Supporting Information for

Catalytic chemoselective *O*-phosphorylation of alcohols

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Materials and Methods

General

NMR spectra were recorded on JEOL ECX500 (500 MHz for ^{1}H NMR, 126 MHz for ^{13}C NMR), and JEOL ECS400 (400 MHz for ^{1}H NMR, 101 MHz for ^{13}C NMR and 162 MHz for ^{31}P NMR) spectrometers. Chemical shifts were reported in ppm on the δ scale relative to residual $CHD_2S(O)CD_3$ (δ = 2.50 for ^{1}H NMR and δ = 39.5 for ^{13}C NMR), HDO (δ = 4.79 for ^{1}H NMR), CHD_2OD (δ = 3.31 for ^{1}H NMR and δ = 49.0 for ^{13}C NMR), or CHD_2CN (δ = 1.94 for ^{1}H NMR and δ = 118.2 for ^{13}C NMR) as an internal reference, and 85% H_3PO_4 aq. (δ = 0 for ^{31}P NMR) as an external reference, respectively.

Preparative HPLC was conducted by using a JASCO HPLC system equipped with a UV-2075 spectrometer, PU-2086 pumps, a DG-2080-53 degasser, and an MX-2080-32 mixer. General eluent was linear gradient of MeCN in 0.1% TFA (LC-MS grade) aq. (2% acetonitrile for 3 min, followed by a linear gradient of 2–100% acetonitrile over 60 min. YMC-Triart C18, 254 nm), unless otherwise stated. C18 reverse phase column was used at 40 ºC, unless otherwise stated.

Analytical HPLC was conducted by using a JASCO HPLC system equipped with a UV-2075 spectrometer, PU-2080 pumps, a DG-2080-54 degasser, and an MX-2080-32 mixer. General eluent was linear gradient of MeCN in 0.1% TFA (LC-MS grade) aq. (2% acetonitrile for 3 min, followed by a linear gradient of 2–90% acetonitrile over 13 min. YMC-Triart C18, 230 nm), unless otherwise stated. C18 reverse phase column was used at 40 ºC, unless otherwise stated.

MQ means distilled water purified with a Millipore Milli-Q water purification system (Merck K. Ga. Co., Darmstadt, Germany).

LC-MS analysis was conducted by using an Agilent Technologies LC-MS (ESI) system equipped with a 1260 Infinity High Performance Degasser, an Agilent 1260 Infinity Binary Pump, a 1260 Infinity Standard Autosampler, a 1290 Infinity Thermostatted Column Compartment, a 1260 Infinity Variable Wavelength Detector, and an Agilent 6120 Single Quadrupole LC-MS or Shimadzu LCMS-2020. Retention times (Rt/min) were recorded using a gradient elution method of 2－90% B over 13 min, where solution A consisted of water (buffered with 0.1% HCO_2H) and solution B consisted of acetonitrile (LC-MS grade) unless otherwise stated. C18 reverse phase column (2.0 × 50 mm; YMC-Triart C18; YMC Co., Ltd.) was used at 40 ºC at a flow rate of 0.2 mL/min. The eluent was monitored by absorbance at 230 nm, unless otherwise stated.

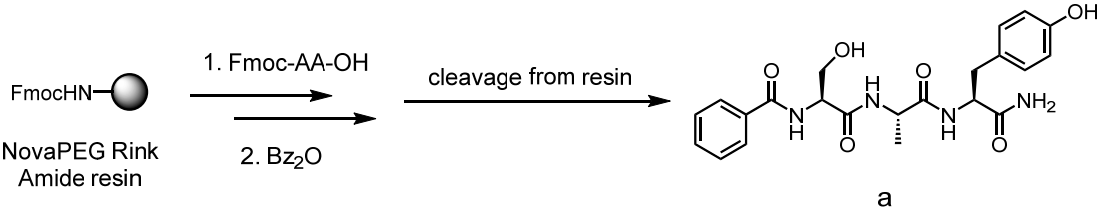
MALDI-TOF MS was obtained with a Shimadzu Biotech Axima ToF^2 spectrometer.

LC–MS/MS analyses were conducted using AB Sciex Triple TOF 4600 equipped with eksigent ekspert microLC 200. LC was carried out as follows: 3C18-CL-120 column (0.5 mm I.D × 100 mm) using a linear gradient of 2–35% acetonitrile with 0.1% formic acid (v/v) versus water with 0.1% formic acid (v/v) over 8 min at 40 °C with a flow rate of 20 μL/min.

Reactions were carried out in dry solvents under an argon atmosphere, unless otherwise stated. ^{34}S-Labeled H_2SO_4 was purchased from Shoko Science. Other reagents were used as received from commercial sources (Aldrich, TCI, or Wako), unless otherwise stated.

Synthesis of peptides

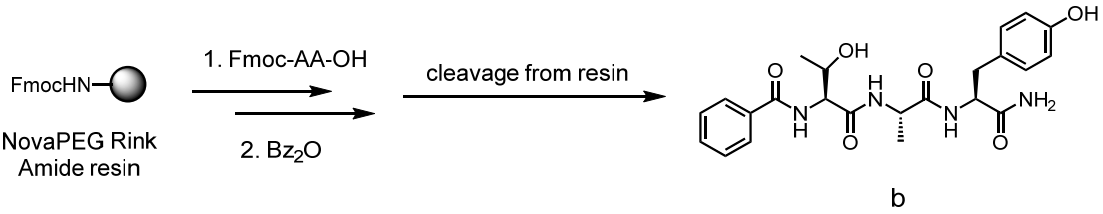
Bz-Ser-Ala-Tyr-NH_2 (a):



Peptide (**a**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **a**, which was purified with preparative HPLC to afford the target peptide (**a**, 23.8 mg, 0.0538 mmol, 27% yield) as white solids after lyophilization.

ESI-MS *m*/z 443.2 $[M+H]^+$, Retention time (LC/MS): 6.9 min.

