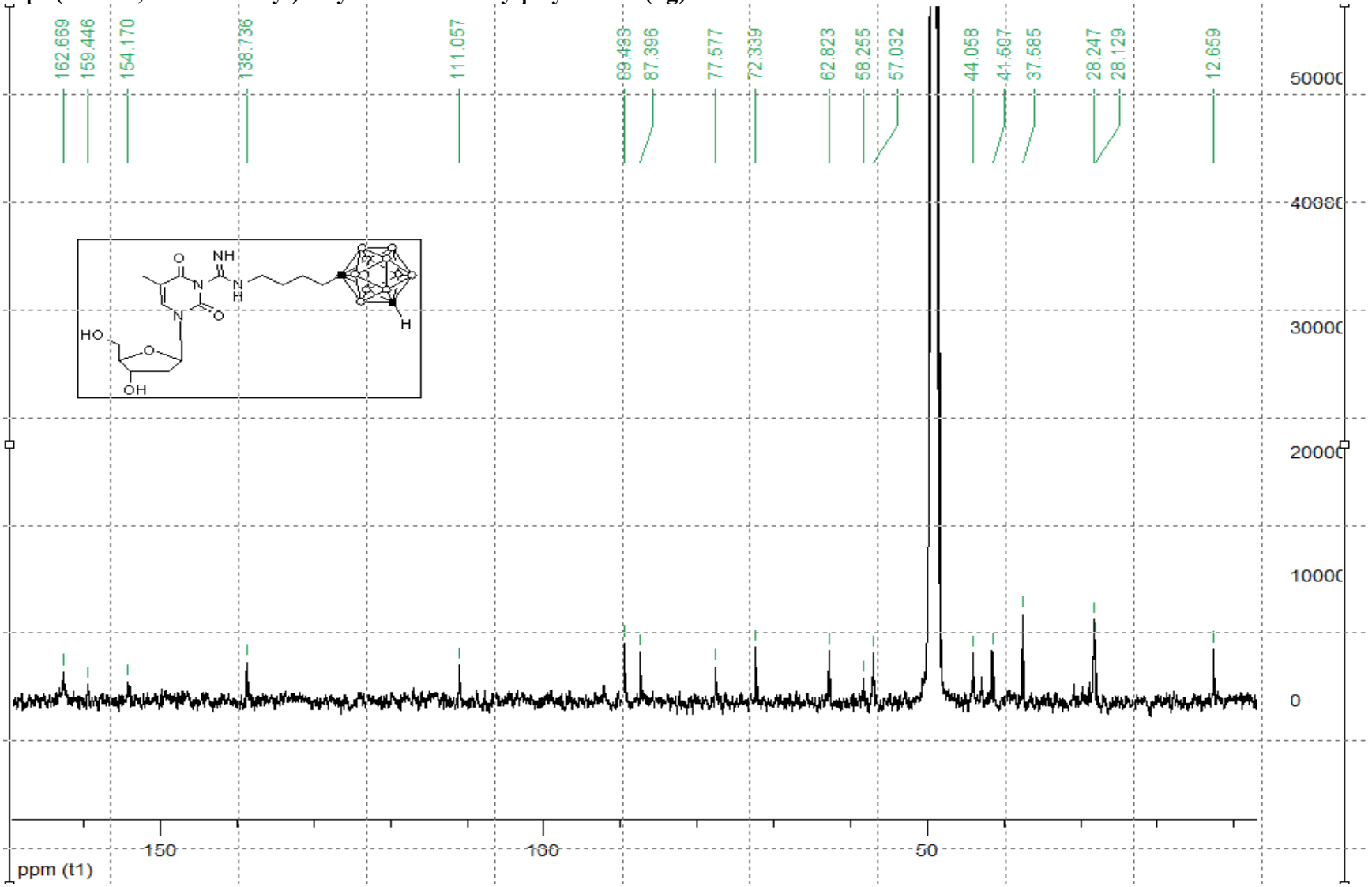
Analytical traces in Water:Methanol gradient



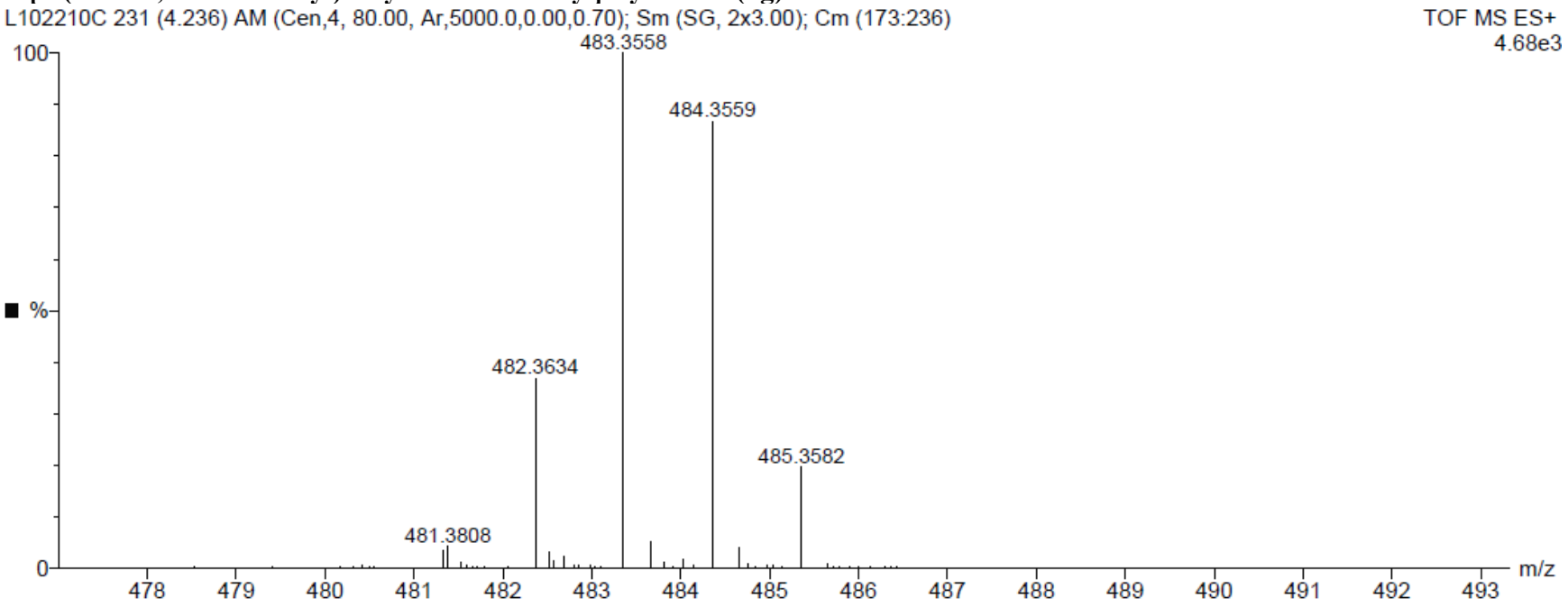
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]thymidine (7g). ^{1}H NMR



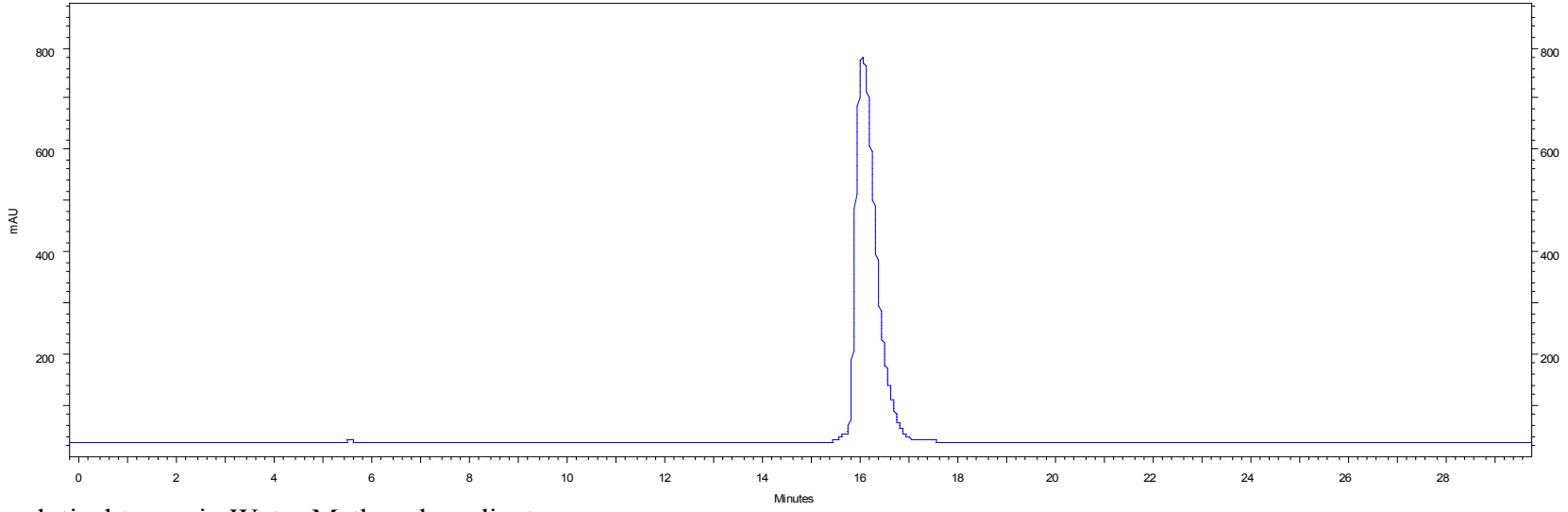
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]thymidine (7g). ^{13}C NMR



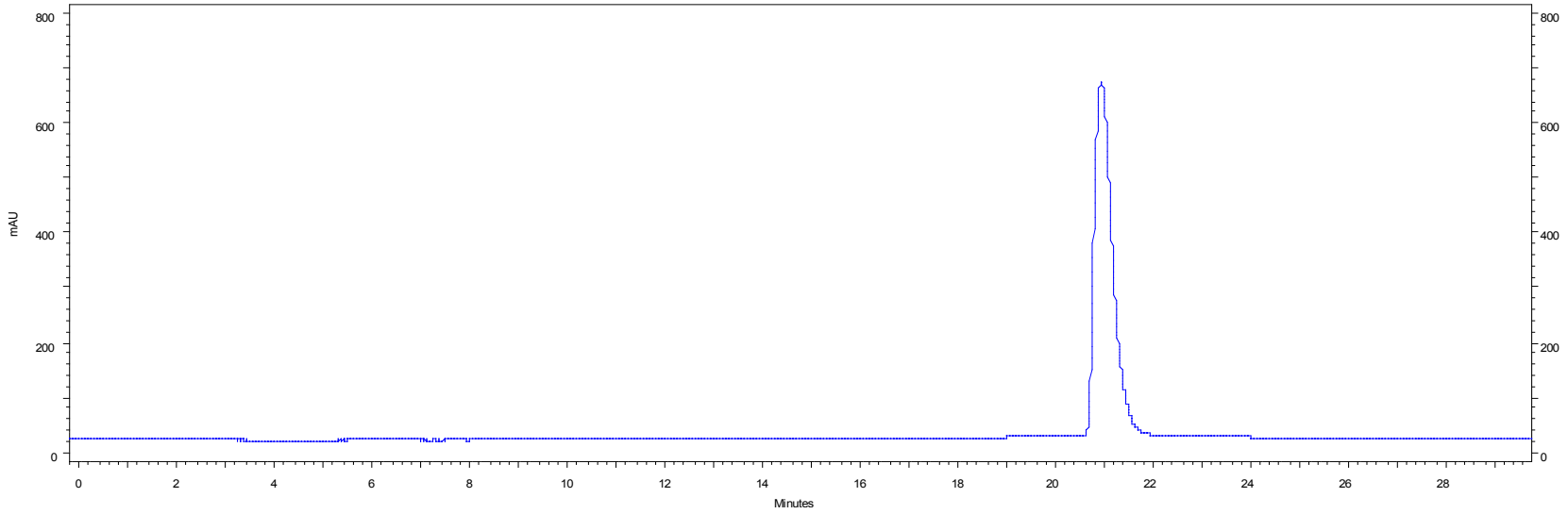
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]thymidine (7g). HR-ESI-MS found: 483.3558.



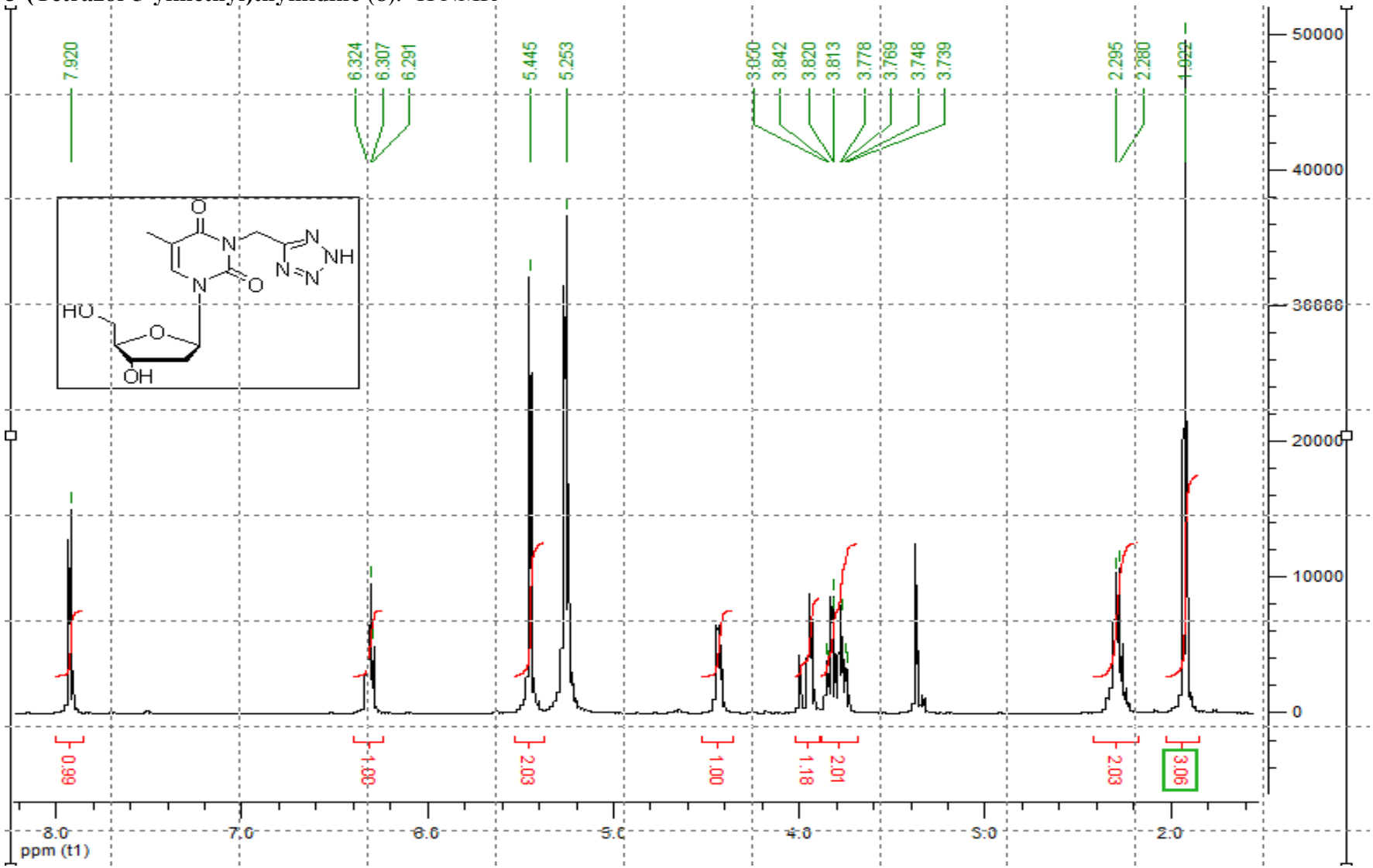
3-[4-(*closo*-1,7-Carboranyl)butylcarbamimidoyl]thymidine (7g). Analytical traces in Water:Acetonitrile gradient



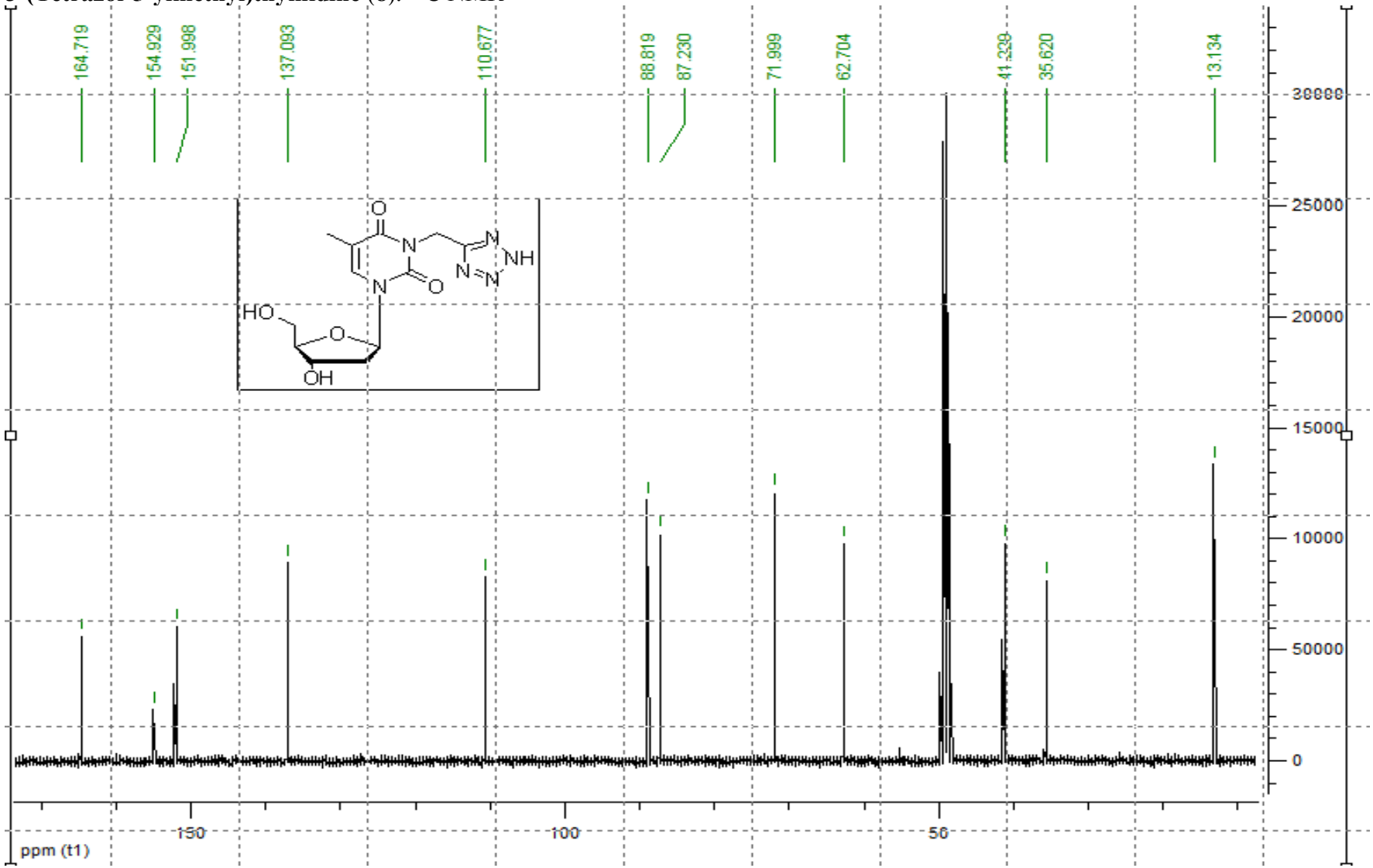
Analytical traces in Water:Methanol gradient



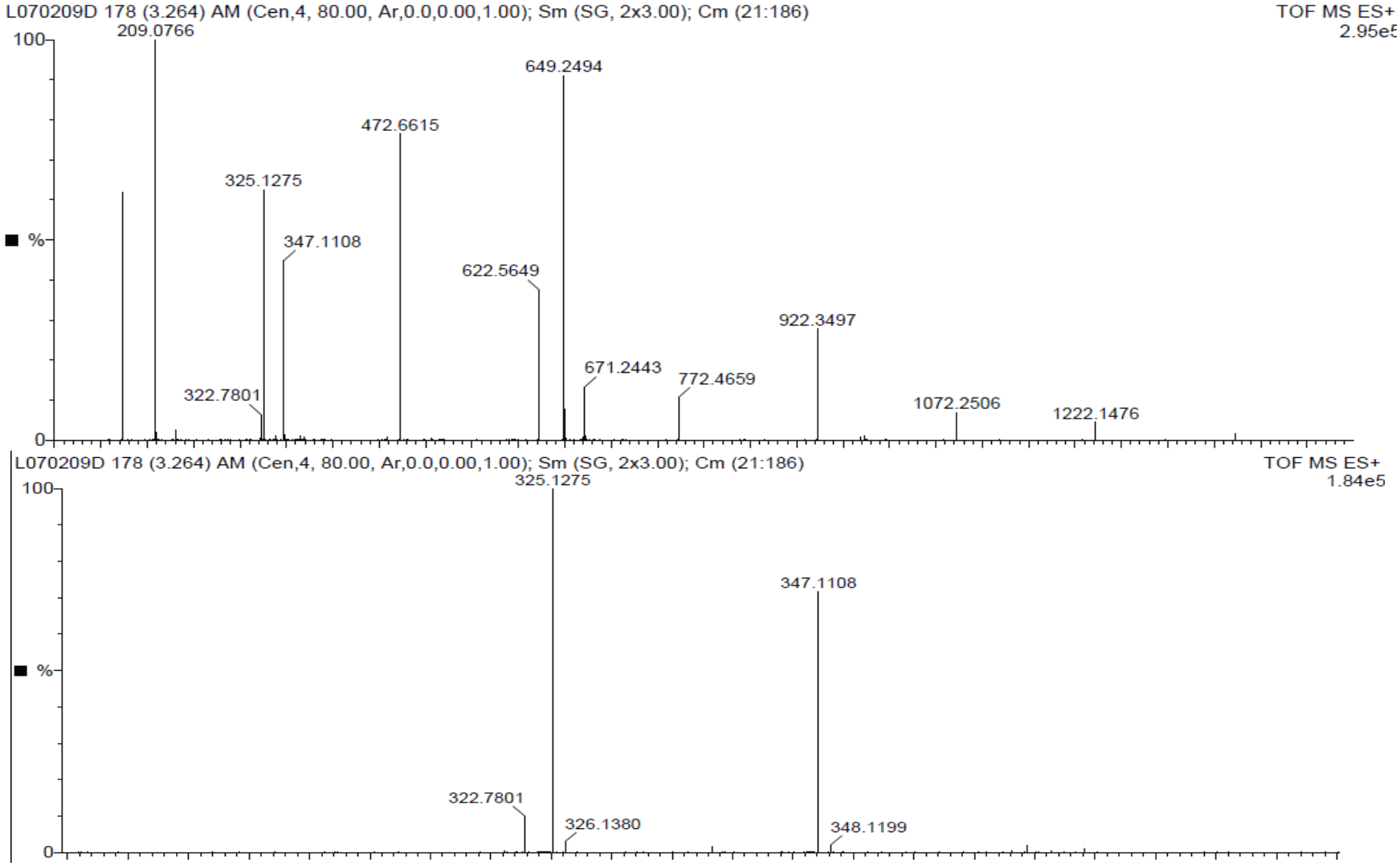
3-(Tetrazol-5-ylmethyl)thymidine (8). ^{1}H NMR