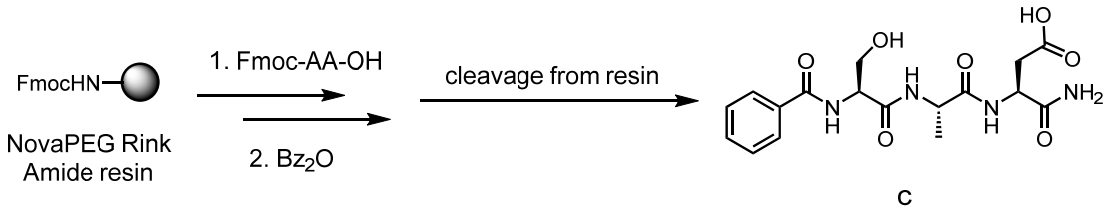
Bz-Thr-Ala-Tyr-NH_2 (b):



Peptide (**b**) was synthesized on a solid phase in 0.294 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **b**, which was purified with preparative HPLC to afford the target peptide (**b**, 20.9 mg, 0.0458 mmol, 16% yield) as white solids after lyophilization.

ESI-MS *m*/z 457.4 $[M+H]^+$, Retention time (LC/MS): 6.7 min.

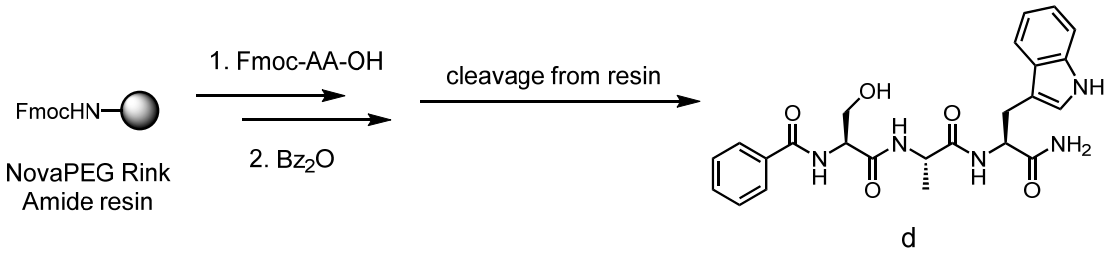
Bz-Ser-Ala-Asp-NH_2 (c):



Peptide (**c**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **c**, which was purified with preparative HPLC to afford the target peptide (**c**, 17.9 mg, 0.0454 mmol, 23% yield) as white solids after lyophilization.

ESI-MS *m*/z 395.2 $[M+H]^+$, Retention time (LC/MS): 5.8 min.

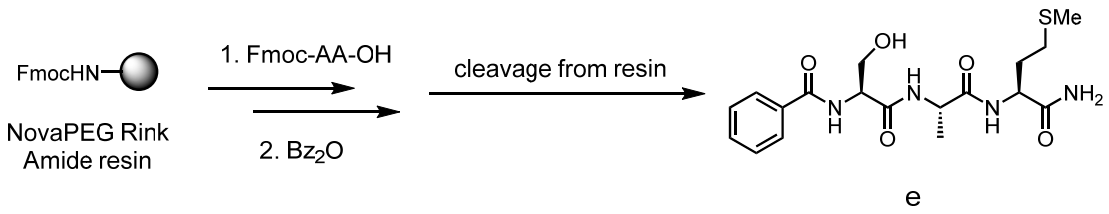
Bz-Ser-Ala-Trp-NH_2 (d):



Peptide (**d**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **d**, which was purified with preparative HPLC to afford the target peptide (**d**, 21.4 mg, 0.0460 mmol, 23% yield) as white solids after lyophilization.

ESI-MS *m*/z 466.2 $[M+H]^+$, Retention time (LC/MS): 6.9 min.

Bz-Ser-Ala-Met-NH_2 (e):

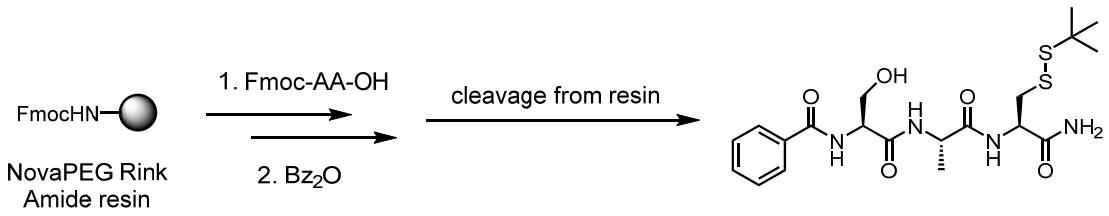


e

Peptide (**e**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **e**, which was purified with preparative HPLC to afford the target peptide (**e**, 28.0 mg, 0.0682 mmol, 35% yield) as white solids after lyophilization.

ESI-MS *m*/z 411.2 $[M+H]^+$, Retention time (LC/MS): 7.0 min.

Bz-Ser-Ala-Cys(*t*BuS)-NH_2 (g):

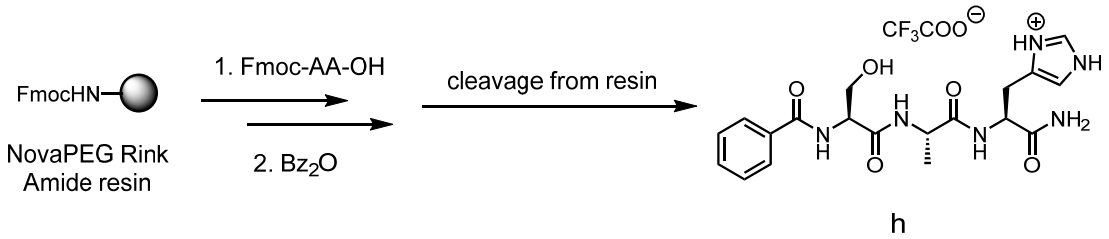


g

Peptide (**g**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **g**, which was purified with preparative HPLC to afford the target peptide (**g**, 24.5 mg, 0.0521 mmol, 27% yield) as white solids after lyophilization.

ESI-MS *m*/z 471.2 $[M+H]^+$, Retention time (LC/MS): 7.6 min.

Bz-Ser-Ala-His-NH_2 TFA salt (h):

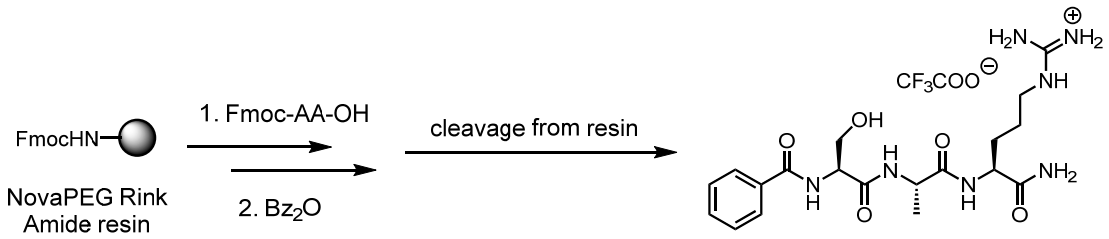


h

Peptide (**h**) was synthesized on a solid phase in 0.147 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **h**, which was purified with preparative HPLC to afford the target peptide (**h**, 18.7 mg, 0.0353 mmol, 24% yield) as white solids after lyophilization.

ESI-MS *m*/z 417.2 $[M+H]^+$, Retention time (LC/MS): 5.6 min.

Bz-Ser-Ala-Arg-NH_2 TFA salt (i):

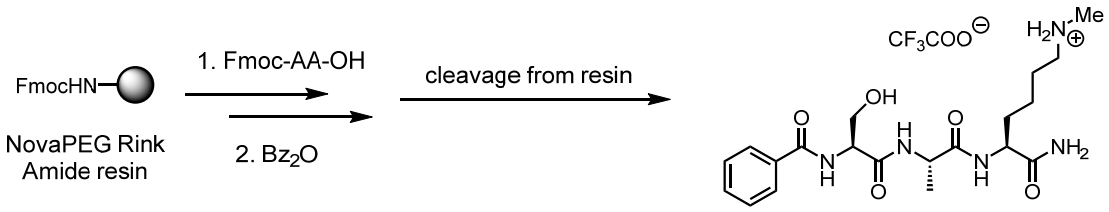


i

Peptide (**i**) was synthesized on a solid phase in 0.147 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **i**, which was purified with preparative HPLC to afford the target peptide (**i**, 14.3 mg, 0.0260 mmol, 18% yield) as white solids after lyophilization.

ESI-MS *m*/z 436.3 $[M+H]^+$, Retention time (LC/MS): 5.6 min.

Bz-Ser-Ala-Lys(Me)-NH_2 TFA salt (j):

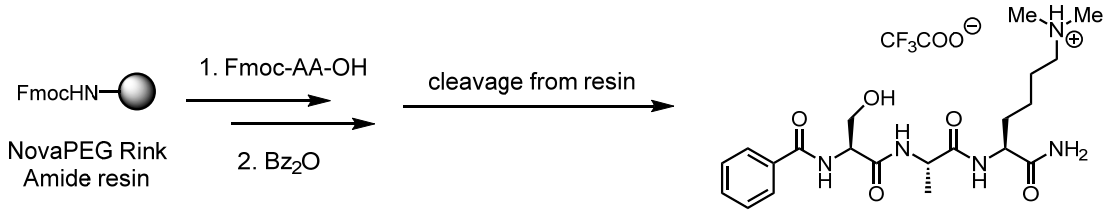


j

Peptide (**j**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **j**, which was purified with preparative HPLC to afford the target peptide (**j**, 12.0 mg, 0.0224 mmol, 11% yield) as white solids after lyophilization.

ESI-MS *m*/z 422.3 $[M+H]^+$, Retention time (LC/MS): 5.7 min.

Bz-Ser-Ala-Lys(Me)$_2$-NH_2 TFA salt (k):

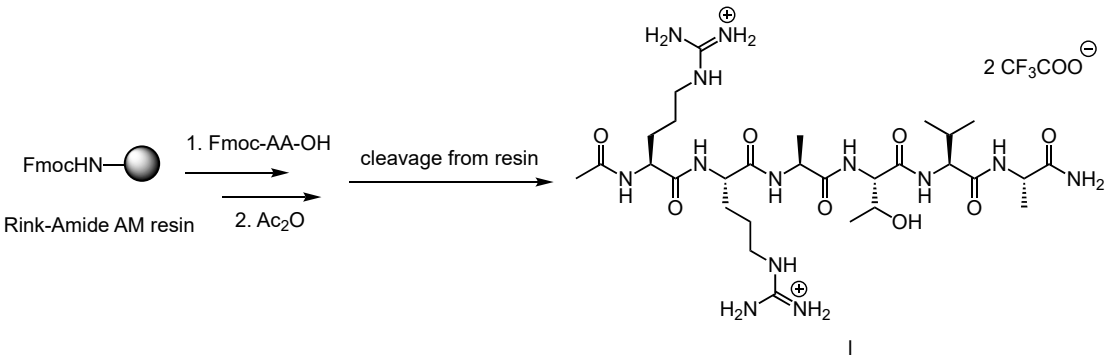


k

Peptide (**k**) was synthesized on a solid phase in 0.196 mmol scale using NovaPEG Rink Amide resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, benzoic anhydride (5.0 equiv.) in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **k**, which was purified with preparative HPLC to afford the target peptide (**k**, 23.5 mg, 0.0428 mmol, 22% yield) as white solids after lyophilization.

ESI-MS *m*/z 436.3 $[M+H]^+$, Retention time (LC/MS): 5.8 min.