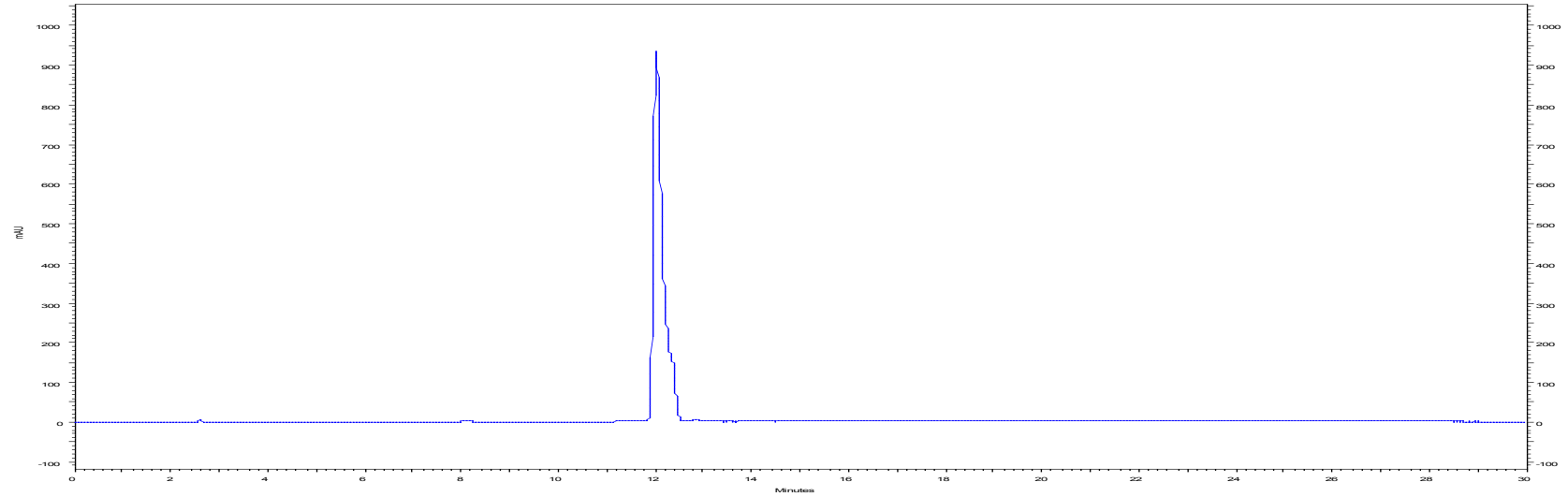
3-(Tetrazol-5-ylmethyl)thymidine (8). ^{13}C NMR



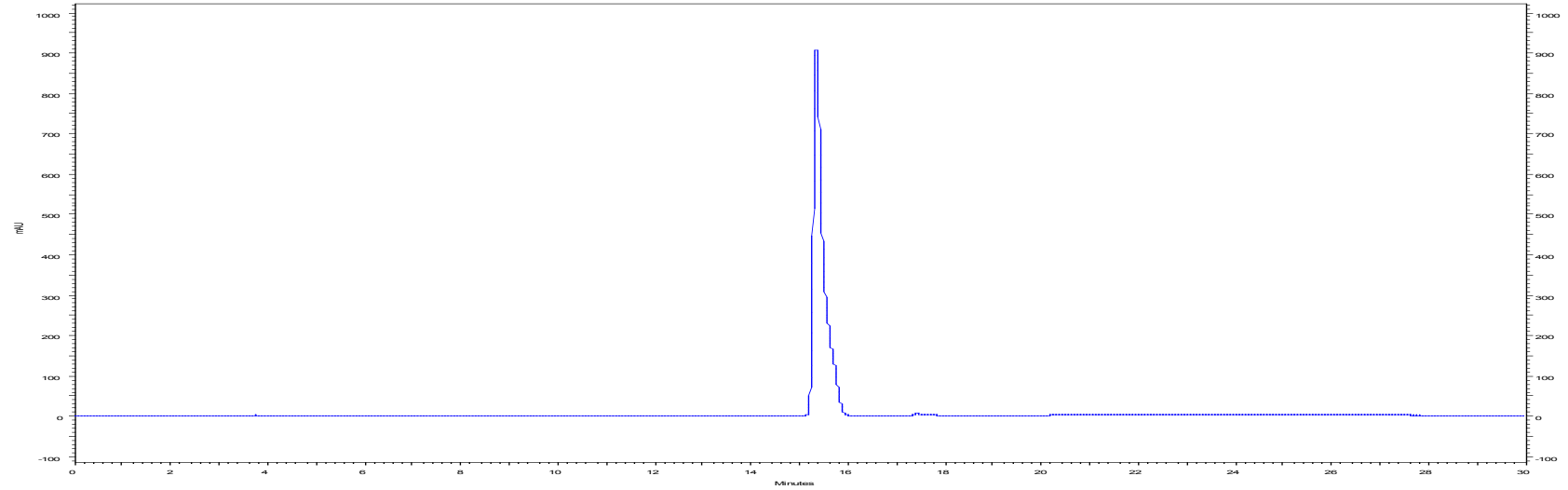
3-(Tetrazol-5-ylmethyl)thymidine (**8**). HR-ESI-MS found: 325.1275, 347.1108 and 649.2494.



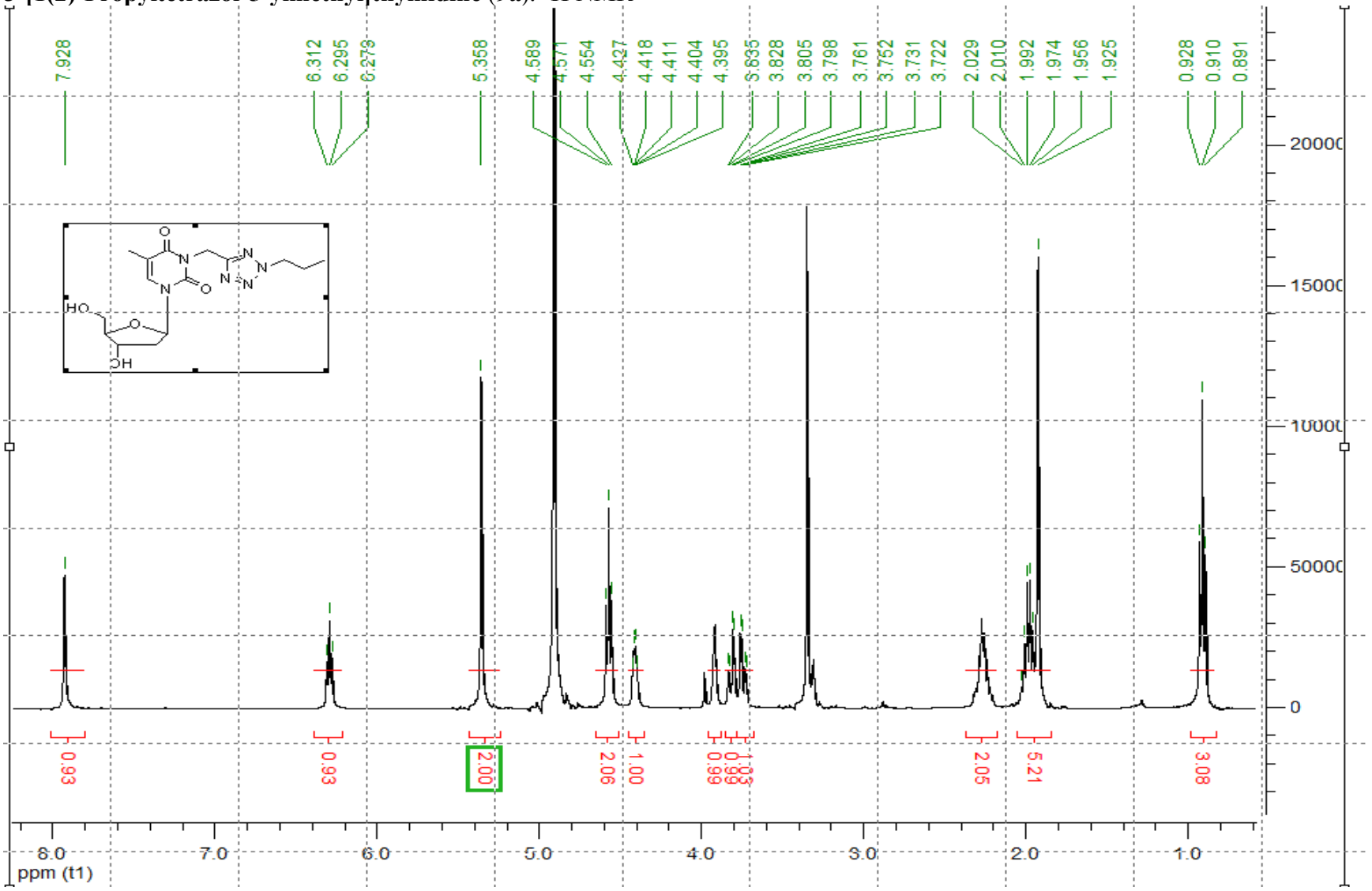
3-(Tetrazol-5-ylmethyl)thymidine (**8**). Analytical traces in Water:Acetonitrile gradient



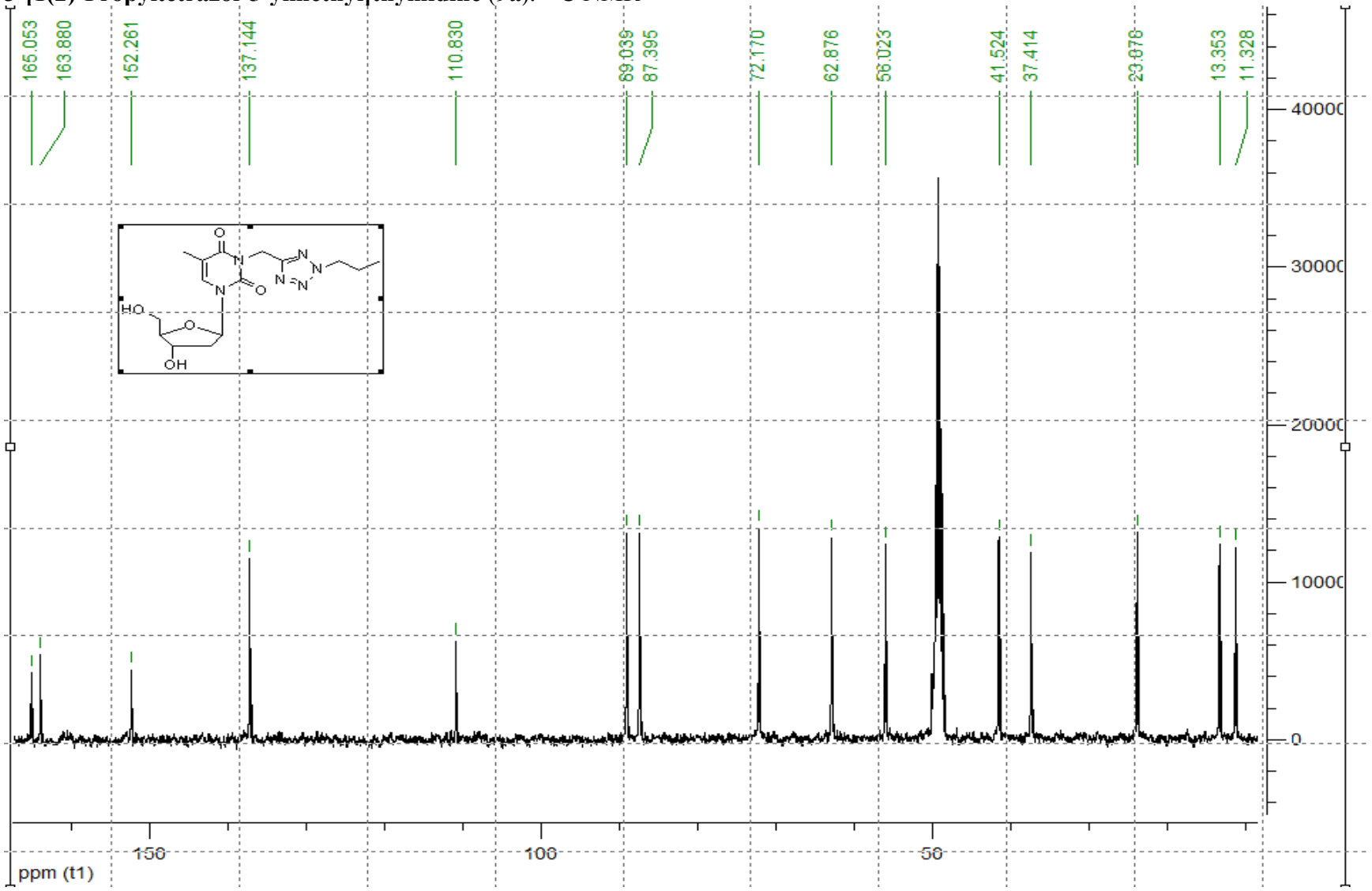
Analytical traces in Water: Methanol gradient



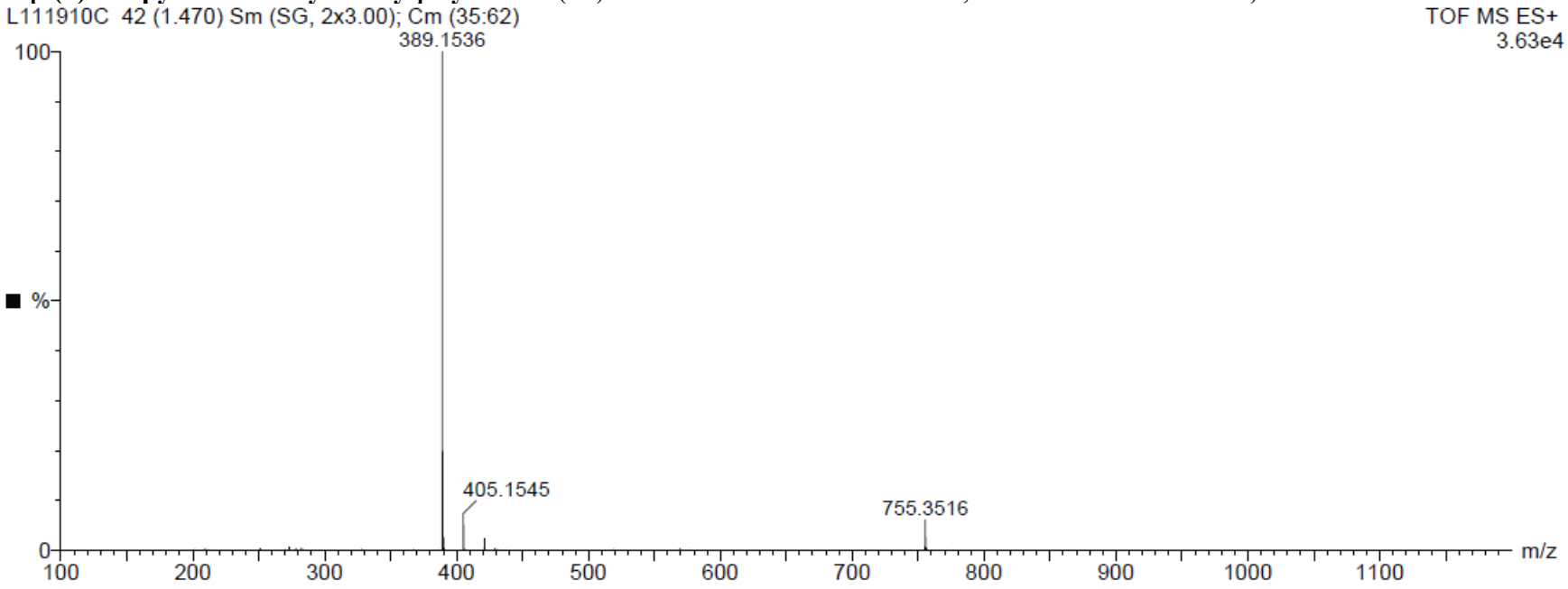
3-[1(2)-Propyltetrazol-5-ylmethyl]thymidine (9a). ^{1}H NMR



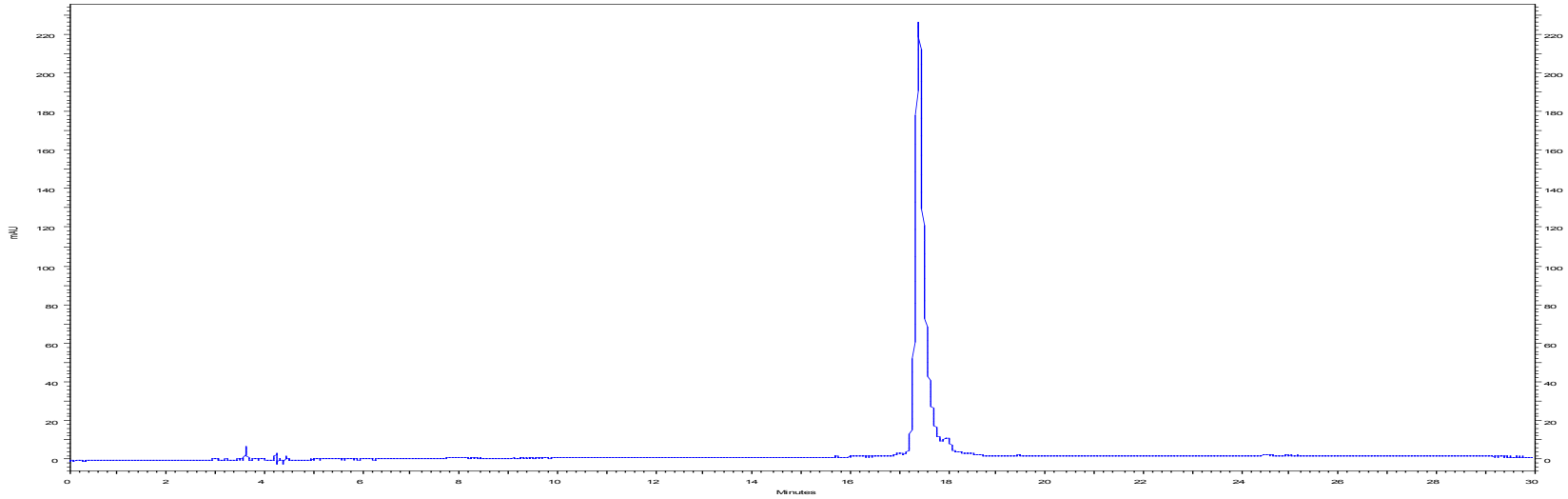
3-[1(2)-Propyltetrazol-5-ylmethyl]thymidine (9a). ^{13}C NMR



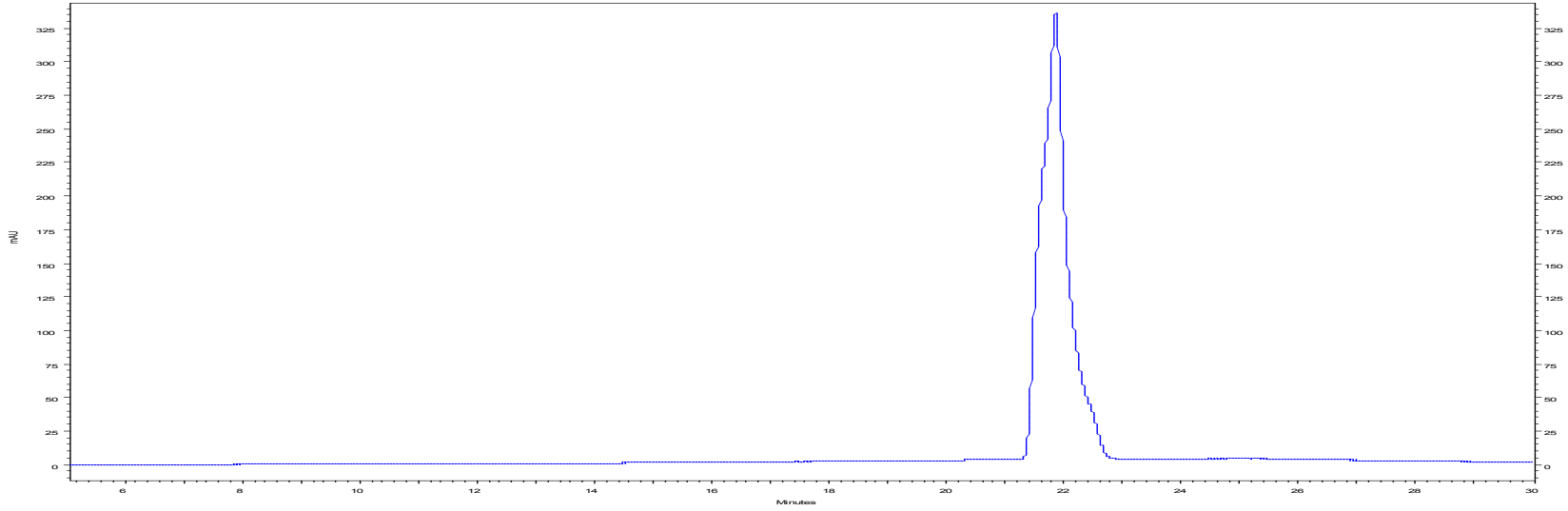
3-[1(2)-Propyltetrazol-5-ylmethyl]thymidine (**9a**). HR-ESI-MS found: 389.1536, 405.1545 and 755.3516)