Ac-Arg-Arg-Ala-Thr-Val-Ala-NH_2 TFA salt (l):

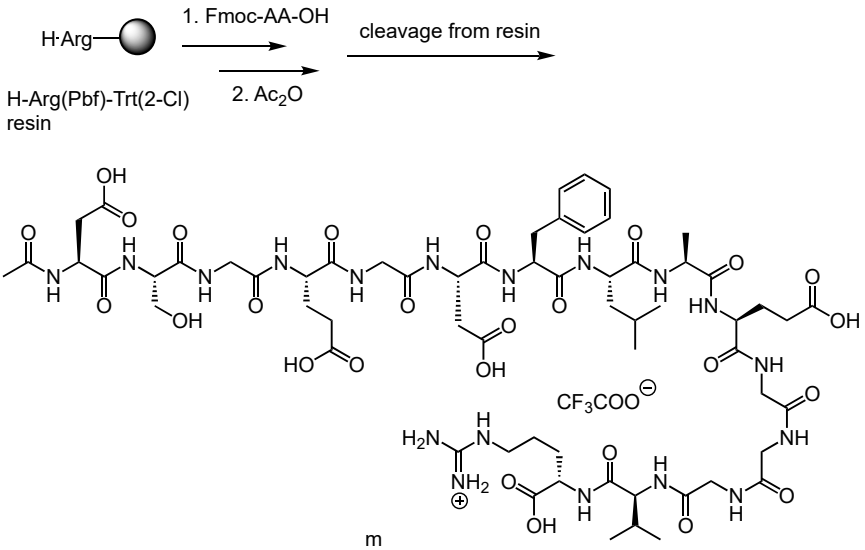


l

Peptide (**l**) was synthesized on a solid phase in 0.350 mmol scale using Rink Amide AM resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, 25% acetic anhydride in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under reduced pressure, and precipitated with ether to afford crude **l**, which was purified with preparative HPLC to afford the target peptide (**l**, 164.4 mg, 0.174 mmol, 50% yield) as white solids after lyophilization.

MALDI-TOF MS *m*/z 714.4 $[M+H]^+$, Retention time (Analytical HPLC): 8.9 min.

Ac-Asp-Ser-Gly-Glu-gly-Asp-Phe-Leu-Ala-Glu-Gly-Gly-Gly-Val-Arg-OH TFA salt (m):

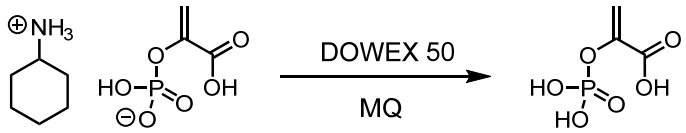


m

Peptide (**m**) was synthesized on a solid phase in 0.320 mmol scale using Rink Amide AM resin. Fmoc-amino acid (3.0 equiv.) was sequentially coupled using a DIEA-COMU method in DMF for 60 min (3.0 equiv. each) at r.t. after removal of each Fmoc group with 20% piperidine-DMF for 10 min. After the last removal of Fmoc group, 25% acetic anhydride in CH_2Cl_2 was added, and stirred for 10 min. The peptide was cleaved from the resin by treatment with TFA in the presence of TIPS and H_2O (95:2.5:2.5) for 90 min at r.t., concentrated under

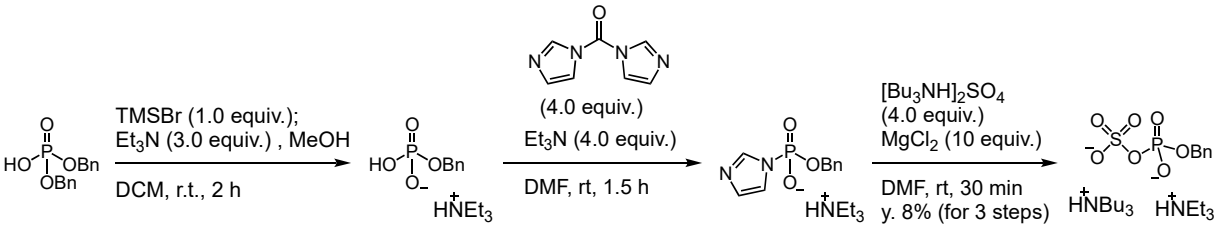
reduced pressure, and precipitated with ether to afford crude **m**, which was purified with preparative HPLC to afford the target peptide (**m**, 25.3 mg, 0.0144 mmol, 5% yield) as white solids after lyophilization.
MALDI-TOF MS *m*/z 1507.6 $[M+H]^+$, Retention time (Analytical HPLC): 10.7 min.

Preparation of PEP-H



To a stirred solution of phosphoenolpyruvic acid cyclohexylammonium salt (534.4 mg, 2.00 mmol) in MQ, ion-exchange resin (DOWEX 50WX2-200) was added. After the mixture was stirred at r.t. for 1 min, resin was removed by filtration and washed with MQ three times. The filtrate was lyophilized to afford **PEP-H** (296.8 mg, 1.77 mmol, 88% yield) as white solid. ^{1}H NMR (D_2O, 500 MHz) δ 5.76 (d, J = 2.3 Hz, 1H), 5.40 (d, J = 2.3 Hz, 1H)

Synthesis of *O*-benzyl phosphosulfate



Benzyl hydrogen phosphate triethylammonium salt (S1):

An argon-flushed flask equipped with a magnetic stirrer bar was charged with dibenzyl phosphate (1.39 g, 5.00 mmol) and CH_2Cl_2 (25.0 ml). To the reaction mixture, bromotrimethylsilane (638 μl, 5.00 mmol) was added dropwise at 0 °C, and the mixture was warmed to r.t.. After stirring for 2 h, Et_3N (2.12 ml, 15.0 mmol) and MeOH (5.0 ml) were added. The reaction mixture was concentrated under vacuum to give crude **S1**, which was separated by preparative HPLC (Eluent was linear gradient of MeCN in 50 mM triethylammonium acetate aq. and C18 reverse phase column was used at r.t..) to give **S1** (1.39 g) as white solid, which was used for the next reaction without further purification. ESI-MS *m/z* 187.0 $[M-H]^-$.