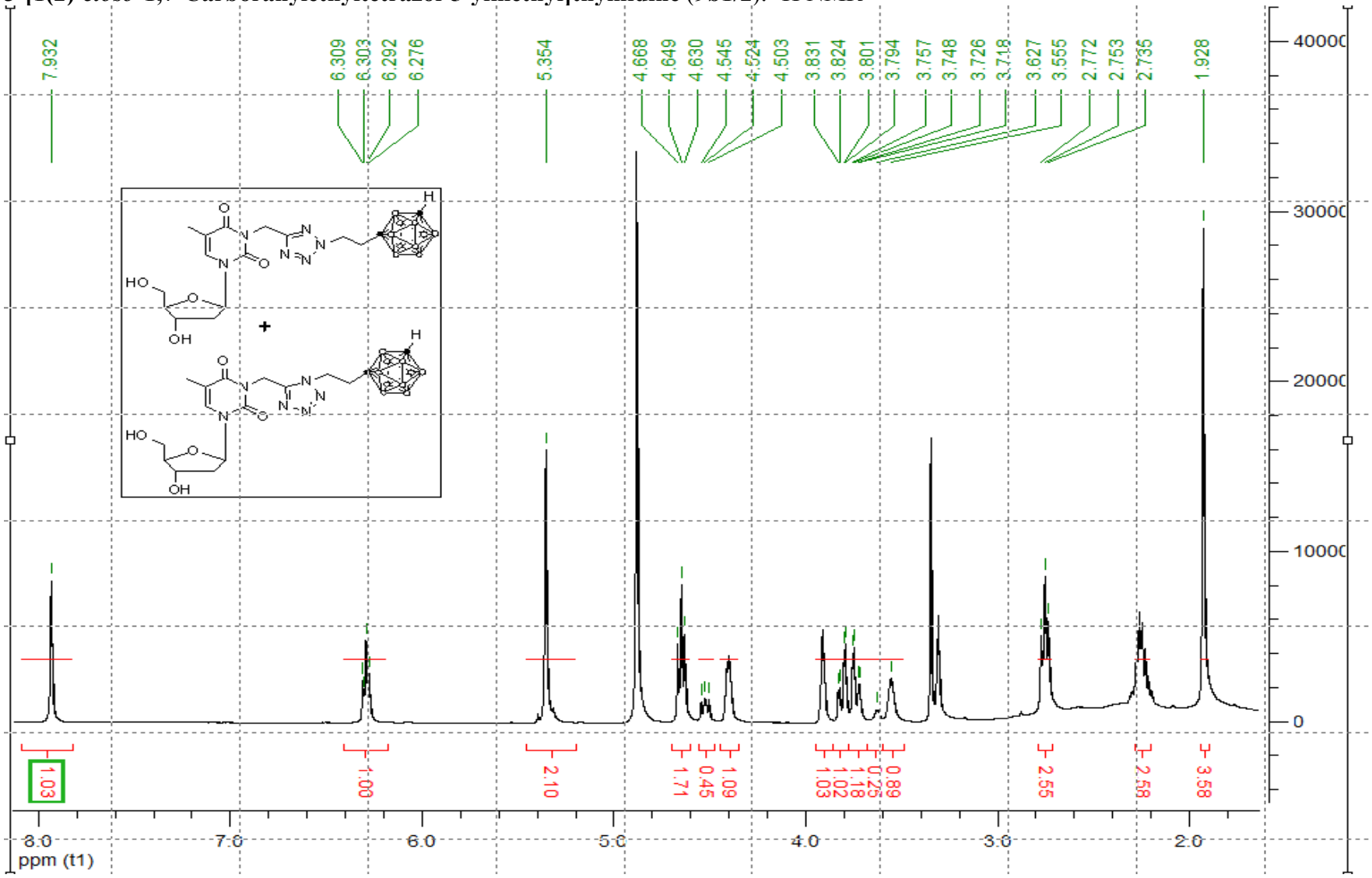
3-[1(2)-Propyltetrazol-5-ylmethyl]thymidine (**9a**). Analytical traces in Water:Acetonitrile gradient



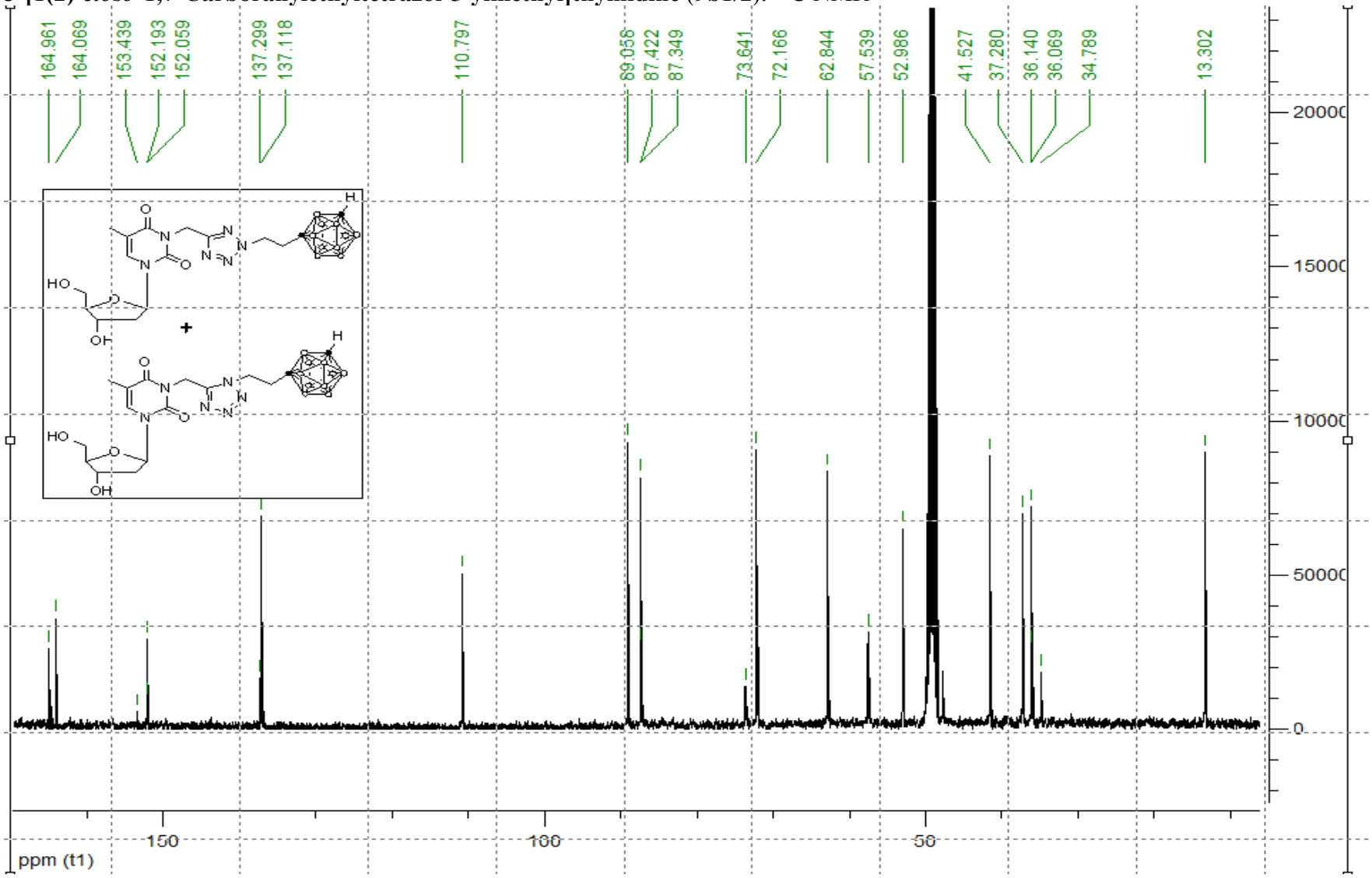
Analytical traces in Water: Methanol gradient



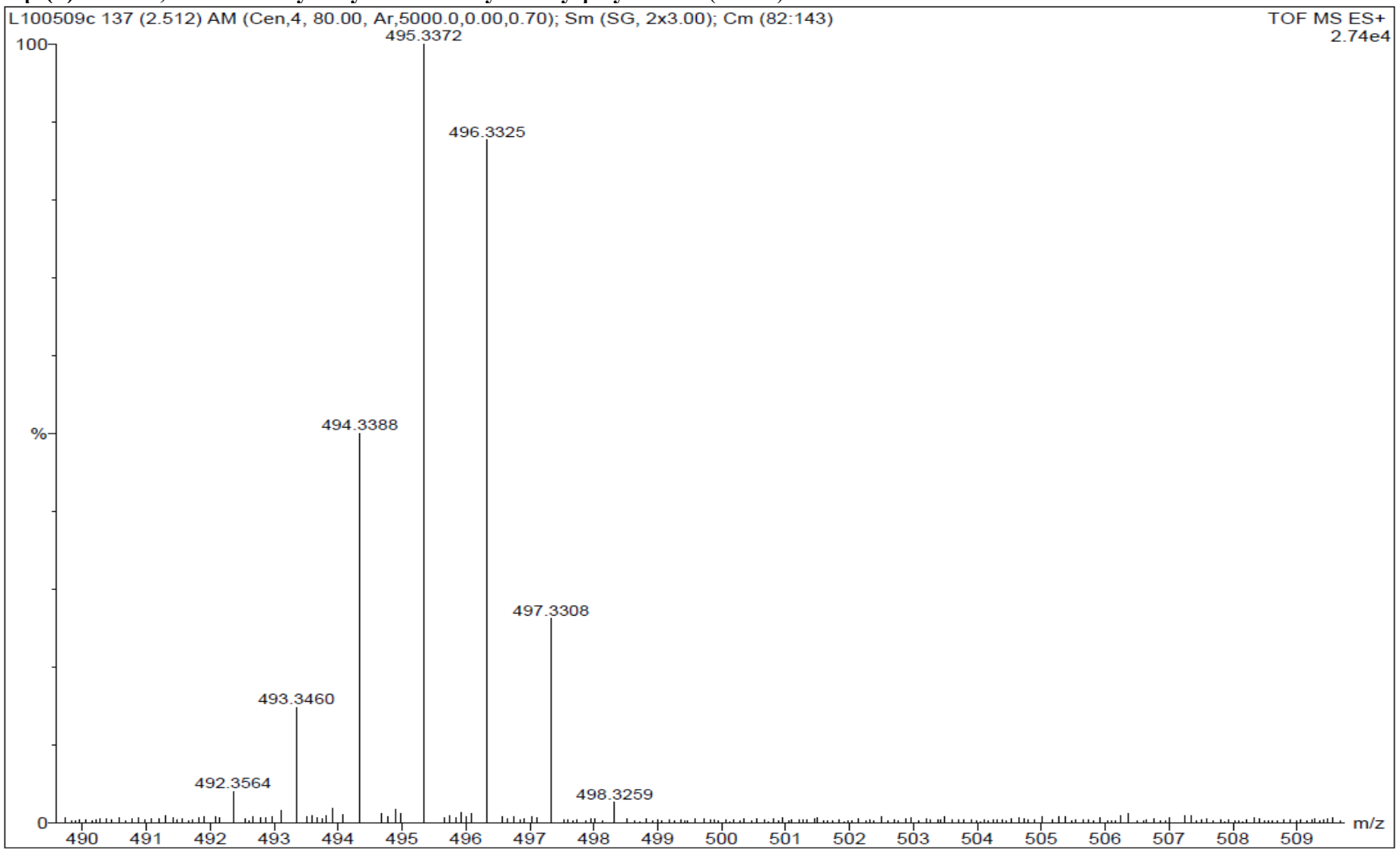
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-ylmethyl]thymidine (9b1/2). ^{1}H NMR



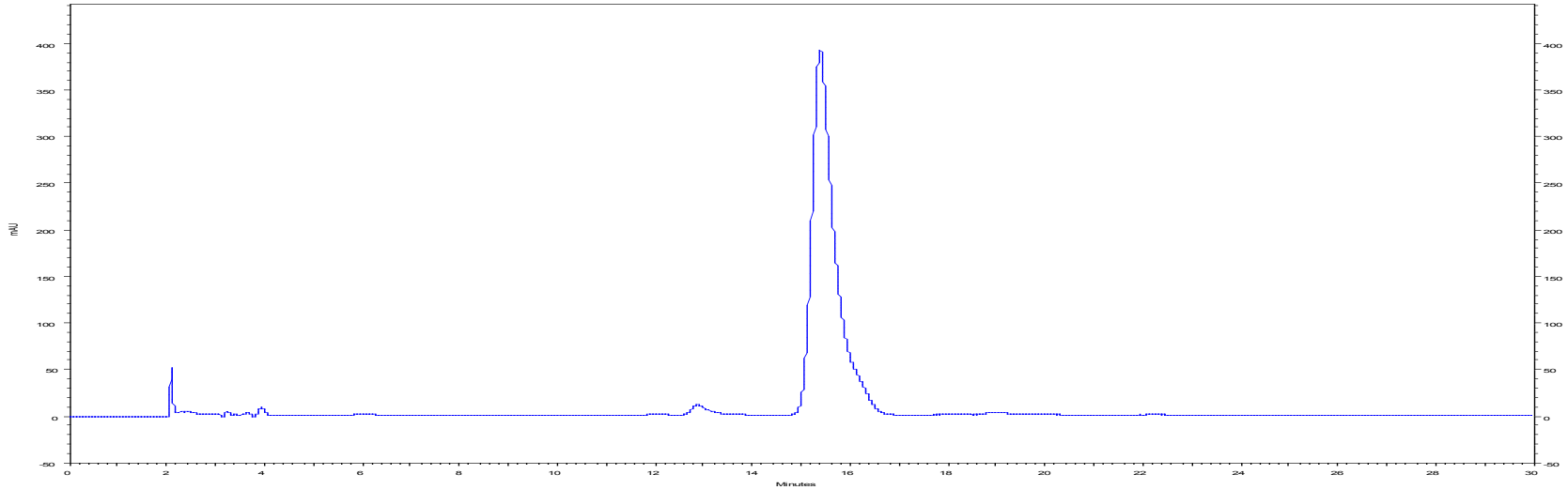
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-ylmethyl]thymidine (9b1/2). ^{13}C NMR



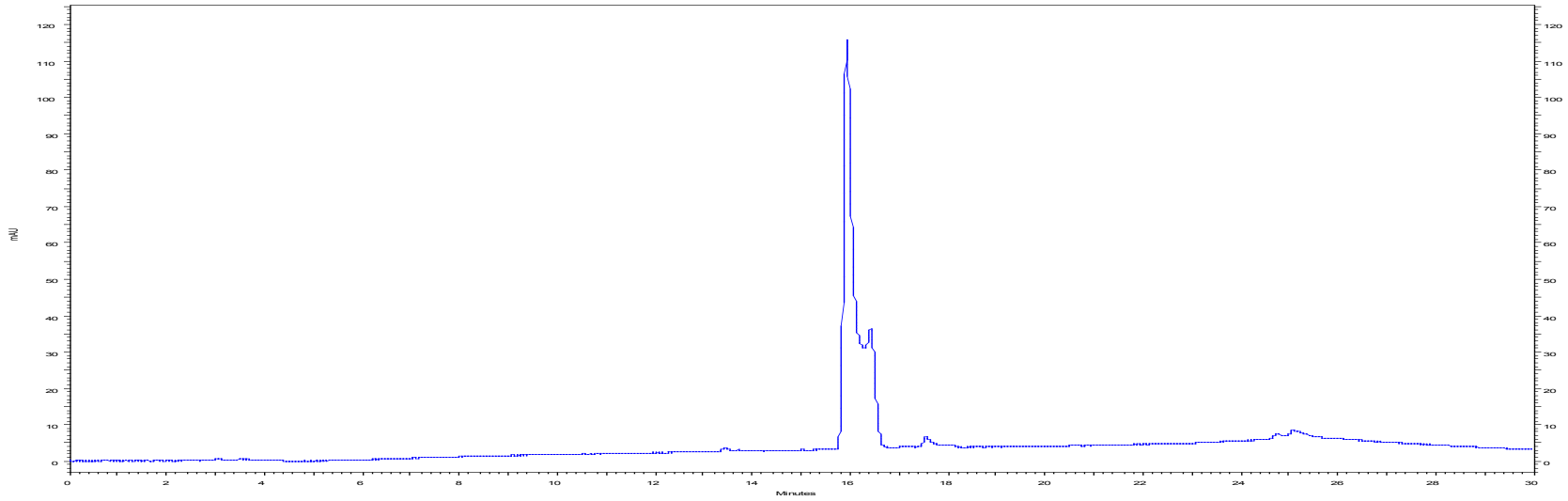
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-ylmethyl]thymidine (**9b1/2**). HR-ESI-MS found: 495.3372.



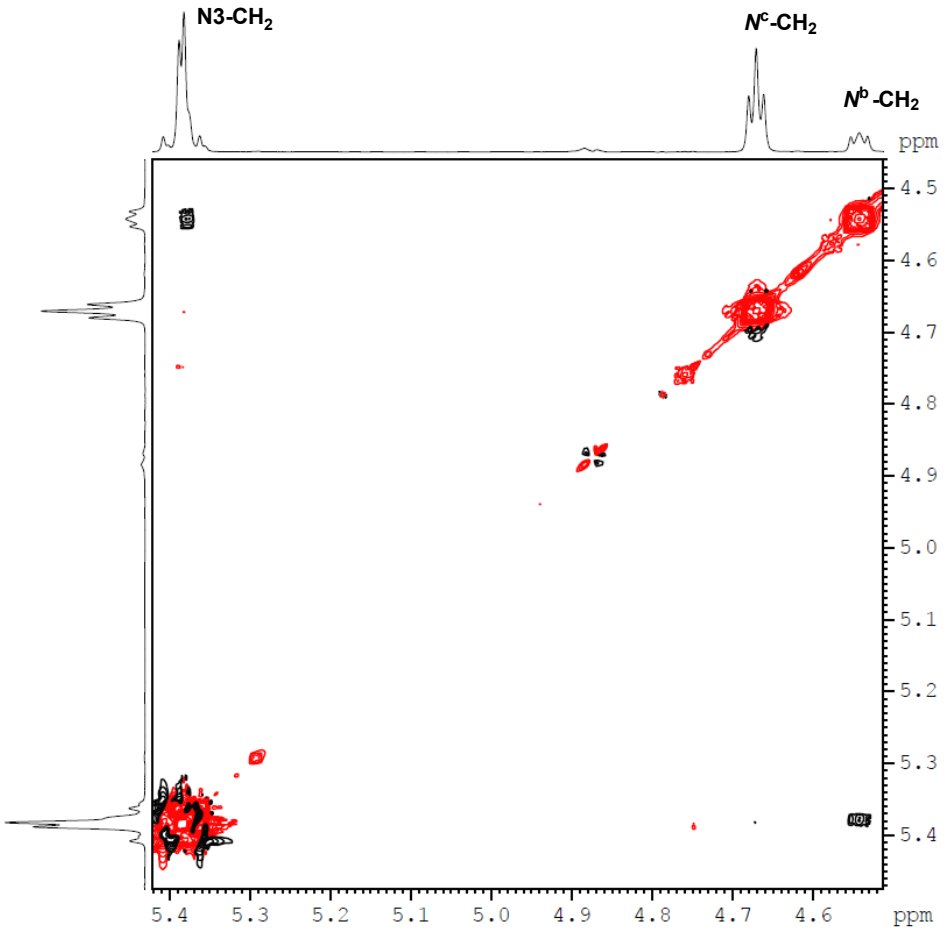
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-ylmethyl]thymidine (**9b1/2**). Analytical traces in Water:Acetonitrile gradient

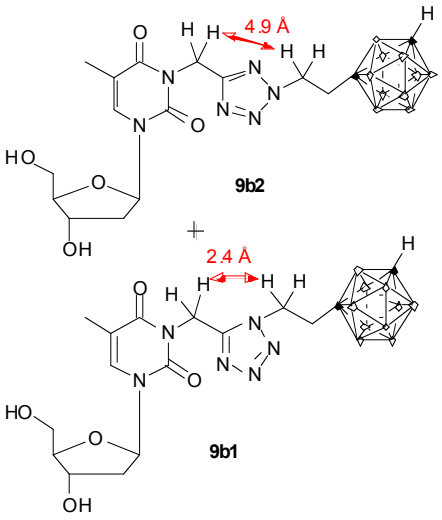


Analytical traces in Water:Methanol gradient

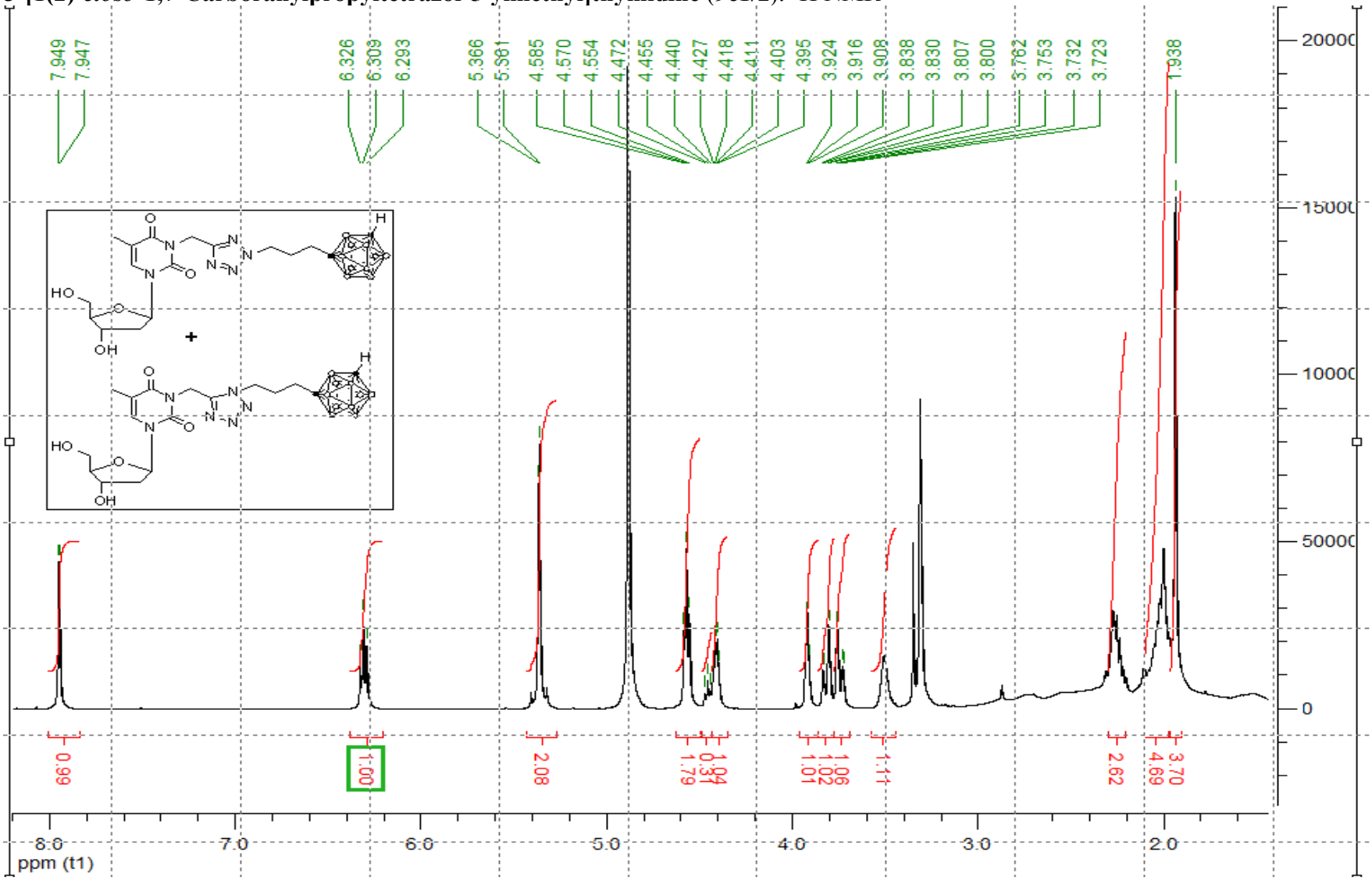


3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-ylmethyl]thymidine (9b1/2). ^{1}H-^{1}H NOSEY NMR

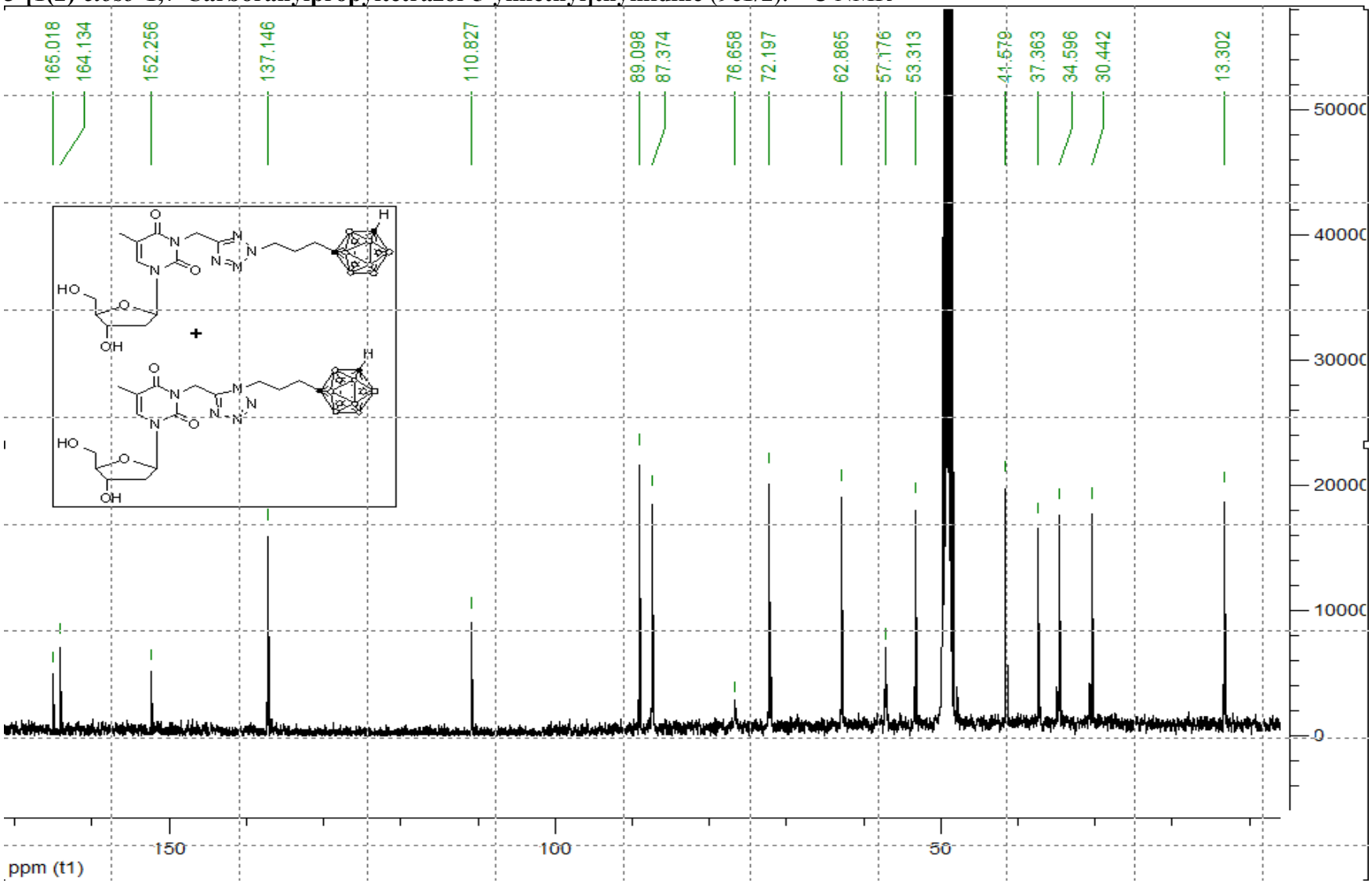




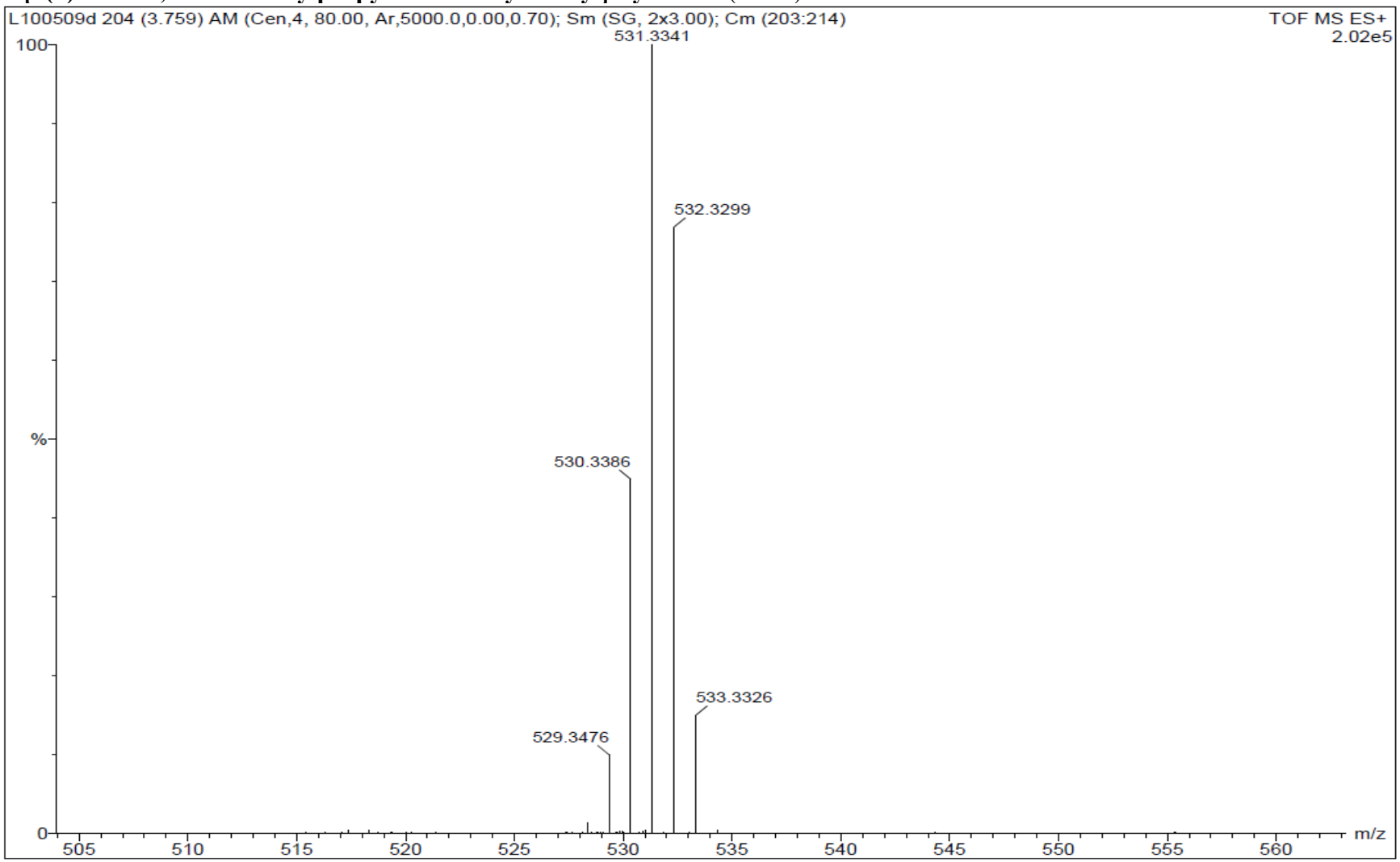
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-ylmethyl]thymidine (9c1/2). ^{1}H NMR



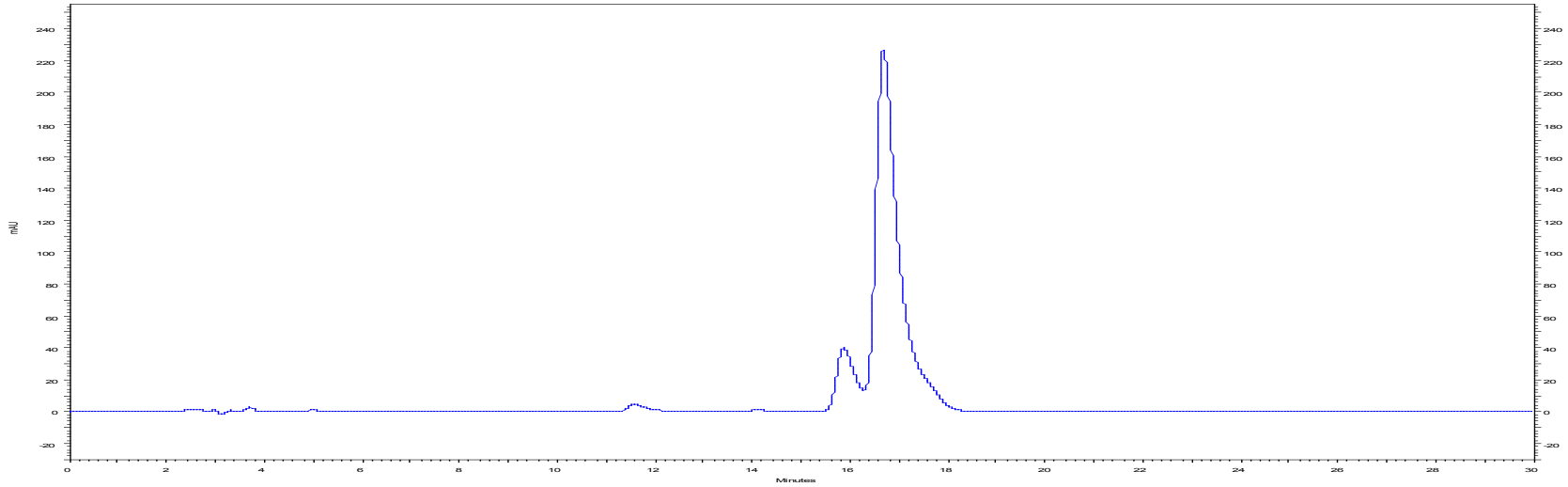
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-ylmethyl]thymidine (9c1/2). ^{13}C NMR



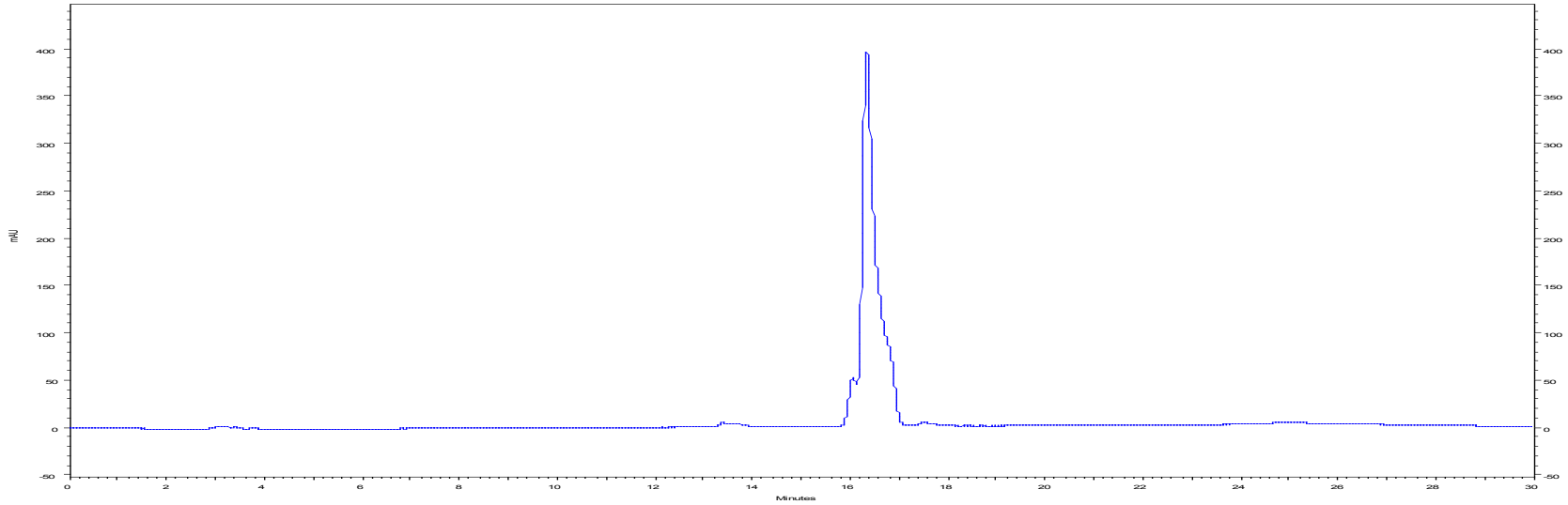
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-ylmethyl]thymidine (**9c1/2**). HR-ESI-MS found: 531.3341.



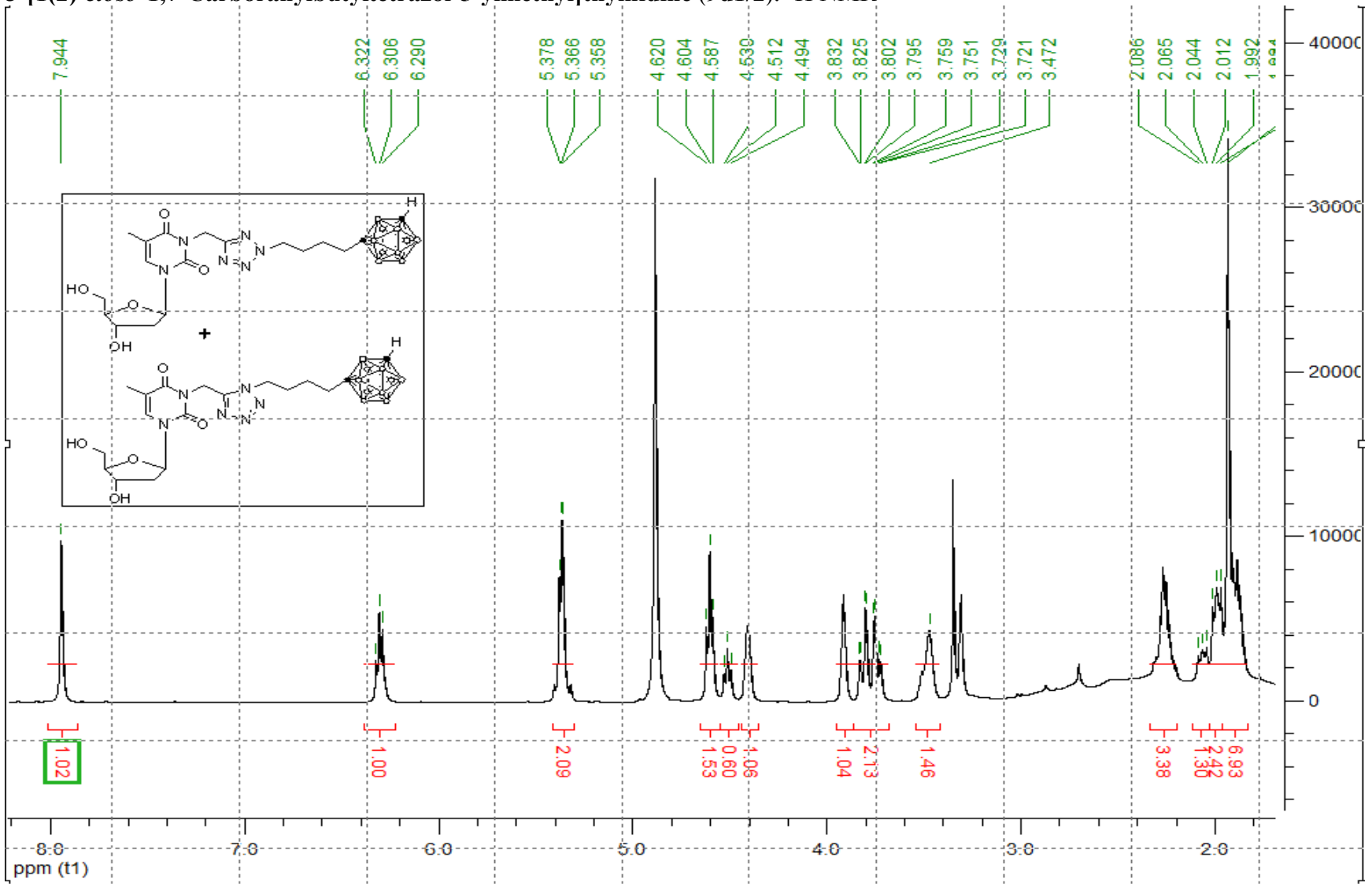
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-ylmethyl]thymidine (**9c1/2**). Analytical traces in Water:Acetonitrile gradient



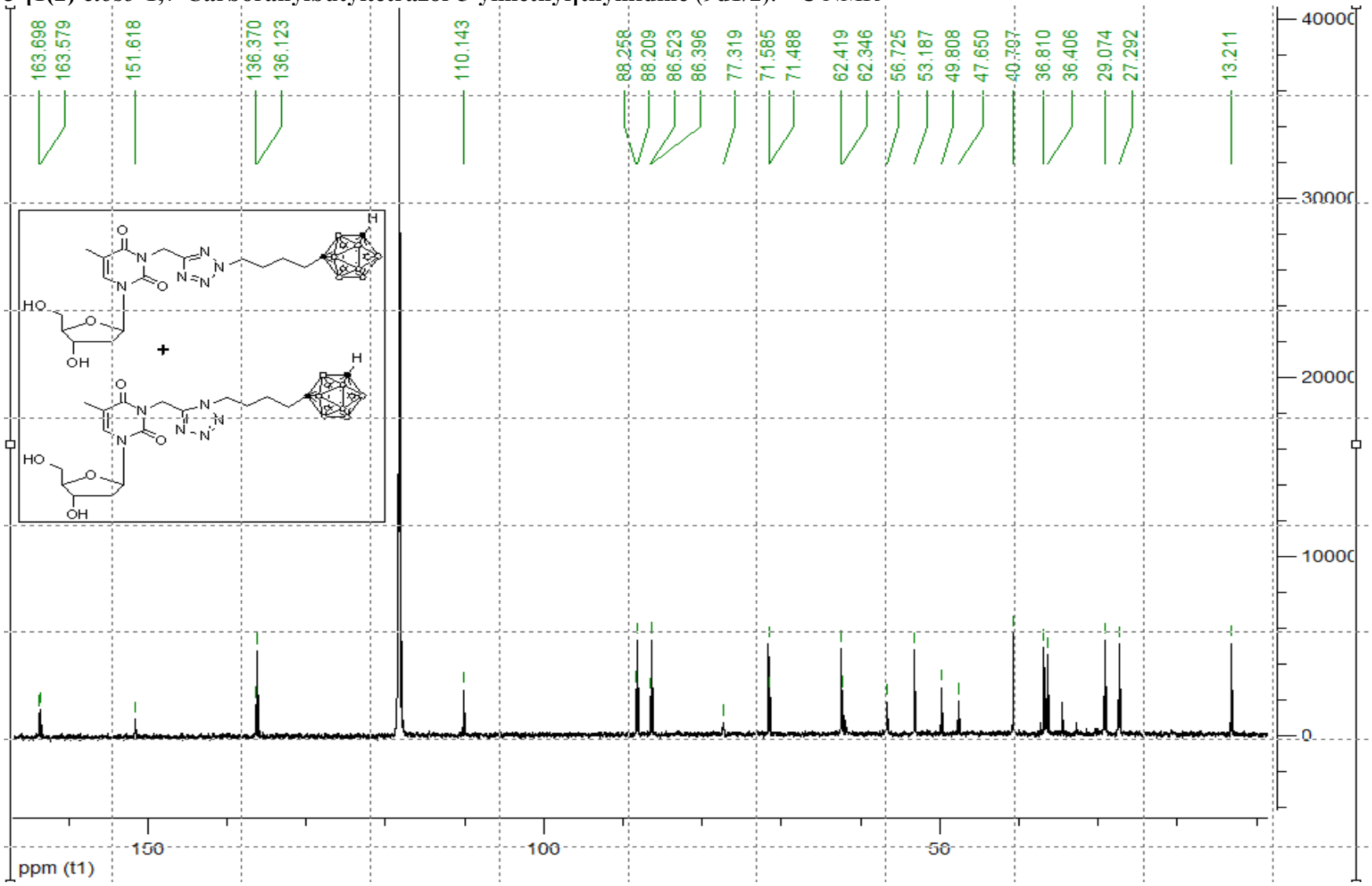
Analytical traces in Water:Methanol gradient