Benzyl (1*H*-imidazol-1-yl)phosphonate triethylammonium salt (S2):

To a stirred solution of **S1** (1.18 g) in DMF (11.8 ml), 1,1'-carbonyldiimidazole (1.52 g, 9.40 mmol) and Et_3N (1.32 ml, 9.65 mmol) were added at r.t.. After stirring for 2 h, MeOH (10.0 ml) was added to the reaction mixture. The reaction mixture was concentrated under vacuum to give crude **S2**, which was separated by preparative HPLC (Eluent was linear gradient of MeCN in 50 mM triethylammonium acetate aq. and C18 reverse phase column was used at r.t..) to give **S2** (560 mg) as colorless oil, which was used for the next reaction without

further purification. ESI-MS *m/z* 237.1 $[M–H]^–$.

***O*-Benzyl phosphosulfate (S3):**

To a stirred solution of **S2** (560 mg) in DMF (4.17 ml), $(Bu_3NH)_2SO_4$ (1.56 g, 3.33 mmol) and $MgCl_2$ (794 mg, 8.34 mmol) were added at r.t.. After stirring for 30 min, water (5.0 ml) was added to the reaction mixture, and the mixture was purified by preparative HPLC (Eluent was linear gradient of MeCN in 50 mM triethylammonium acetate aq. and C18 reverse phase column was used at r.t..) to give *O*-benzyl phosphosulfate (**S3**, 215 mg, 0.388 mmol, 8% yield for 3 steps) as colorless oil. ^{1}H NMR (CD_3CN, 500 MHz) δ 7.40 (d, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 2H), 4.95 (d, *J* = 6.9 Hz, 2H), 3.05 (q, *J* = 7.4 Hz, 6H), 2.96 (t, *J* = 8.6 Hz, 2H), 1.64 (m, 6H) 1.31 (q, *J* = 7.4 Hz, 6H), 1.21 (t, *J* = 7.4 Hz, 9H), 0.91 (t, *J* = 7.4 Hz, 9H); ^{13}C NMR (CD_3CN, 126 MHz) δ 174.4, 139.8, 129.1, 128.3, 128.3, 68.2, 52.6, 46.5, 25.7, 21.9, 20.6, 13.9, 8.8; ^{31}P NMR (CD_3OD, 162 MHz) δ –40.7; ESI-MS *m/z* 267.0 $[M–H]^–$; HRMS calcd for $[C_7H_8O_7PS]^–$ requires *m/z* 266.9734; found 266.9734.

Synthesis of ^{34}S-labeled tetrabutylammonium hydrogen sulfate (^{34}S-TBAHS)

To a stirred solution of ^{34}S-sufluric acid aq. (2.6%, 1.20 mL, 312 μmol), tetrabutylammonium hydroxide aq. (40%, 202 μL, 312 μmol) was added at 4 °C, and the mixture was stirred for 1 h at the same temperature. Lyophilization of the mixture afforded ^{34}S-TBAHS (106 mg, 312 μmol, y. quant.) as white solids.

General procedures for catalytic phosphorylation of alcohols

Procedure S (Standard)

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (0.30 equiv.) and phosphoenolpyruvate monopotassium salt (4.5 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.20 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 6 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Procedure A

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (0.60 equiv.) and phosphoenolpyruvate monopotassium salt (6.0 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.20 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 6 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Procedure B

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (0.60 equiv.) and phosphoenolpyruvate monopotassium salt (6.0 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.20 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 3 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Procedure C

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (0.60 equiv.) and phosphoenolpyruvate monopotassium salt (10 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.20 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 4.5 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Procedure D

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (0.60 equiv.) and phosphoenolpyruvate monopotassium salt (10 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.20 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 3 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Procedure E

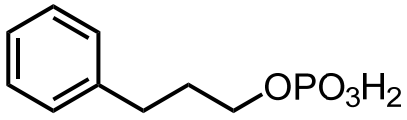
An argon-flushed test tube equipped with a magnetic stirrer bar was charged with substrate (1.0 equiv.), tetrabutylammonium hydrogen sulfate (2.0 equiv.) and phosphoenolpyruvate monopotassium salt (50 equiv.). To the reaction mixture, *N*,*N*-dimethylformamide (0.0125 M) was added at r.t., and the mixture was warmed to 100 °C. After stirring for 3 h, the reaction mixture was cooled to r.t. and purified by preparative HPLC to give the corresponding phosphorylated product.

Reaction of POS (42) with 3-phenyl-1-propanol with varied amount of PEP-K

An argon-flushed test tube equipped with a magnetic stirrer bar was charged with *O*-benzyl phosphosulfate (**S3**, 1.0 equiv.), Pd/C (30 wt%) and DMF (0.20 M). Hydrogen gas was, then, flushed, and the reaction mixture was stirred at r.t. for 30 min. The obtained crude solution of POS **42** was immediately used for the next reaction without further purification. To a stirred solution of the crude POS **42** in DMF (0.2 M) at r.t., 3-phenyl-1-propanol (1.0 equiv.) and PEP-K (0-4.5 equiv.) were added. The reaction mixture was stirred for 3 h at 100 °C, diluted with water/MeCN, and purified by preparative HPLC to give the corresponding phosphorylated (or sulfurylated) product.

Characterization of phosphorylated products

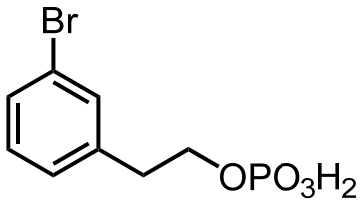
3-Phenylpropyl dihydrogen phosphate (2):



General procedure S (15.5 mg, 0.0717 mmol, 72% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.25 (t, *J* = 7.4 Hz, 2H), 7.20 (d, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.4 Hz, 1H), 3.97 (q, *J* = 6.3 Hz, 2H), 2.71 (t, *J* = 7.4 Hz, 2H), 1.95 (tt, *J* = 6.3 Hz, 7.4 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 142.7, 129.5, 129.4, 127.0, 66.9 (d, *J* = 4.8 Hz), 33.4 (d, *J* = 7.2 Hz), 32.7; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.2; ESI-MS *m/z* 215.1 $[M–H]^–$; HRMS calcd for $[C_9H_{12}O_4P]^–$ requires *m/z* 215.0473; found 215.0474.