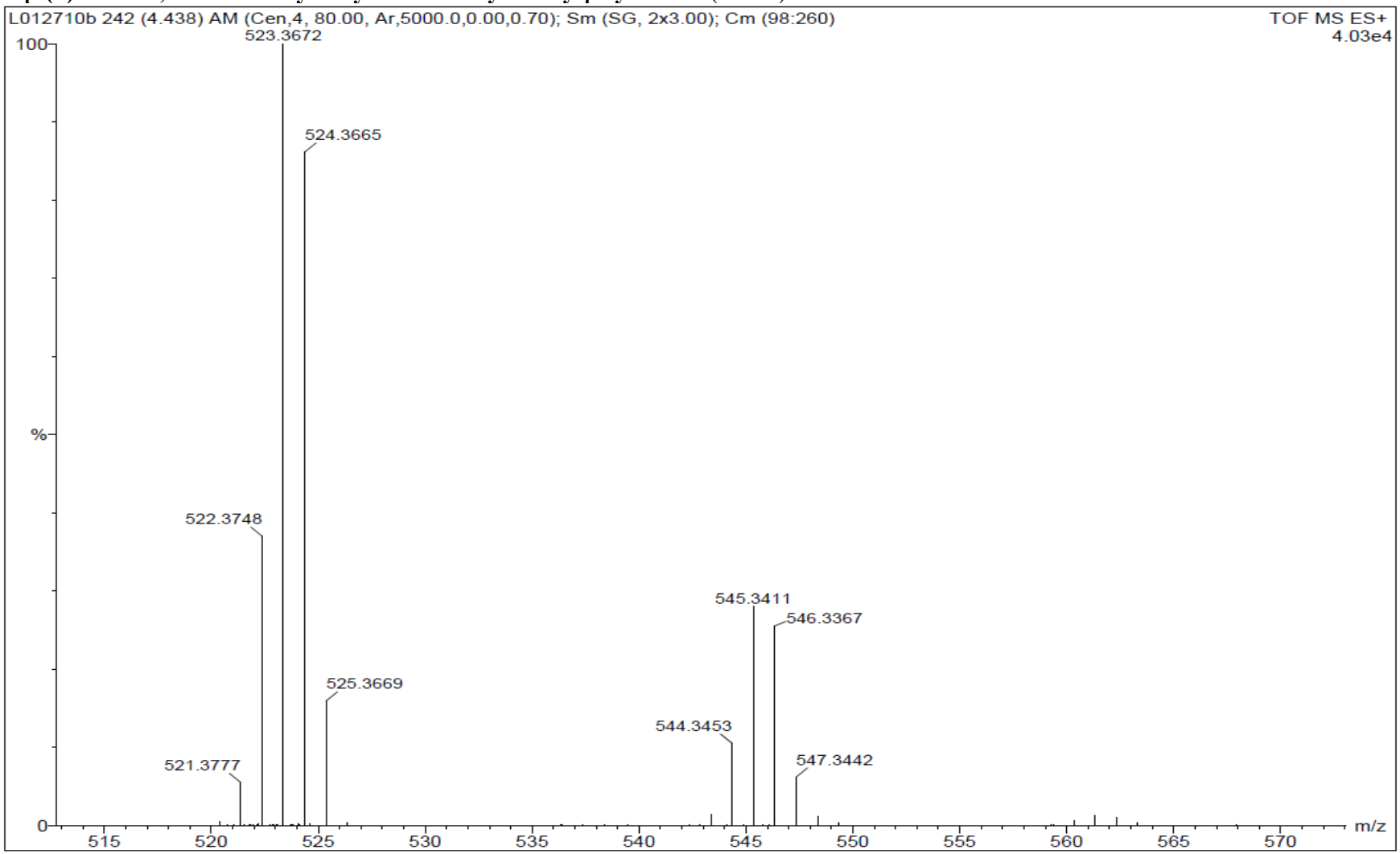
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-ylmethyl]thymidine (9d1/2). ^{1}H NMR



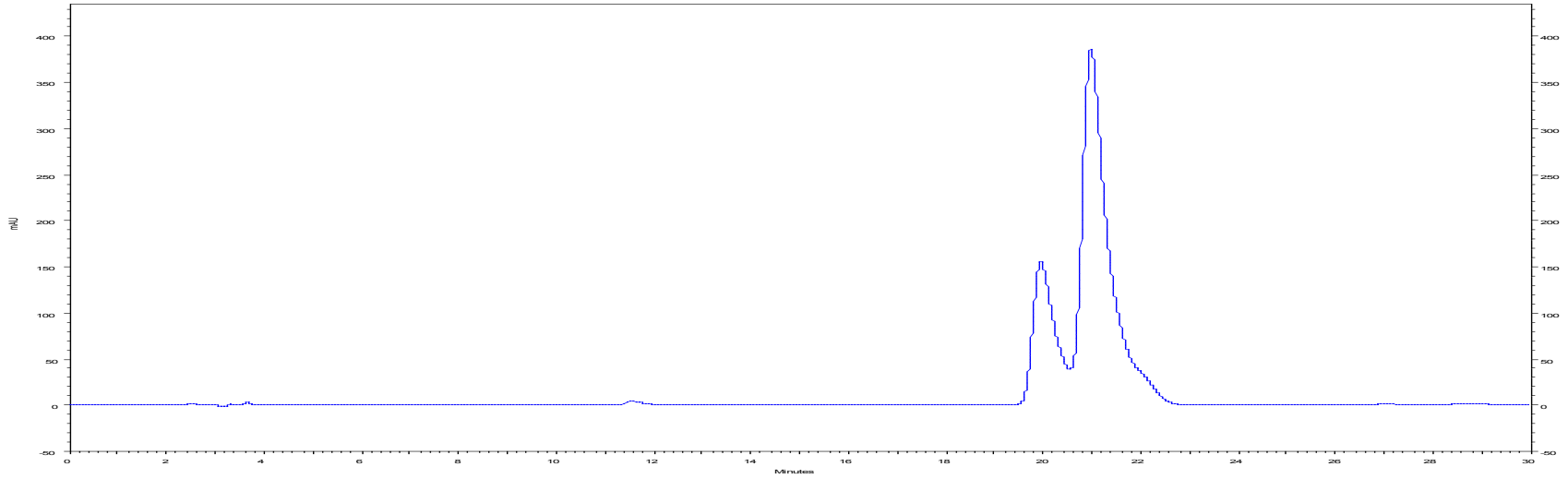
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-ylmethyl]thymidine (9d1/2). ^{13}C NMR



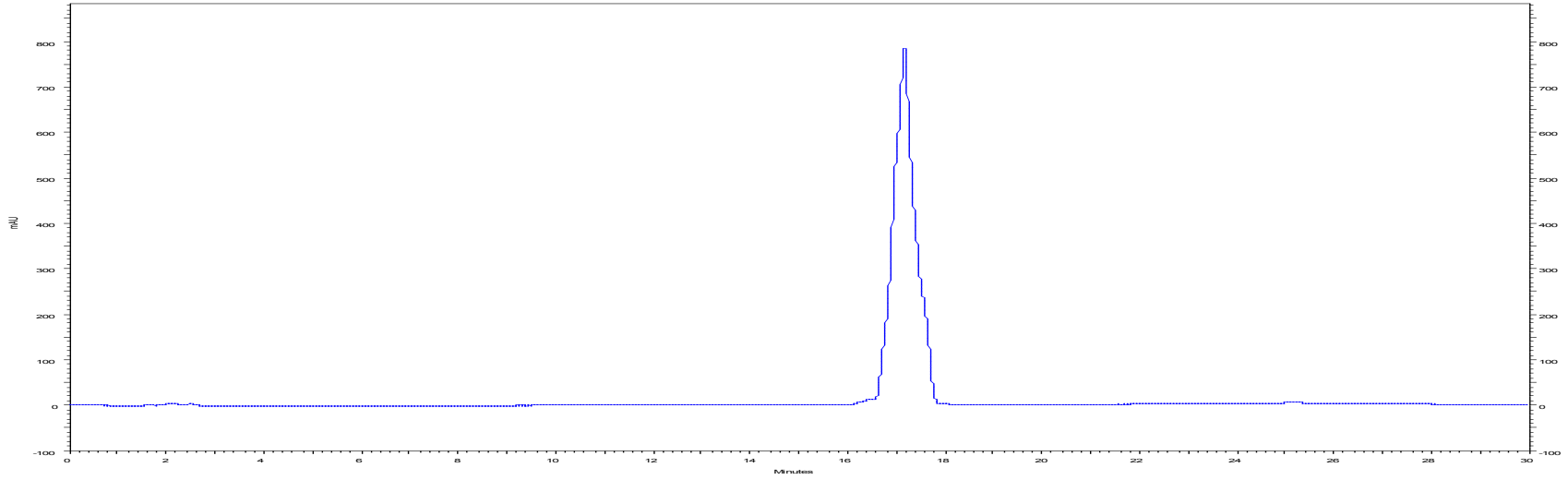
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-ylmethyl]thymidine (**9d1/2**). HR-ESI-MS found: 523.3672 and 545.3411.



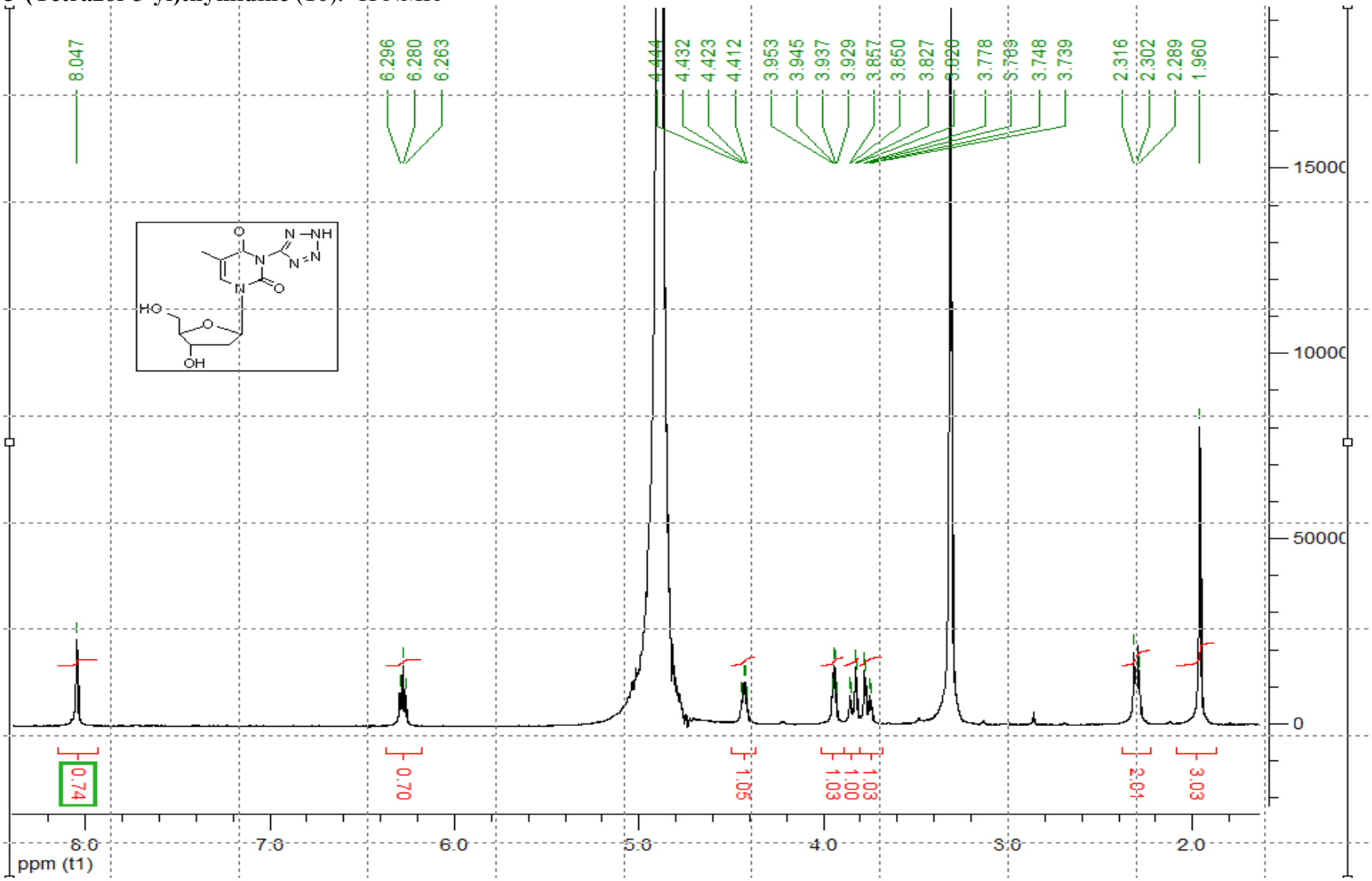
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-ylmethyl]thymidine (**9d1/2**). Analytical traces in Water:Acetonitrile gradient



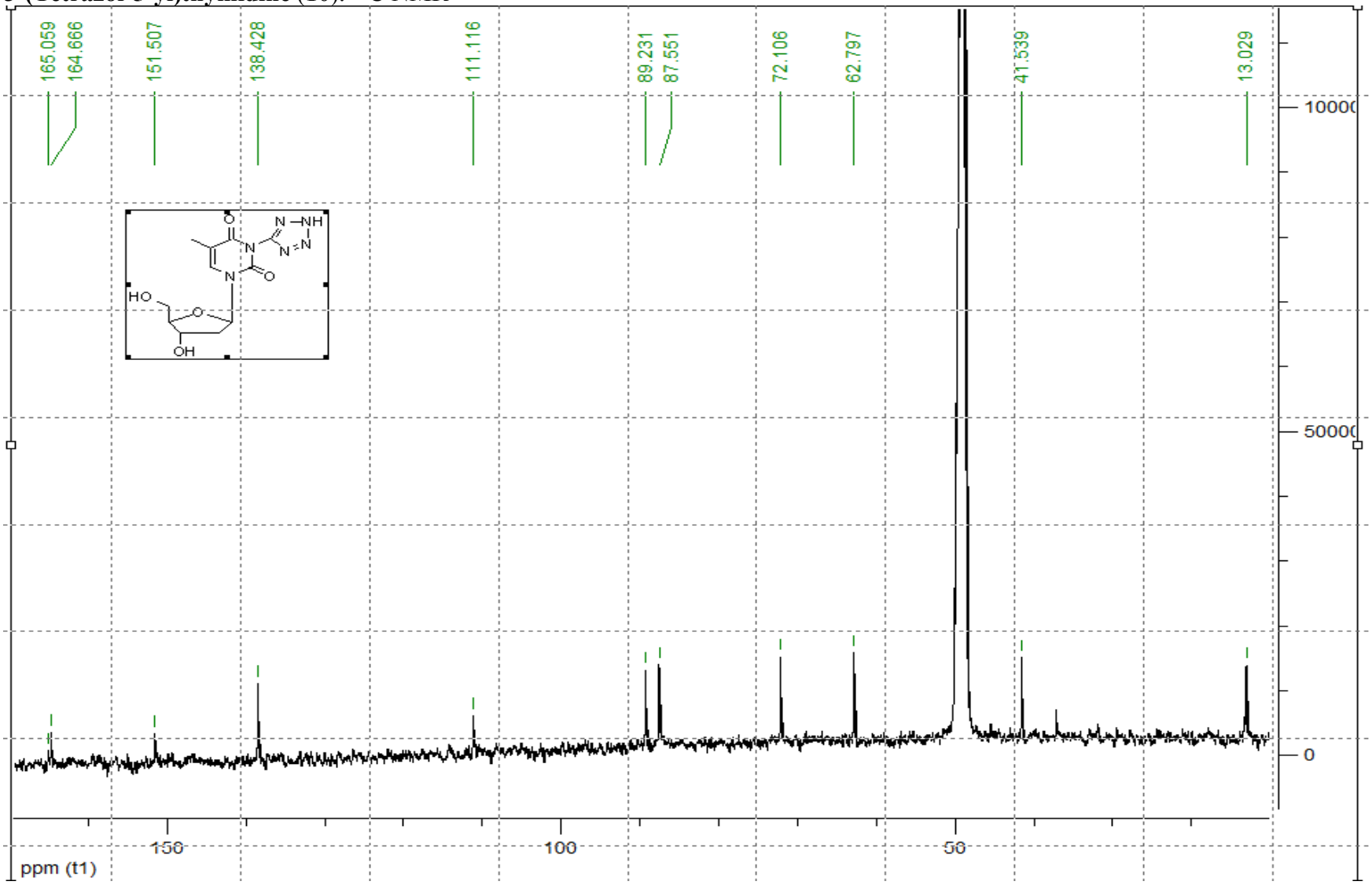
Analytical traces in Water:Methanol gradient



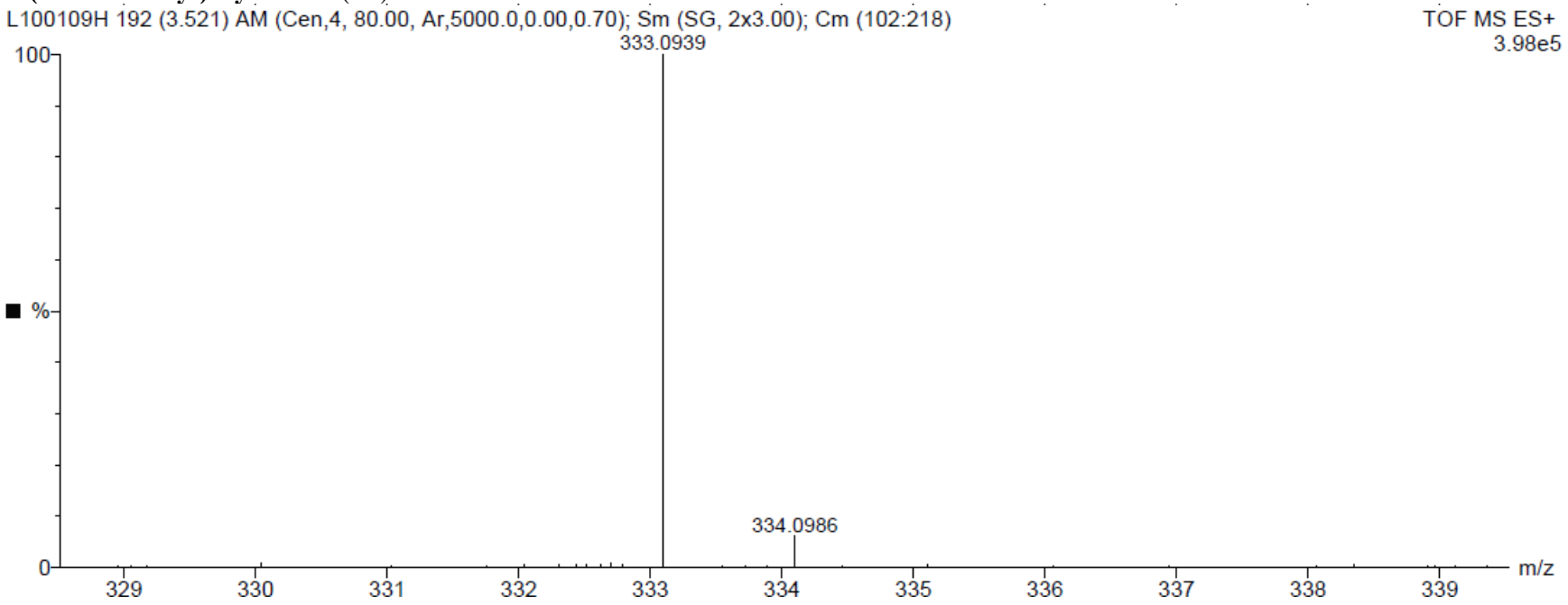
3-(Tetrazol-5-yl)thymidine (10). ^{1}H NMR



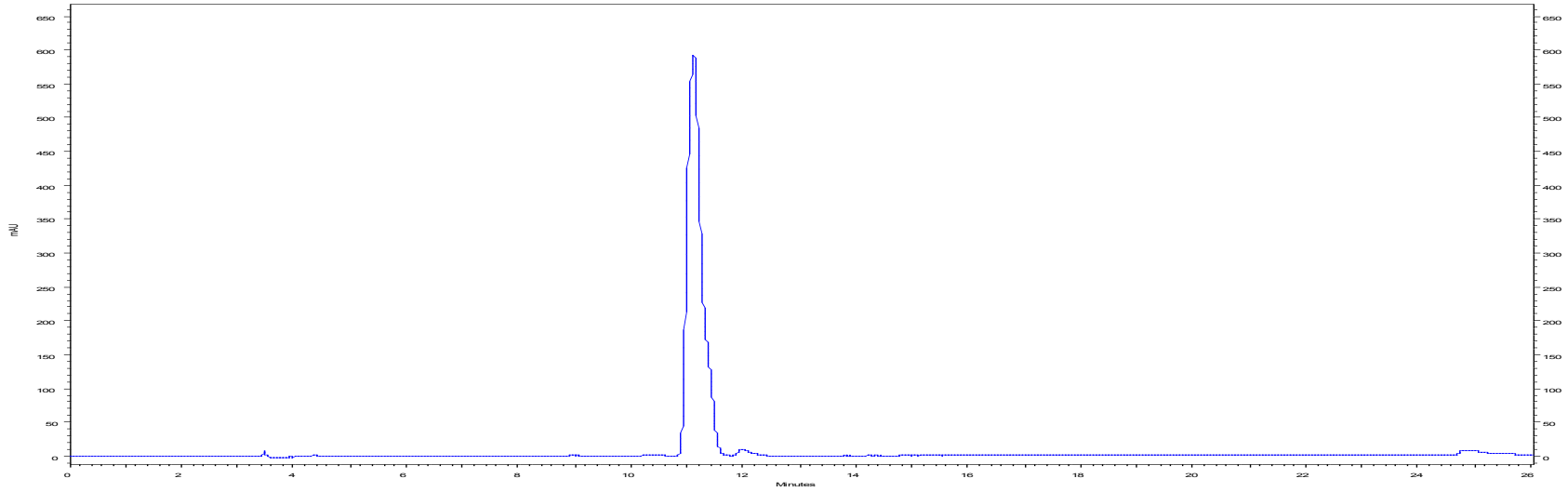
3-(Tetrazol-5-yl)thymidine (10). ^{13}C NMR



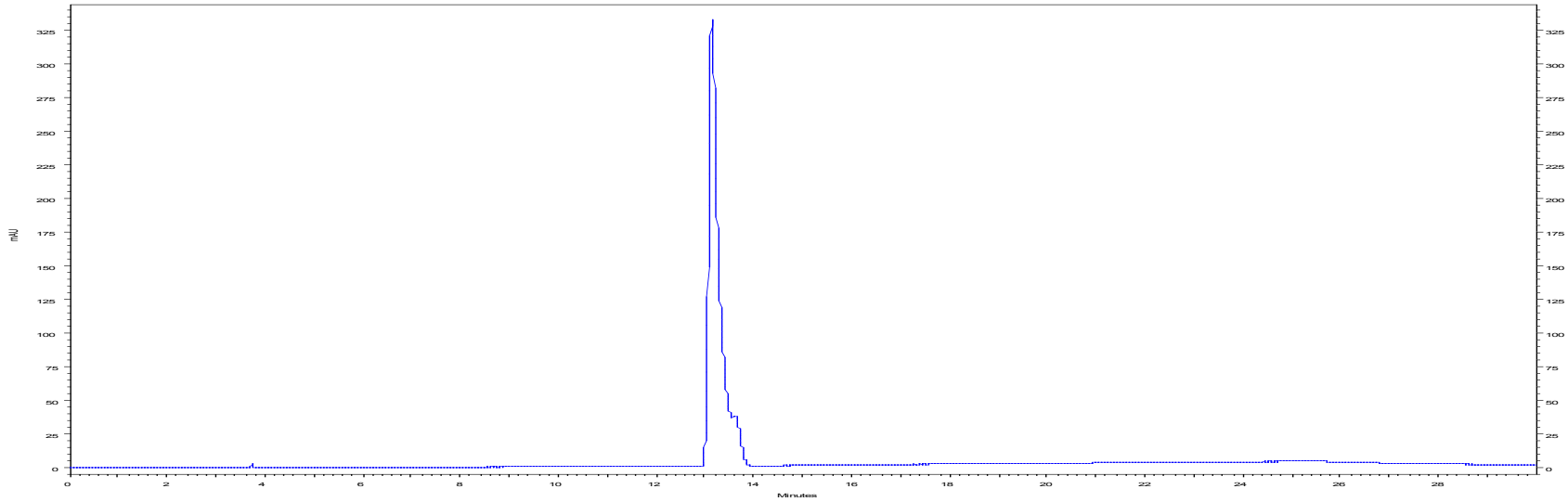
3-(Tetrazol-5-yl)thymidine (**10**). HR-ESI-MS found: 333.0939.



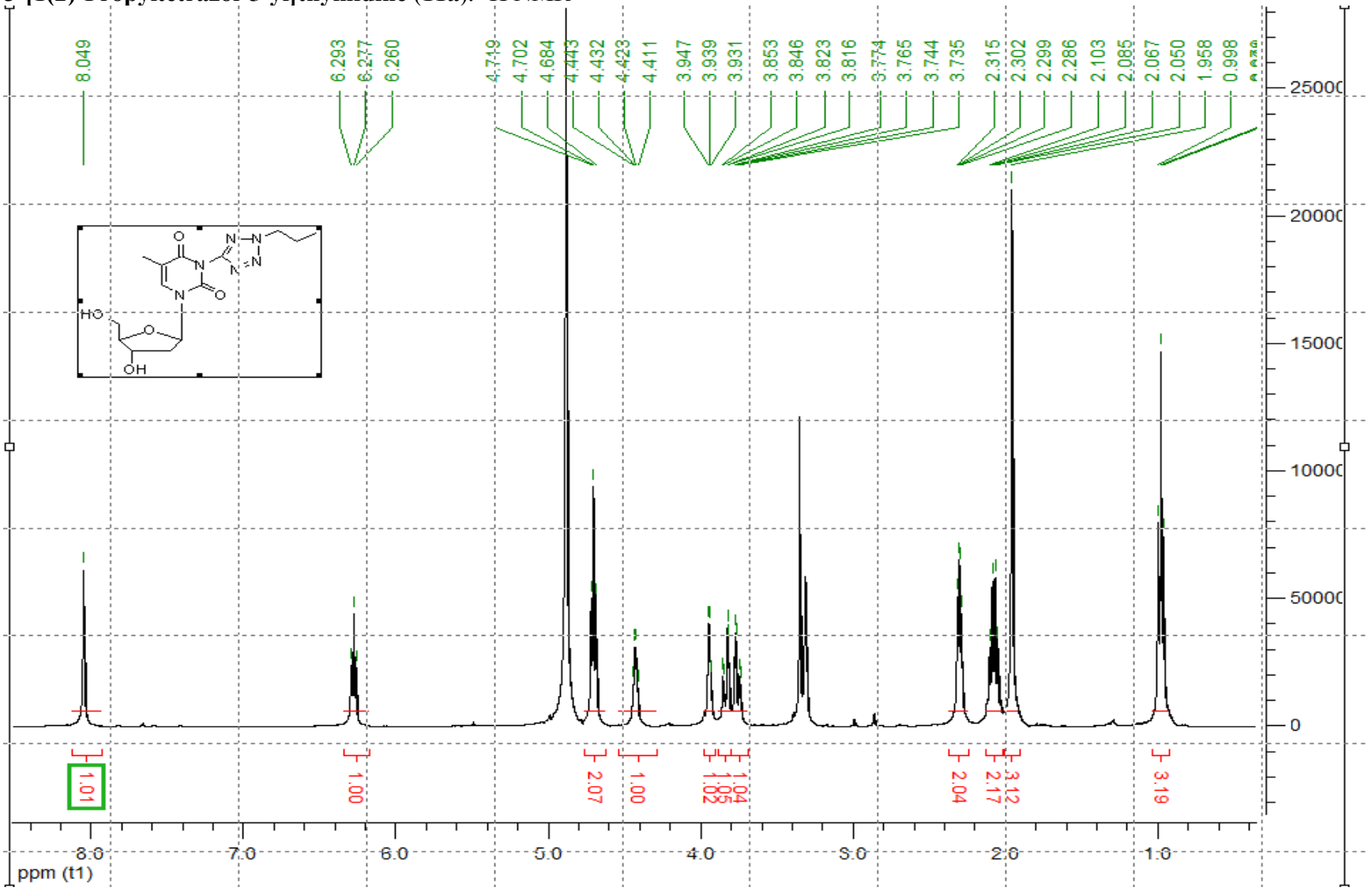
3-(Tetrazol-5-yl)thymidine (**10**). Analytical traces in Water:Acetonitrile gradient



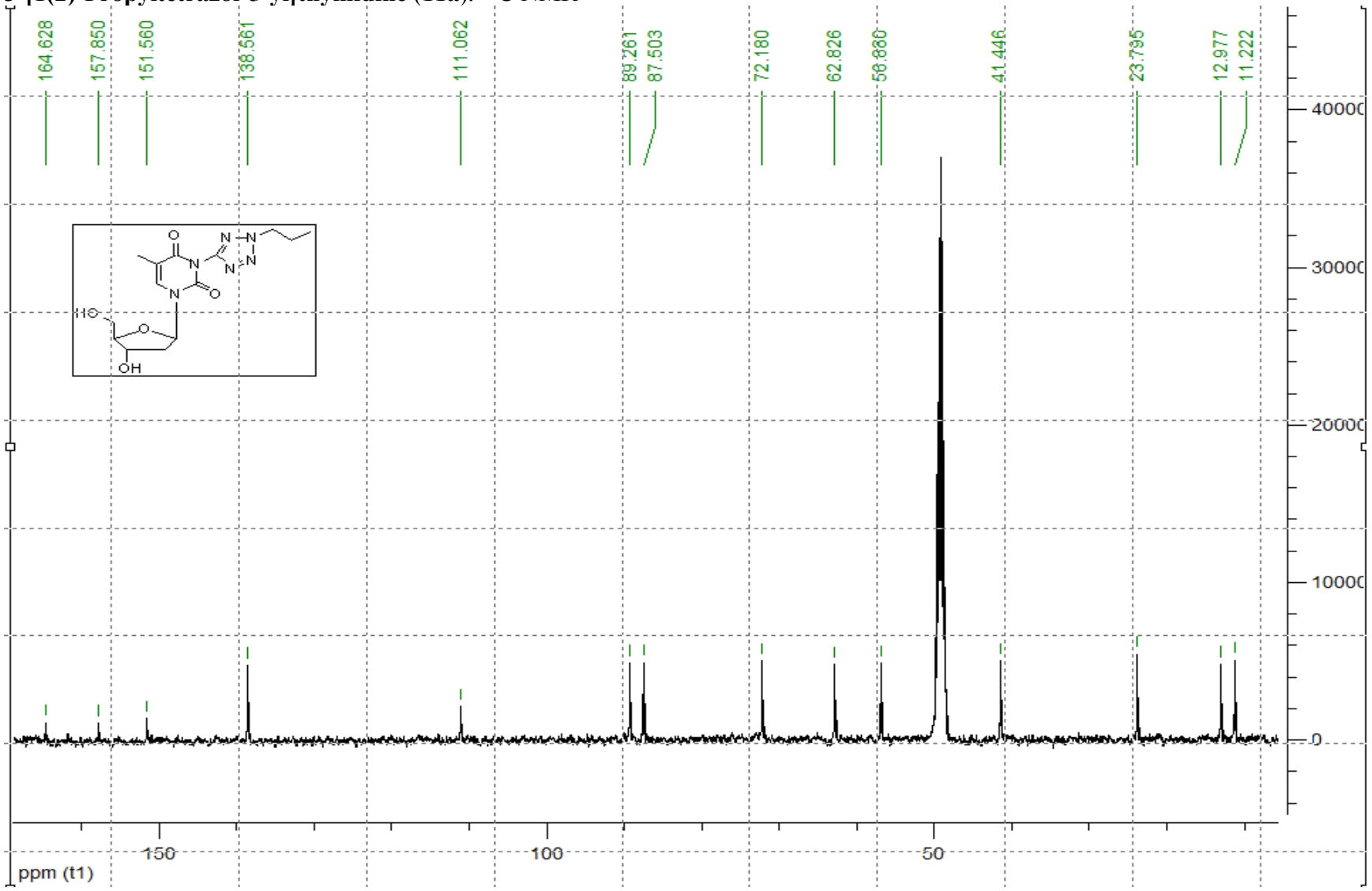
Analytical traces in Water:Methanol gradient



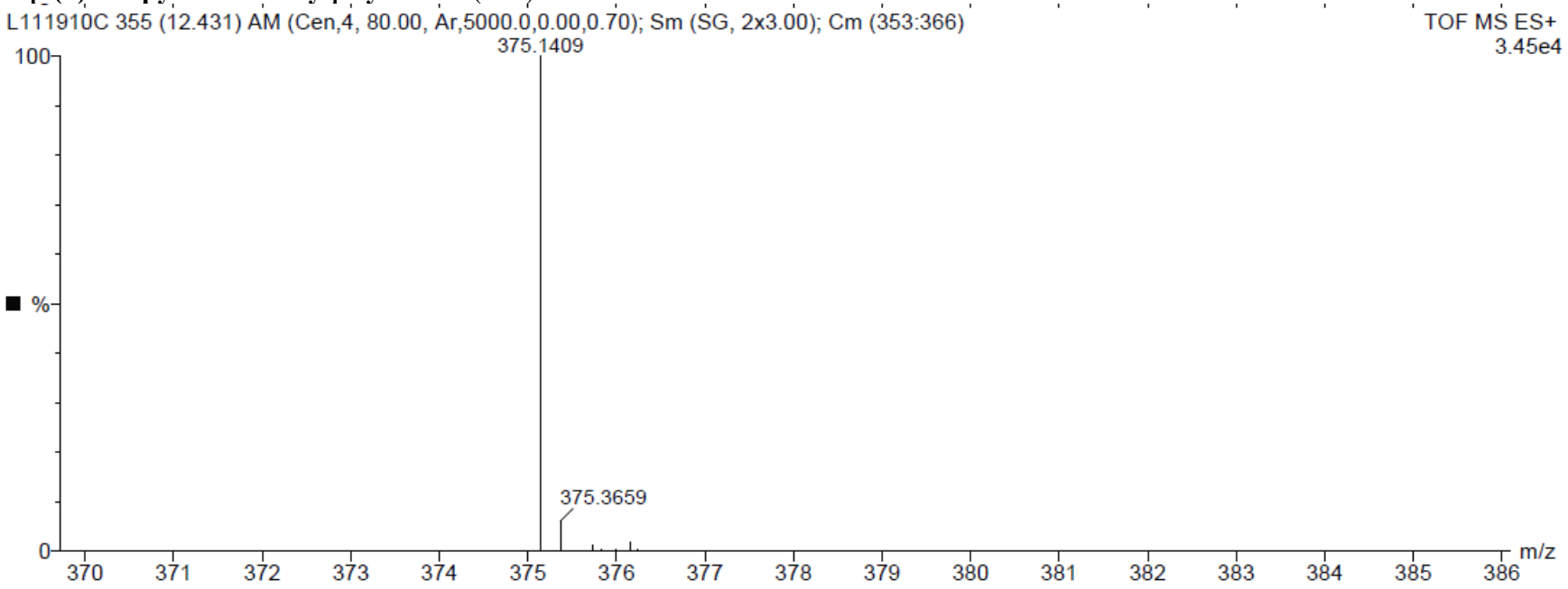
3-[1(2)-Propyltetrazol-5-yl]thymidine (11a). ^{1}H NMR



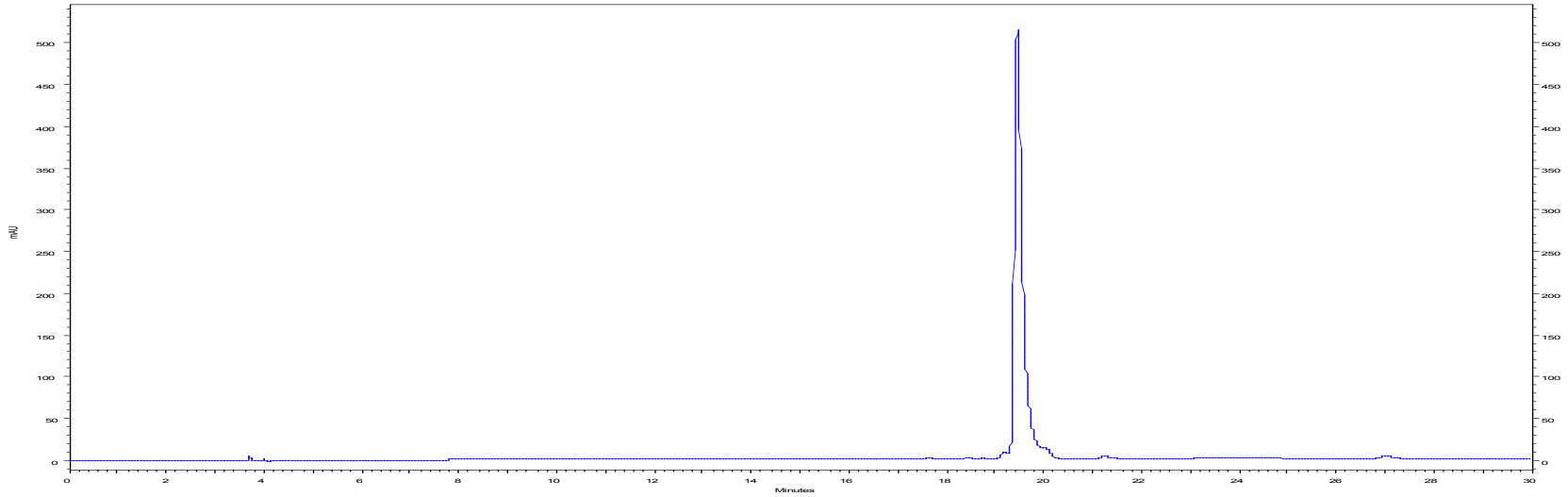
3-[1(2)-Propyltetrazol-5-yl]thymidine (11a). ^{13}C NMR



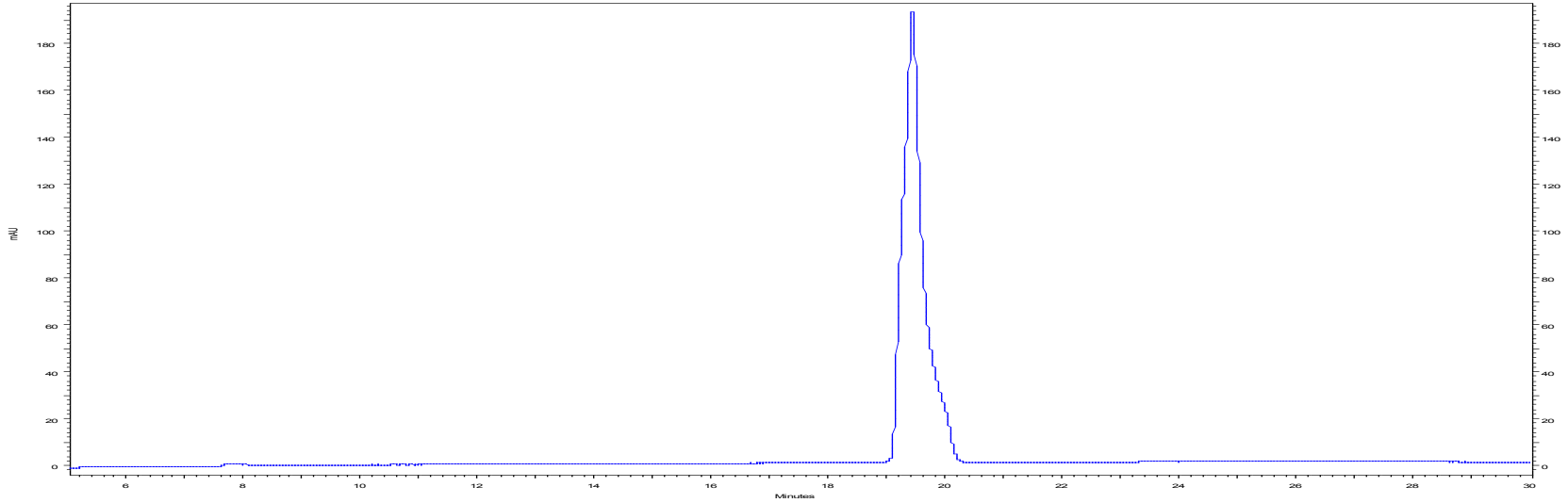
3-[1(2)-Propyltetrazol-5-yl]thymidine (**11a**). HR-ESI-MS: 375.1409.



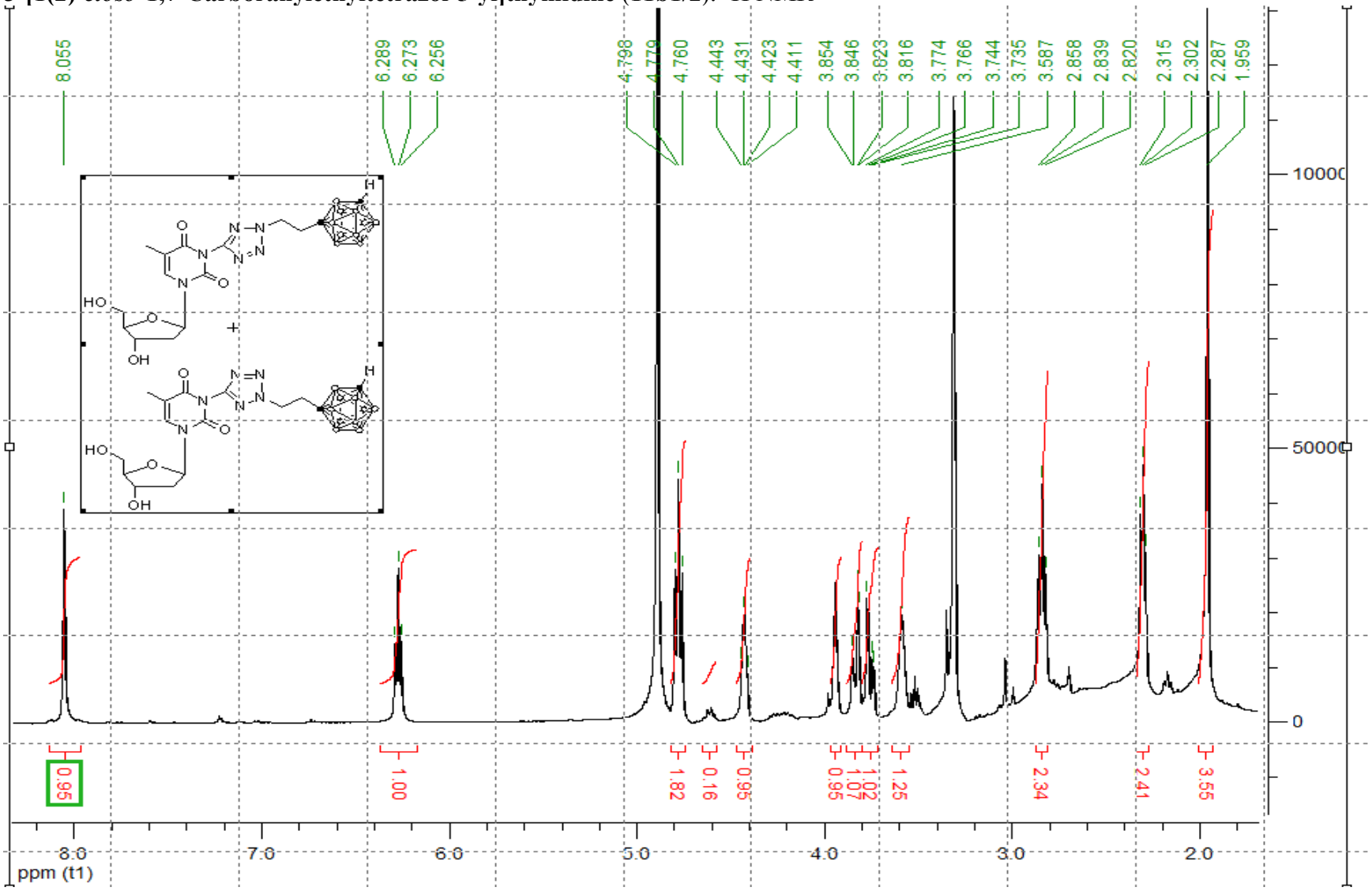
3-[1(2)-Propyltetrazol-5-yl]thymidine (**11a**). Analytical traces in Water:Acetonitrile gradient



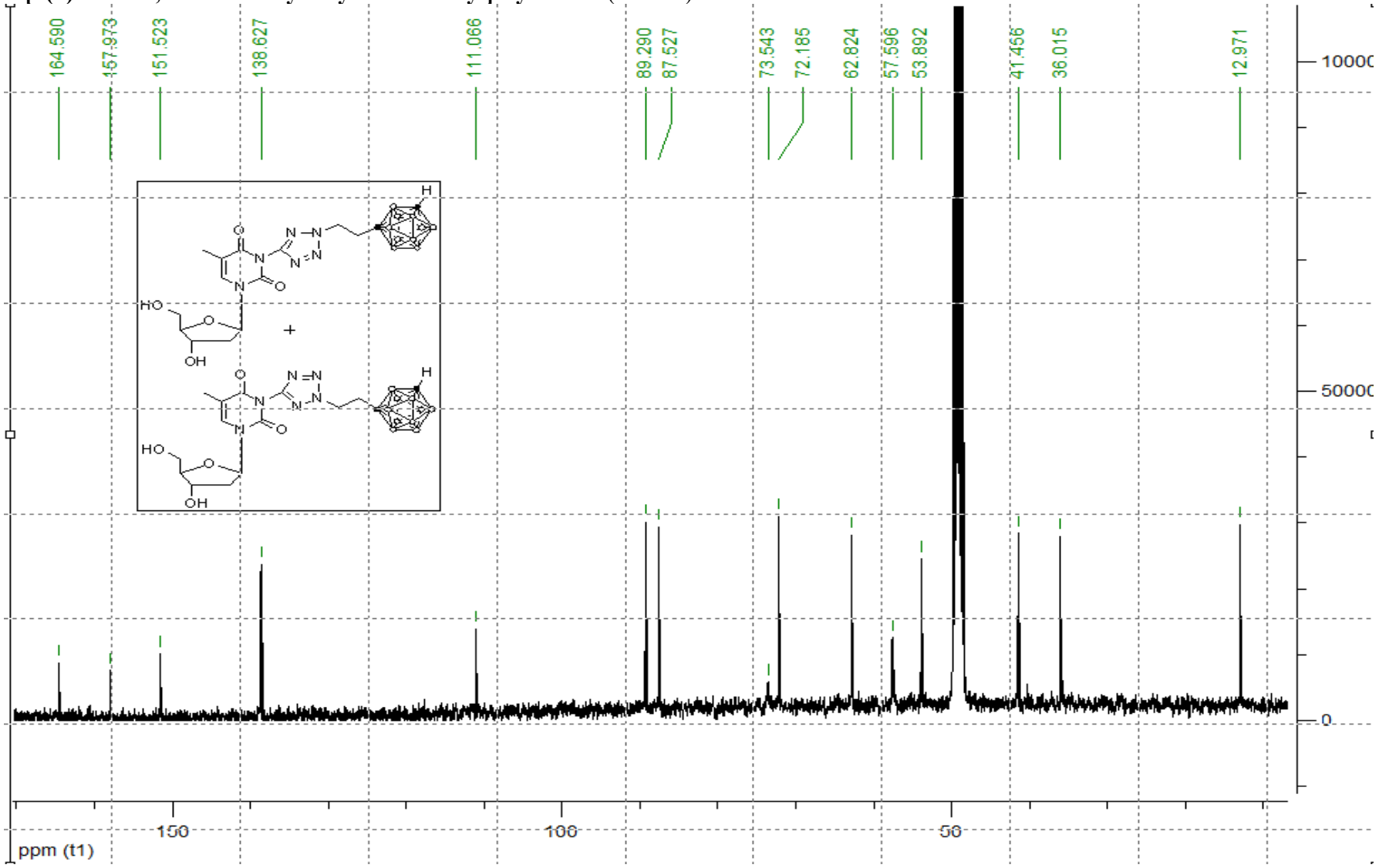
Analytical traces in Water:Methanol gradient