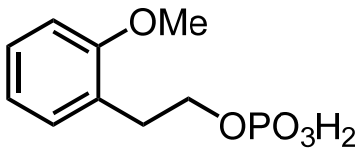
3-Bromophenethyl dihydrogen phosphate (3):



General procedure S (24.0 mg, 0.0853 mmol, 85% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.45 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.25-7.16 (m, 2H), 4.15 (q, *J* = 6.9 Hz, 2H), 2.95 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 142.1, 133.0, 131.4, 130.6, 128.9, 123.2, 67.8 (d, *J* = 5.7 Hz), 37.2 (d, *J* = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.0; ESI-MS *m/z* 279.0 $[M–H]^–$; HRMS calcd for $[C_8H_9BrO_4P]^–$ requires *m/z* 278.9422; found 278.9424.

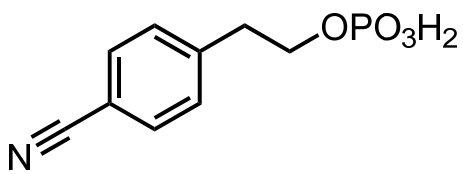
2-Methoxyphenethyl dihydrogen phosphate (4):



General procedure S (20.8 mg, 0.0897mmol, 90% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.21-7.14 (m, 2H), 6.92 (d, *J* = 7.7 Hz, 1H), 6.85 (dd, *J* = 6.3 Hz, 7.7 Hz, 1H), 4.10 (q, *J* = 7.4 Hz, 2H), 3.81 (s, 3H), 2.97 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 159.3, 131.9, 129.1, 126.4, 121.5, 111.4, 67.0 (d, *J* = 5.7 Hz), 55.8, 32.7 (d, *J* = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.1; ESI-MS *m/z* 231.1 $[M–H]^–$; HRMS calcd for $[C_9H_{12}O_5P]^–$ requires *m/z* 231.0422; found 231.0423.

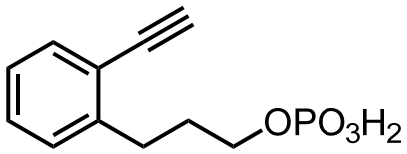
4-Cyanophenethyl dihydrogen phosphate (5):



General procedure S (17.4 mg, 0.0765mmol, 77% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 8.3 Hz, 2H), 4.19 (q, *J* = 6.9 Hz, 2H), 3.05 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 145.8, 133.3, 131.3, 120.0, 111.3, 67.4 (d, *J* = 5.7 Hz), 37.7 (d, *J* = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.2; ESI-MS *m/z* 226.1 $[M–H]^–$; HRMS calcd for $[C_9H_9NO_4P]^–$ requires *m/z* 226.0269; found 226.0277.

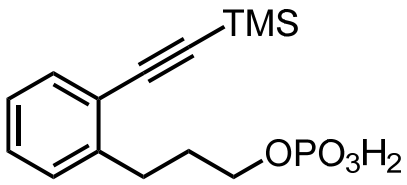
3-(2-Ethynylphenyl)propyl dihydrogen phosphate (6):



General procedure S (19.4 mg, 0.0806 mmol, 81% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.43 (d, *J* = 8.0 Hz, 1H), 7.27 (dt, *J* = 8.0 Hz, 1.7 Hz, 2H), 7.16 (dt, *J* = 8.0 Hz, 1.7 Hz, 1H), 3.98 (q, *J* = 6.7 Hz, 2H), 3.67 (s, 1H), 2.90 (t, *J* = 8.0 Hz, 2H), 1.99 (tt, *J* = 6.7 Hz, 8.0 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 145.3, 133.9, 130.2, 130.0, 127.2, 123.0, 82.9, 82.6, 67.1 (d, *J* = 5.7 Hz), 32.3 (d, *J* = 7.7 Hz), 31.5; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.2; ESI-MS *m/z* 239.1 $[M-H]^-$; HRMS calcd for $[C_{11}H_{12}O_4P]^-$ requires *m/z* 239.0473; found 239.0474.

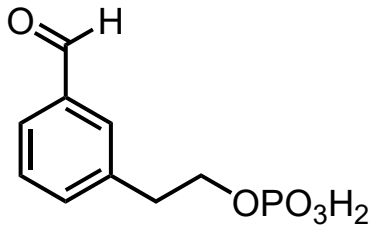
3-(2-((Trimethylsilyl)ethynyl)phenyl)propyl dihydrogen phosphate (7):



General procedure S (24.1 mg, 0.0772 mmol, 77% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.14 (d, *J* = 7.4 Hz, 1H), 7.04-6.99 (m, 2H), 6.91 (dt, *J* = 6.3 Hz, 2.3 Hz, 1H), 3.74 (q, *J* = 6.6 Hz, 2H), 2.63 (t, *J* = 7.7 Hz, 2H), 1.75 (tt, *J* = 6.6 Hz, 7.7 Hz, 2H), 0.00 (s, 9H); ^{13}C NMR (CD_3OD, 126 MHz) δ 145.1, 133.4, 130.2, 129.9, 127.2, 123.7, 104.8, 98.7, 67.1 (d, *J* = 5.8 Hz), 32.2 (d, *J* = 7.7 Hz), 31.7, 0.0; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.2; ESI-MS *m/z* 311.1 $[M-H]^-$; HRMS calcd for $[C_{14}H_{20}O_4PSi]^-$ requires *m/z* 311.0868; found 311.0871.

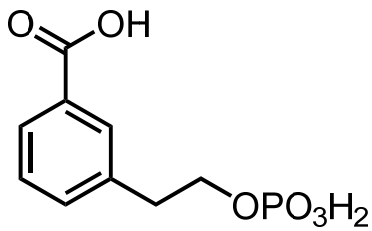
3-Formylphenethyl dihydrogen phosphate (8):



General procedure S (23.1 mg, 0.1004 mmol, 73% yield)

^{1}H NMR (CD_3CN, 500 MHz) δ 9.95 (s, 1H), 7.76 (s, 1H), 7.74 (d, *J* = 7.4 Hz, 1H), 7.55 (d, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 4.20 (q, *J* = 6.9 Hz, 2H), 3.03 (t, *J* = 6.3 Hz, 2H); ^{13}C NMR (CD_3CN, 126 MHz) δ 193.7, 140.1, 137.7, 136.1, 130.8, 130.1, 128.9, 67.9 (d, *J* = 4.8 Hz), 36.6 (d, *J* = 7.2 Hz); ^{31}P NMR (CD_3CN, 162 MHz) δ 1.8; ESI-MS *m/z* 229.1 $[M-H]^-$; HRMS calcd for $[C_9H_{10}O_5P]^-$ requires *m/z* 229.0266; found 229.0265.

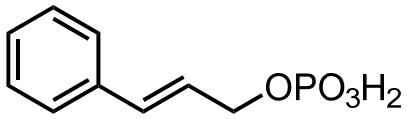
3-(2-(Phosphonooxy)ethyl)benzoic acid (9):



General procedure S (17.5 mg, 0.0710 mmol, 71% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.93 (s, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 4.18 (q, *J* = 6.9 Hz, 2H), 3.04 (t, *J* = 6.9 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 169.9, 139.8, 134.8, 132.1, 131.3, 129.6, 129.0, 68.0 (d, *J* = 5.8 Hz), 37.5 (d, *J* = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.0; ESI-MS *m/z* 245.1 $[M-H]^-$; HRMS calcd for $[C_9H_{10}O_6P]^-$ requires *m/z* 245.0215; found 245.0216.

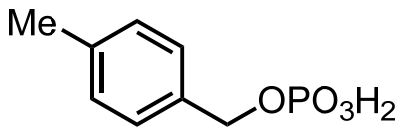
Cinnamyl dihydrogen phosphate (10):



General procedure S (16.6 mg, 0.0777 mmol, 78% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.41 (d, *J* = 8.3 Hz, 2H), 7.31 (dd, *J* = 8.3 Hz, 7.4 Hz, 2H), 7.24 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 16.0 Hz, 1H), 6.36 (dt, *J* = 16.0 Hz, 6.3 Hz, 1H), 4.62 (dd, *J* = 6.3 Hz, 8.0 Hz, 1H); ^{13}C NMR (CD_3OD, 126 MHz) δ 137.7, 133.9, 129.6, 129.0, 127.6, 125.5 (d, *J* = 7.2 Hz), 68.1 (d, *J* = 6.0 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.1; ESI-MS *m/z* 213.1 $[M–H]^–$; HRMS calcd for $[C_9H_{10}O_4P]^–$ requires *m/z* 213.0317; found 213.0316.

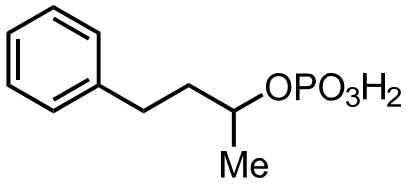
4-Methylbenzyl dihydrogen phosphate (11):



General procedure S (14.1 mg, 0.0698 mmol, 70% yield)

^{1}H NMR (CD_3CN, 500 MHz) δ 7.26 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 4.95 (d, *J* = 6.9 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (CD_3OD, 126 MHz) δ 139.1, 135.2, 130.1, 128.8, 69.1 (d, *J* = 6.0 Hz), 21.2; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.9; ESI-MS *m/z* 201.1 $[M–H]^–$; HRMS calcd for $[C_8H_{10}O_4P]^–$ requires *m/z* 201.0317; found 201.0317.

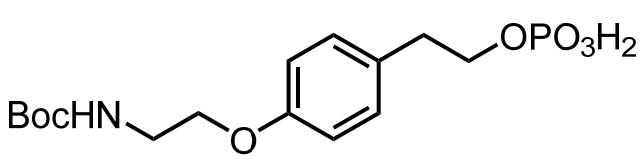
4-Phenylbutan-2-yl dihydrogen phosphate (12):



General procedure S (16.4 mg, 0.0712 mmol, 71% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.27-7.10 (m, 5H), 4.44-4.34 (m, 1H), 2.78-2.60 (m, 2H), 1.96-1.76 (m, 2H), 1.34 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (CD_3CN, 101 MHz) δ 142.8, 139.3, 129.2, 126.7, 75.9 (d, *J* = 5.7 Hz), 39.9 (d, *J* = 4.7 Hz), 32.0, 21.7; ^{31}P NMR (CD_3OD, 162 MHz) δ –0.5; ESI-MS *m/z* 229.1 $[M–H]^–$; HRMS calcd for $[C_{10}H_{14}O_4P]^–$ requires *m/z* 229.0630; found 229.0631.

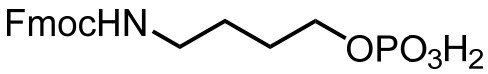
***tert*-Butyl (2-(4-(3-(phosphonooxy)propyl)phenoxy)ethyl)carbamate (13):**



General procedure S (26.1 mg, 0.0723 mmol, 72% yield)

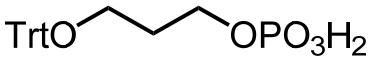
^{1}H NMR (CD_3OD, 400 MHz) δ 7.16 (d, *J* = 9.2 Hz, 2H), 6.86 (d, *J* = 9.2 Hz, 2H), 4.09 (q, *J* = 7.3 Hz, 2H), 3.96 (t, *J* = 5.8 Hz, 2H), 3.40 (t, *J* = 5.8 Hz, 2H), 2.90 (t, *J* = 7.3 Hz, 2H), 1.43 (s, 9H); ^{13}C NMR (CD_3OD, 101 MHz) δ 158.9, 158.6, 131.3, 131.1, 115.6, 80.4, 68.5 (d, *J* = 5.8 Hz), 67.9, 41.0, 36.9 (d, *J* = 7.7 Hz), 28.7; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.0; ESI-MS *m/z* 360.1 $[M–H]^–$; HRMS calcd for $[C_{15}H_{23}NO_7P]^–$ requires *m/z* 360.12121; found 360.1214.