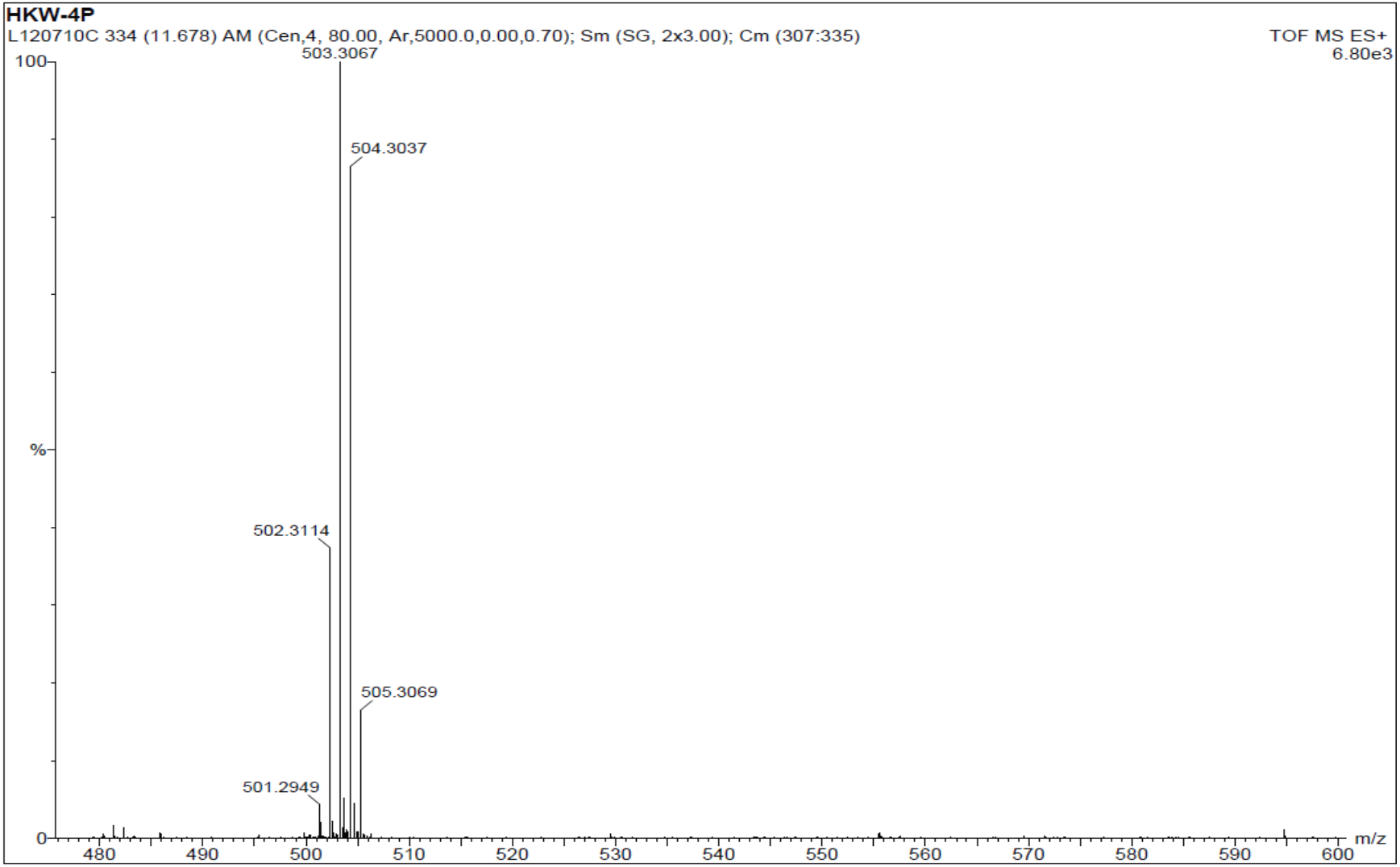
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-yl]thymidine (11b1/2). ^{1}H NMR



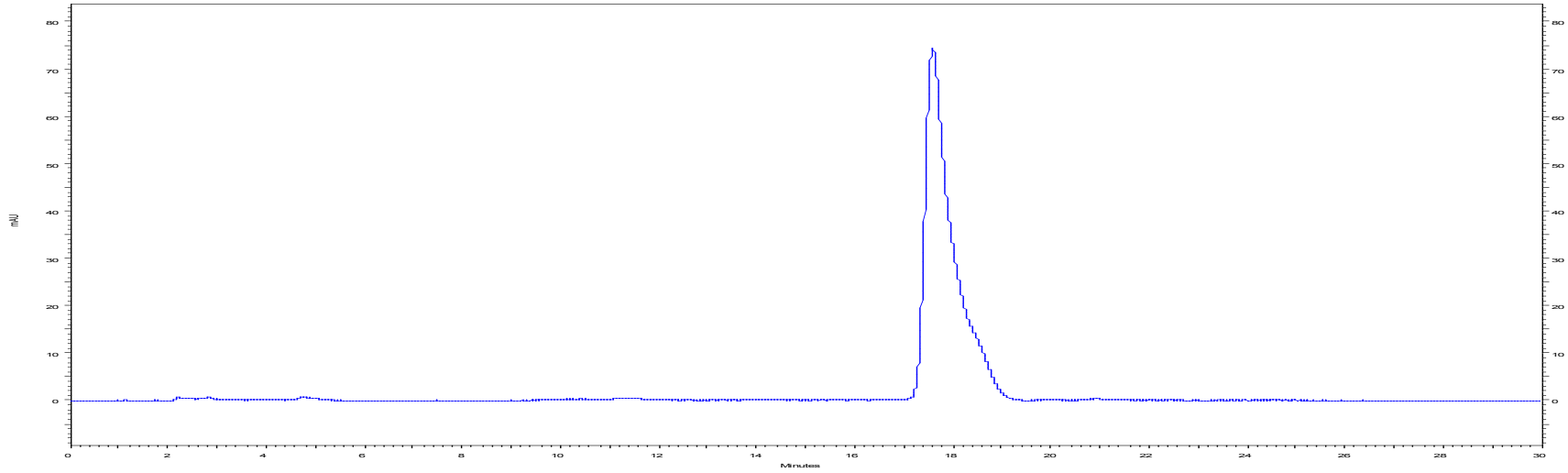
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-yl]thymidine (11b1/2). ^{13}C NMR



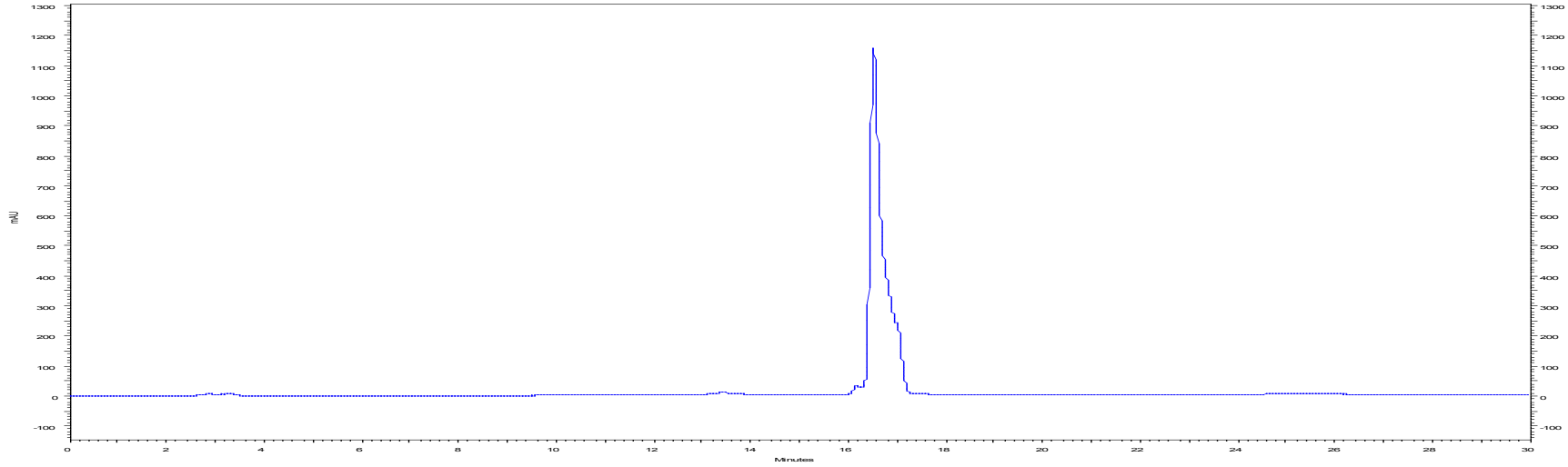
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-yl]thymidine (11b1/2). HR-ESI-MS found: 503.3067.



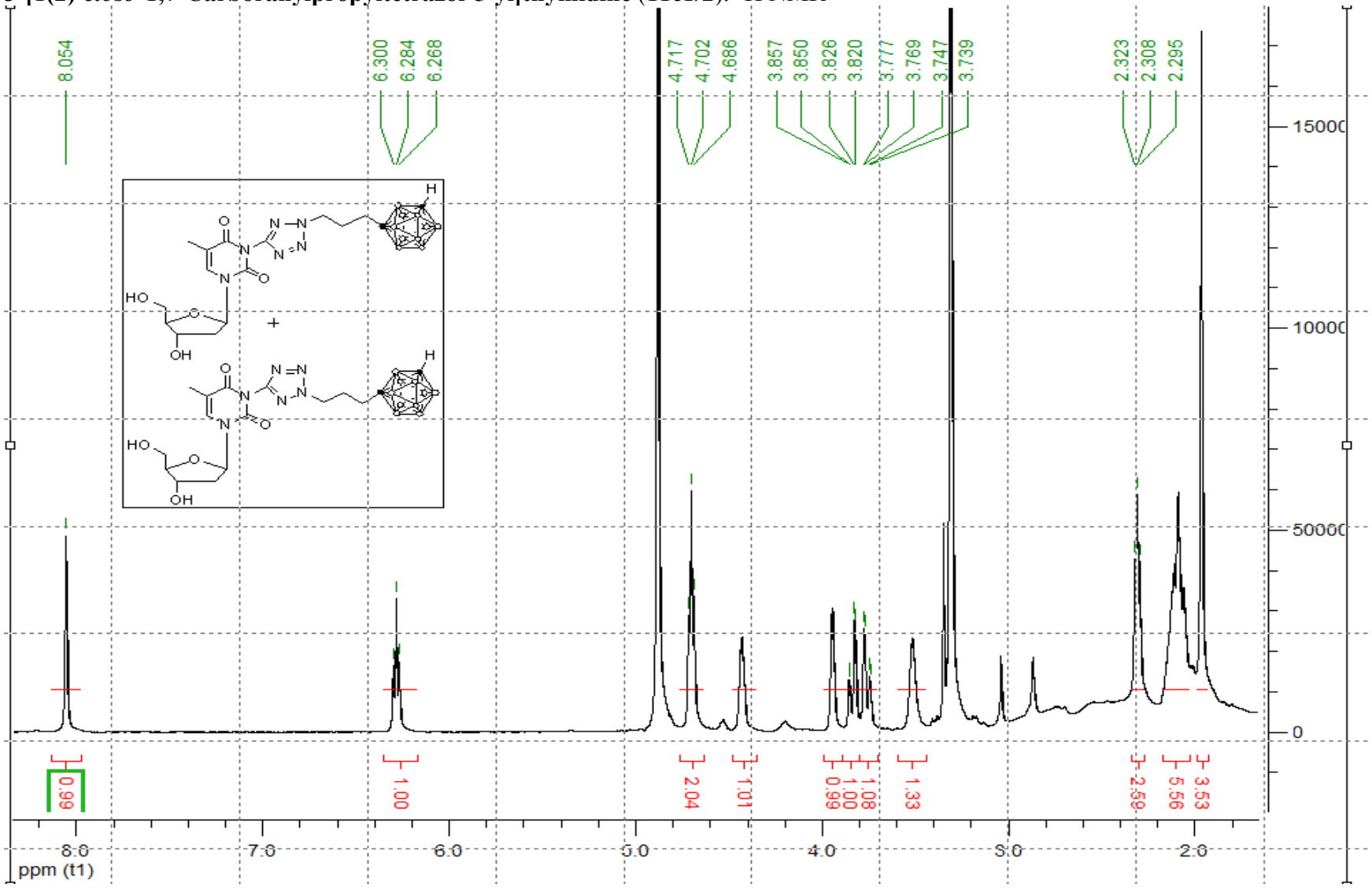
3-[1(2)-*closo*-1,7-Carboranylethyltetrazol-5-yl]thymidine (11b1/2). Analytical traces in Water:Acetonitrile gradient



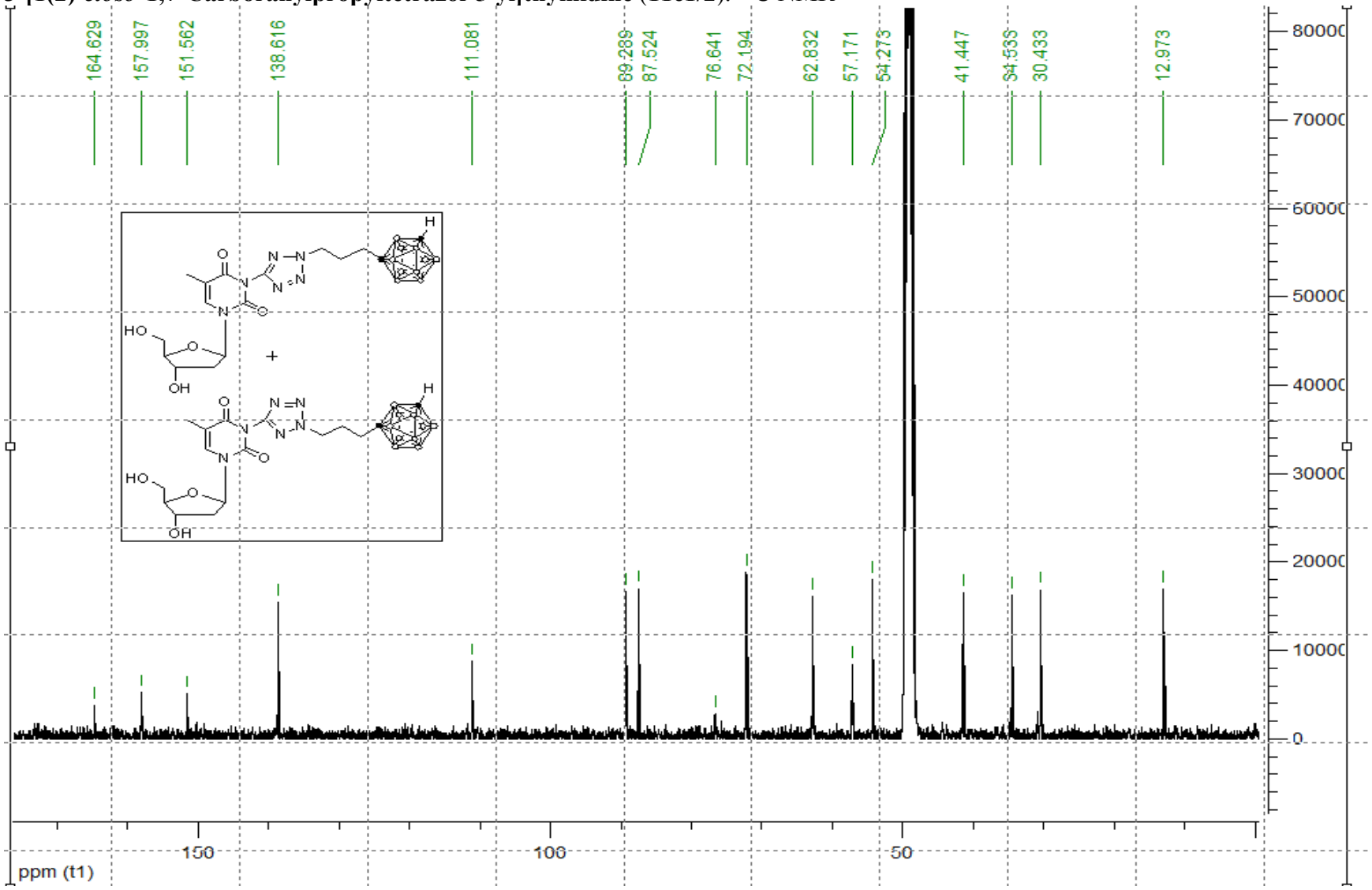
Analytical traces in Water:Methanol gradient



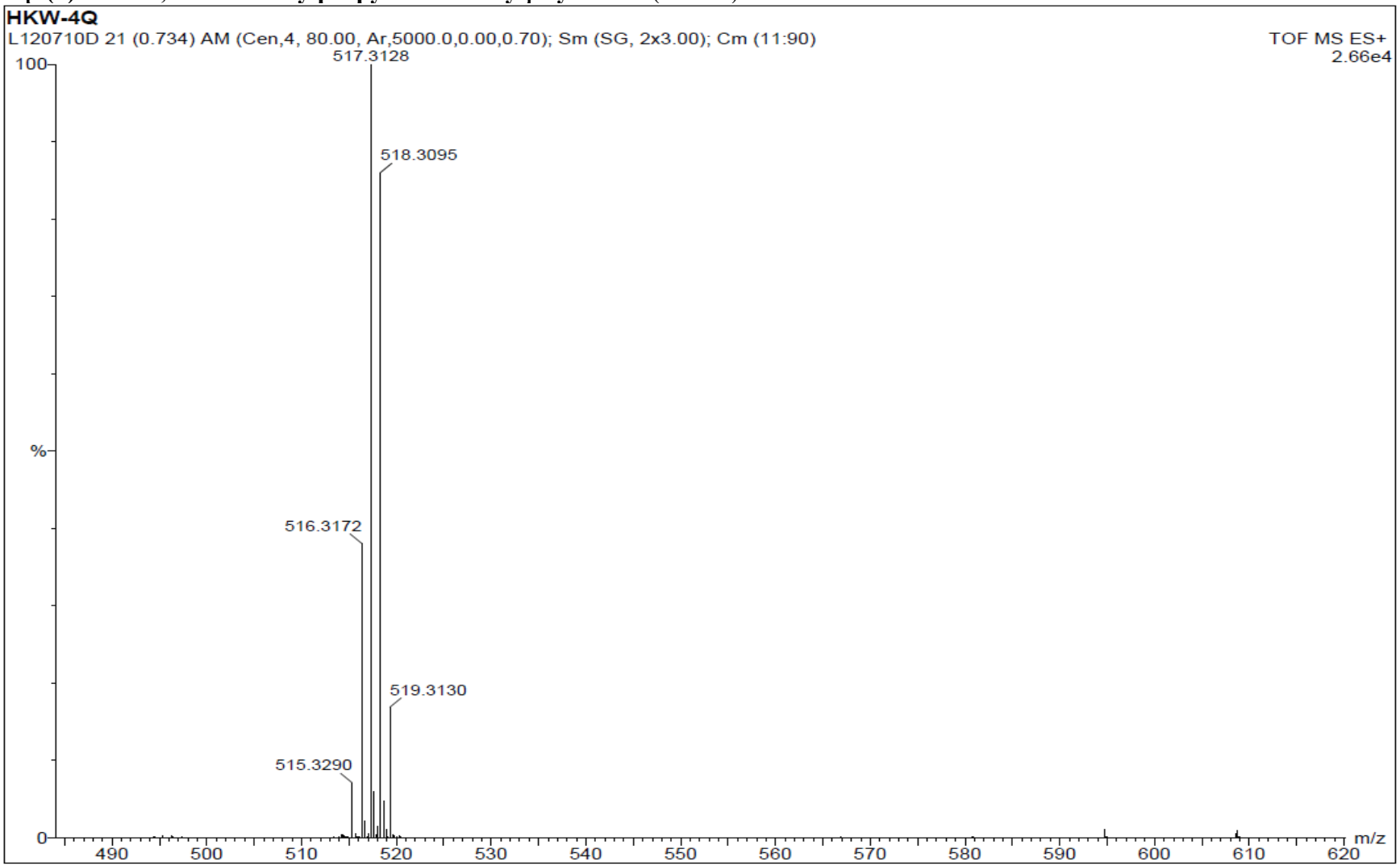
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-yl]thymidine (11c1/2). ^{1}H NMR



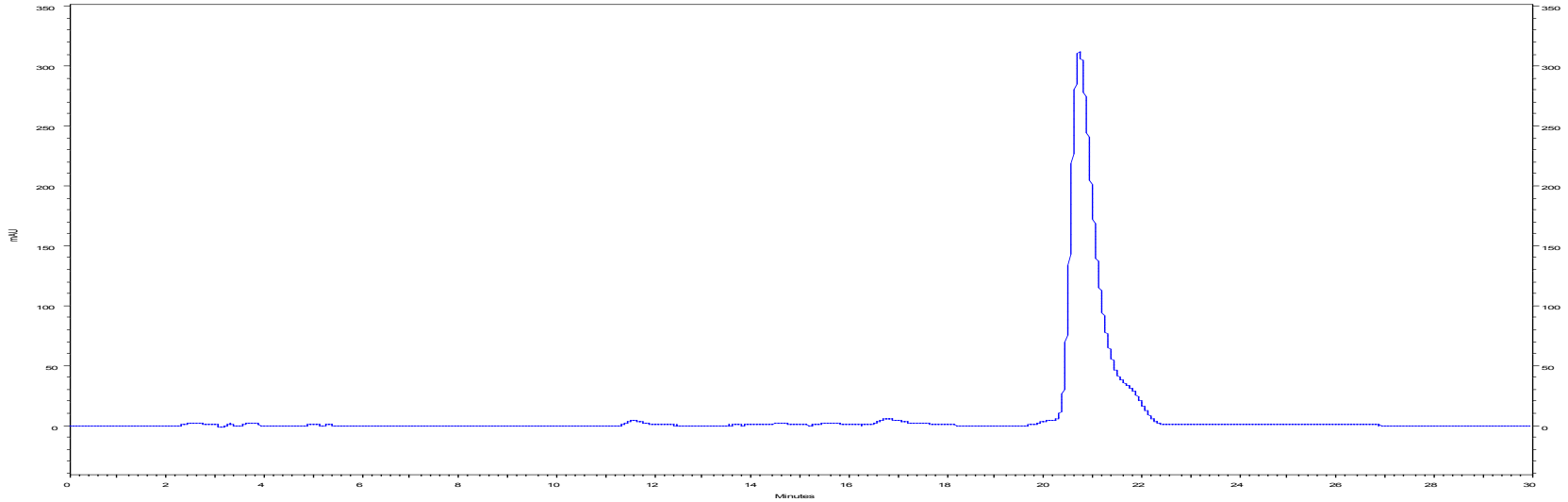
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-yl]thymidine (11c1/2). ^{13}C NMR



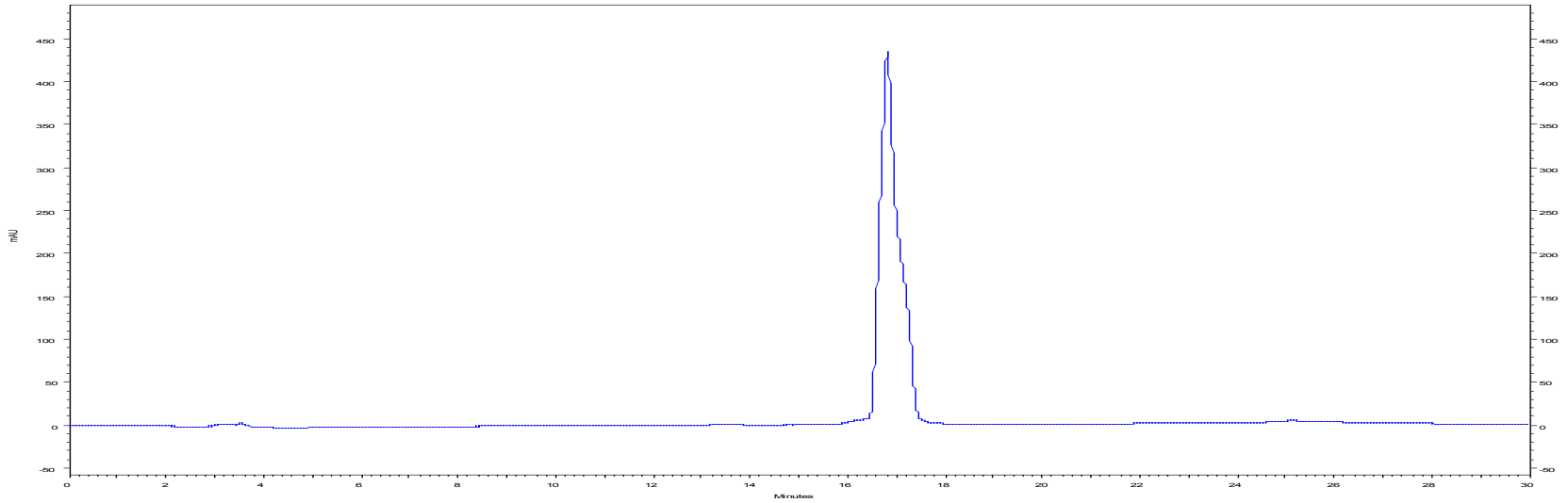
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-yl]thymidine (11c1/2). HR-ESI-MS found: 517.3128.



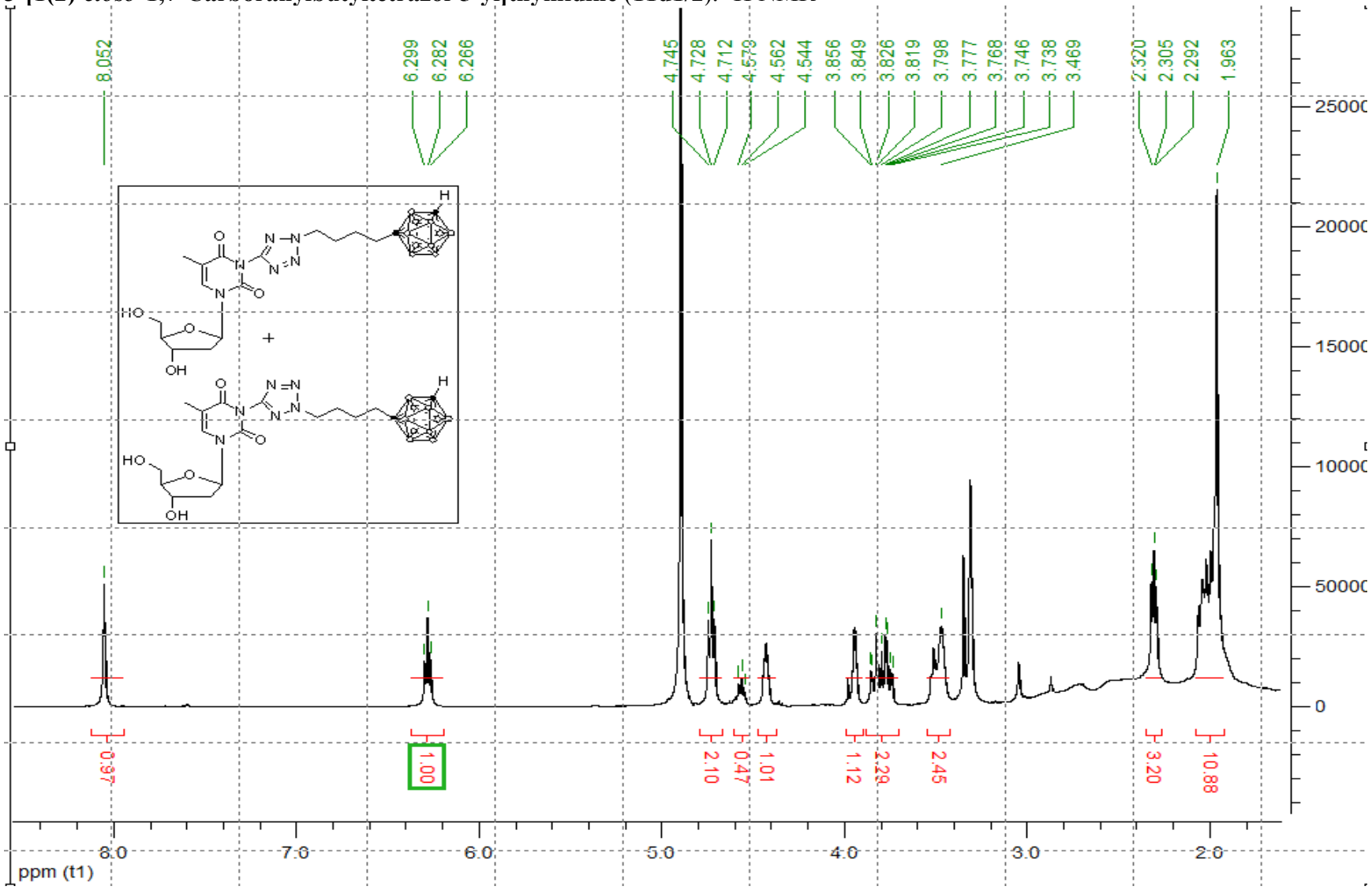
3-[1(2)-*closo*-1,7-Carboranylpropyltetrazol-5-yl]thymidine (**11c1/2**). Analytical traces in Water:Acetonitrile gradient



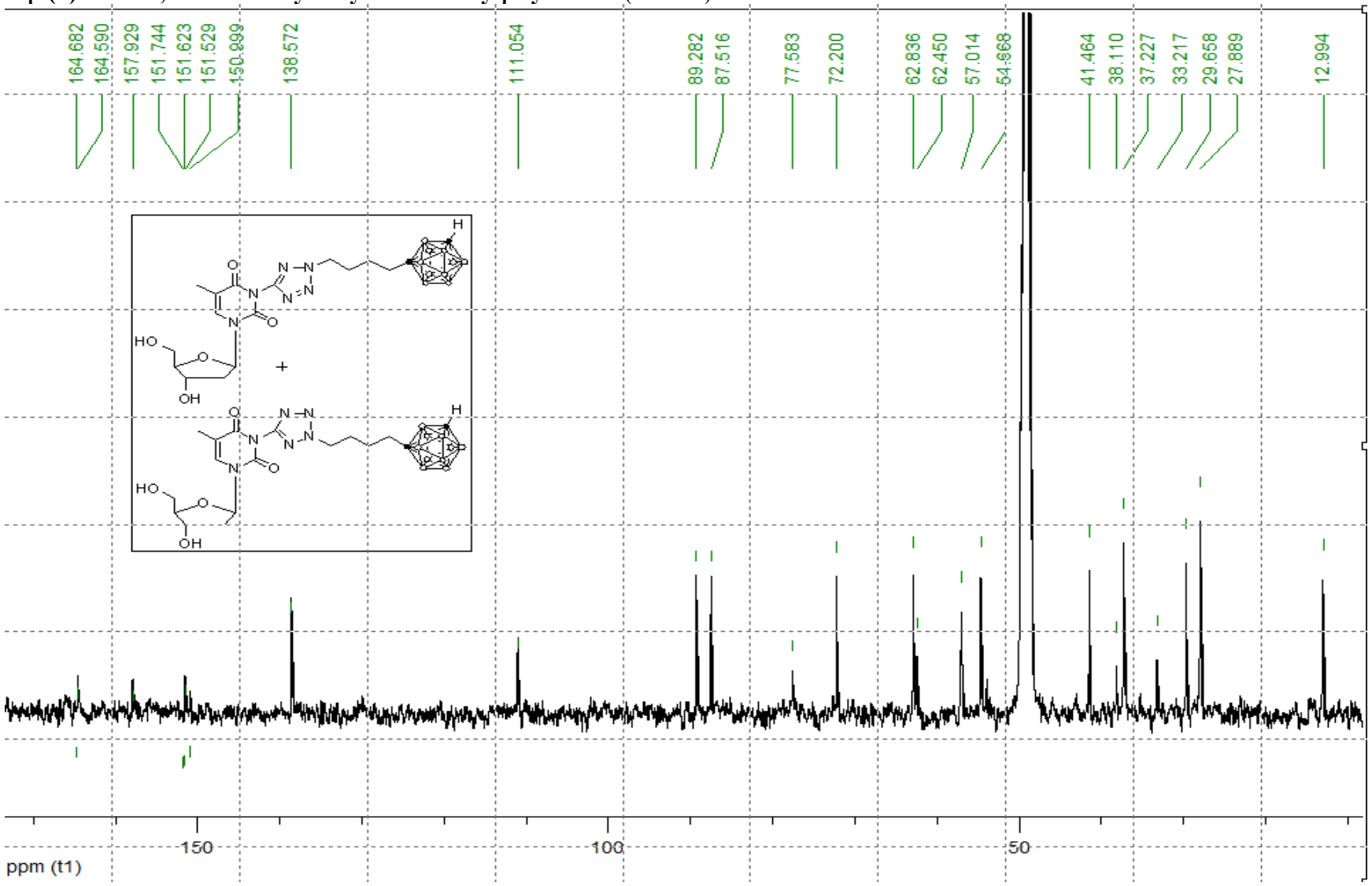
Analytical traces in Water:Methanol gradient



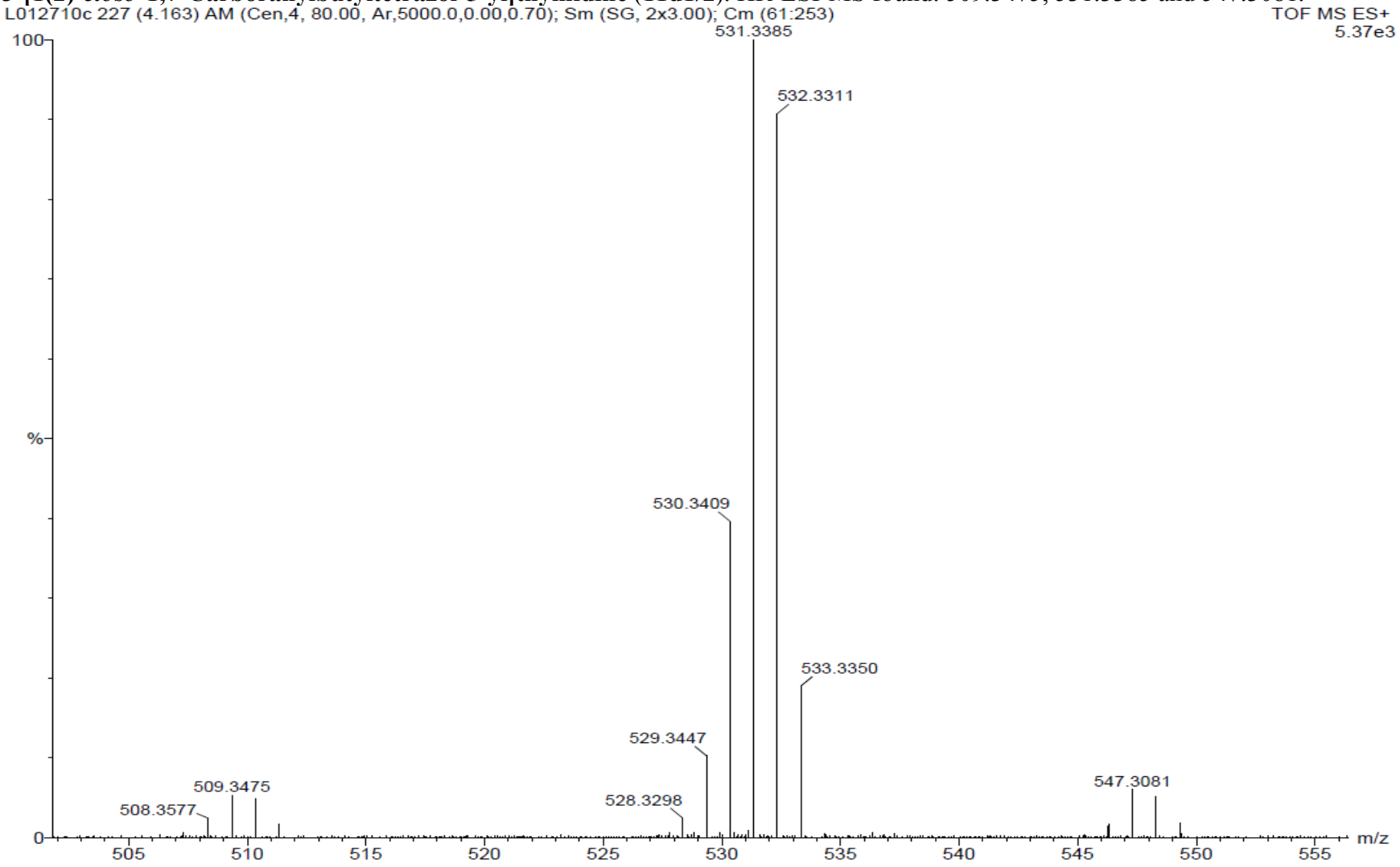
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-yl]thymidine (11d1/2). ^{1}H NMR



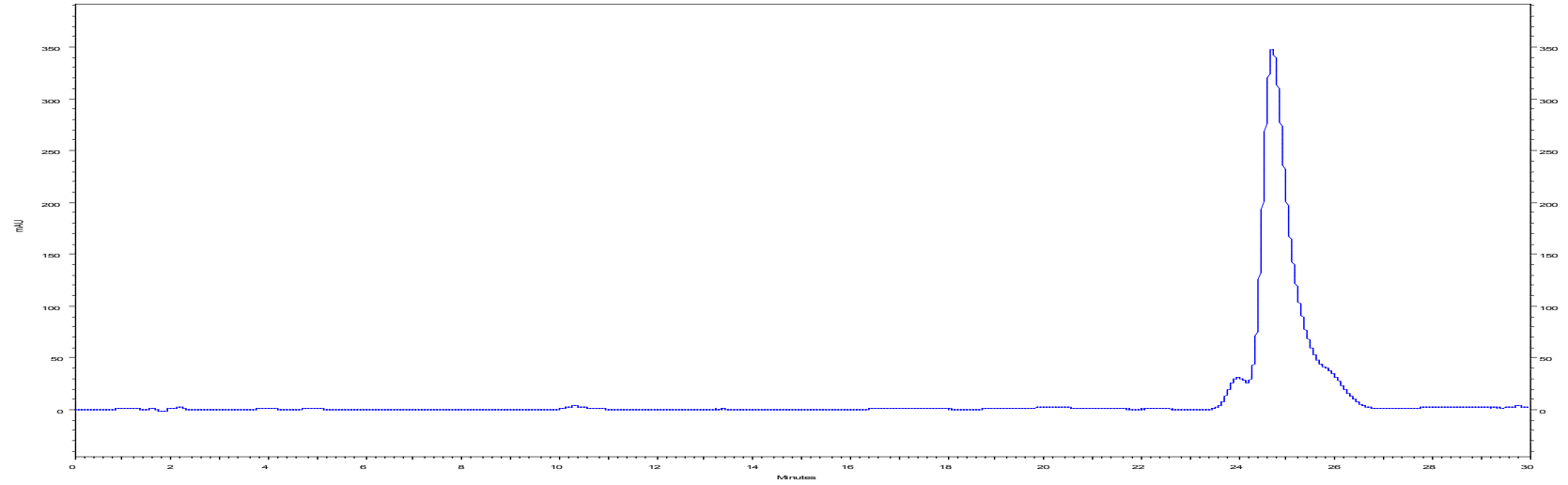
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-yl]thymidine (11d1/2). ^{13}C NMR



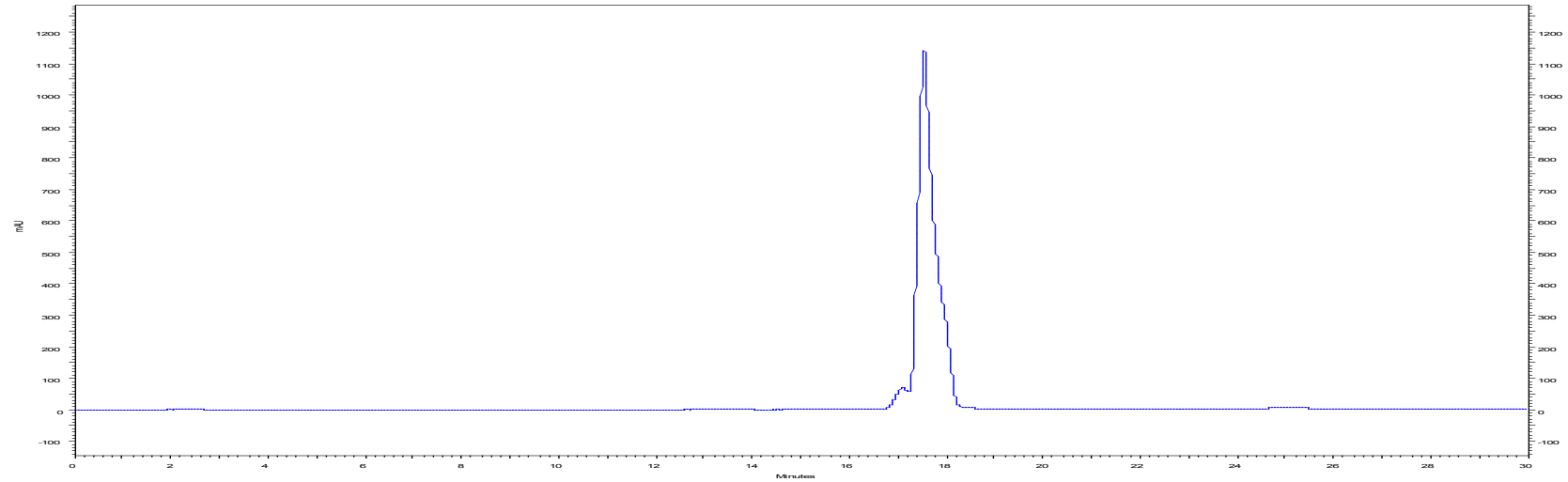
3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-yl]thymidine (**11d1/2**). HR-ESI-MS found: 509.3475, 531.3385 and 547.3081.



3-[1(2)-*closo*-1,7-Carboranylbutyltetrazol-5-yl]thymidine (**11d1/2**). Analytical traces in Water:Acetonitrile gradient



Analytical traces in Water:Methanol gradient



3. Purification of hTK1 and determination of its concentration

The hTK1 content in the enzyme preparation was 538.7 µg/mL (**Table S2**) and was estimated to be ~40% of the purified protein cocktail.

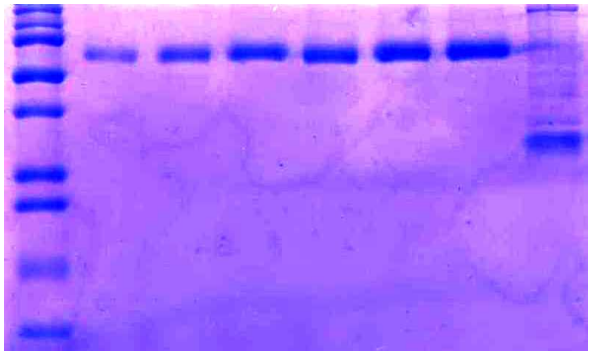


Figure S1. SDS gel with known BSA & hTK1

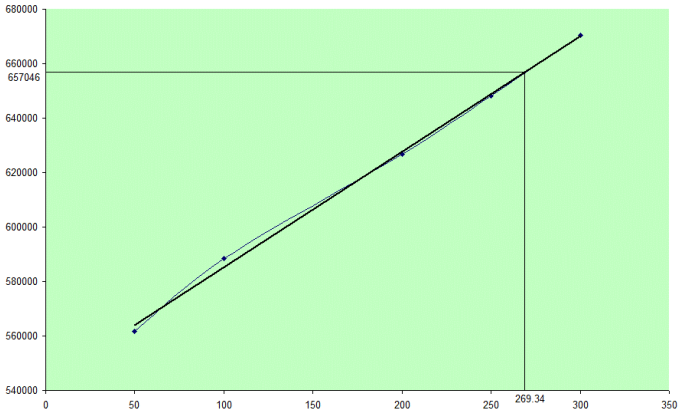


Figure S2. Standard curve for spot intensity of known conc. of BSA & hTK1

Table S2. Protein concentration calculation.

Protein type	Protein Conc. (µg/mL)	Integrated Density
BSA	50	561768
BSA	100	588345
BSA	200	626901
BSA	250	648071
BSA	300	670455
hTK1 (50 % solution in glycerol, v/v)	Unknown	657046

Equation: Y = 424.65X+542670
Conc. of hTK1/mL X = 269.34 µg/mL
(50% in Glycerol, v/v)

Conc. of hTK1 X = 538.68 µg/mL

4. LR-ESI-MS for hTK1 enzyme assay of 7f with ^{31}P-ATP

Thymidine monophosphate and **3-[2-(*closo*-1,7-Carboranyl)propylcarbamimidoyl]thymidine monophosphate (7f-MP).** LR-ESI-MS found: 323.1 $[M+H]^+$ and 549.3 $[M-PO_3H_2 + H]^+$, respectively.