(9*H*-Fluoren-9-yl)methyl (4-(phosphonooxy)butyl)carbamate (14):



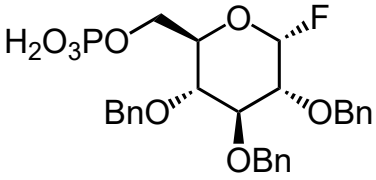
General procedure S (29.1 mg, 0.0745 mmol, 74% yield) ^{1}H NMR (CD_3OD, 500 MHz) δ 7.76 (d, *J* = 7.4 Hz, 2H), 7.61 (d, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 2H), 4.33 (d, *J* = 6.3 Hz, 2H), 4.15 (t, *J* = 6.3 Hz, 1H), 3.96 (q, *J* = 6.3 Hz, 2H), 3.10 (t, *J* = 6.3 Hz, 2H), 1.66-1.50 (m, 4H); ^{13}C NMR (CD_3OD, 126 MHz) δ 158.9, 145.3, 142.6, 128.8, 128.1, 126.1, 120.9, 67.5, 67.3 (d, *J* = 5.8 Hz), 59.4, 41.8, 41.2, 28.7 (d, *J* = 5.8 Hz), 20.1; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.4; ESI-MS *m/z* 390.1 $[M-H]^-$; HRMS calcd for $[C_{19}H_{21}NO_6P]^-$ requires *m/z* 390.1106; found 390.1107.

3-(Trityloxy)propyl dihydrogen phosphate (15):



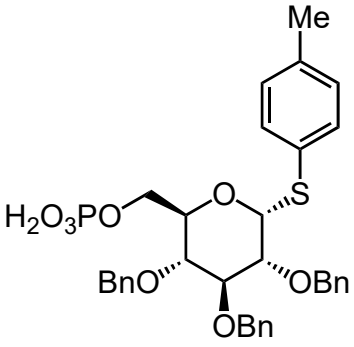
General procedure S (19.6 mg, 0.0492 mmol, 49% yield) ^{1}H NMR (CD_3OD, 500 MHz) δ 7.30-7.18 (m, 15H), 4.07 (q, *J* = 6.9 Hz, 2H), 3.67 (t, *J* = 6.3 Hz, 2H), 1.86 (m, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 148.8, 129.3, 128.6, 128.0, 83.0, 64.6 (d, *J* = 5.7 Hz), 59.1, 34.3 (d, *J* = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.3; ESI-MS *m/z* 397.0 $[M-H]^-$; HRMS calcd for $[C_{22}H_{22}O_5P]^-$ requires *m/z* 397.1205; found 397.1215.

((2*R*,3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-fluorotetrahydro-2*H*-pyran-2-yl)methyl dihydrogen phosphate (16):



General procedure A (19.1 mg, 0.0359 mmol, 72% yield) ^{1}H NMR (CD_3CN, 400 MHz) δ 7.36-7.25 (m, 15H), 5.72 (dd, *J* = 54.5 Hz, 2.3 Hz, 1H), 4.90-4.60 (m, 6H), 4.20-4.11 (m, 2H), 3.90-3.80 (m, 2H), 3.60-3.48 (m, 2H); ^{13}C NMR (CD_3CN, 101 MHz) δ 139.6, 139.1, 139.0, 129.3, 129.2, 129.2, 129.0, 128.8, 128.8, 128.7, 128.6, 128.4, 106.2 (d, *J* = 232.2 Hz), 81.6, 80.3, 80.0, 76.9, 76.0, 75.7, 73.7, 65.8 (d, *J* = 3.9 Hz); ^{31}P NMR (CD_3CN, 162 MHz) δ 0.8; HRMS calcd for $[C_{27}H_{29}FO_8P]^-$ requires *m/z* 531.1584; found 531.1582.

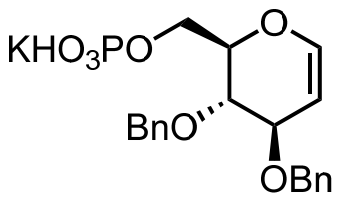
((2*R*,3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-(*p*-tolylthio)tetrahydro-2*H*-pyran-2-yl)methyl dihydrogen phosphate (17):



General procedure A (49.6 mg, 0.0779 mmol, 78% yield) ^{1}H NMR (CD_3CN, 500 MHz) δ 7.43 (d, *J* = 8.0 Hz, 2H), 7.36-7.22 (m, 15H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.85-4.57 (m, 7H), 4.23-4.10 (m, 2H), 3.67 (t, *J* = 8.6 Hz, 1H) , 3.50-3.47 (m, 1H), 3.39 (t, *J* = 9.2 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (CD_3CN, 126 MHz) δ 139.5, 139.3, 139.1, 138.6, 132.5, 131.1, 130.7, 129.2, 129.2, 129.1, 129.0, 128.9, 128.6, 128.5, 128.5, 128.4, 88.2, 86.8, 81.5, 78.1 (d, *J* = 8.4 Hz), 77.9, 76.0, 75.6, 75.4, 66.3 (d, *J* = 4.8 Hz), 21.0; ^{31}P

NMR (CD_3CN, 162 MHz) δ 0.8; HRMS calcd for $[C_{34}H_{36}O_8PS]^-$ requires *m*/*z* 635.1869; found 635.1864.

((2*R*,3*S*,4*R*)-3,4-Bis(benzyloxy)-3,4-dihydro-2*H*-pyran-2-yl)methyl dihydrogen phosphate (18):

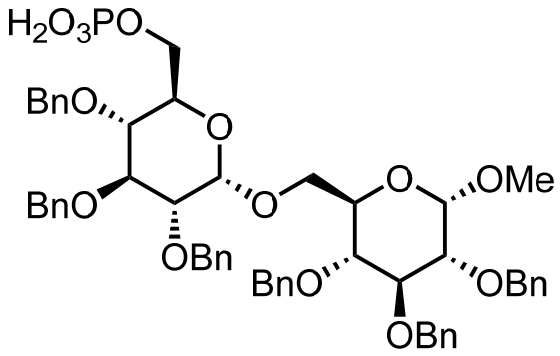


General procedure B (20.8 mg, 0.0468 mmol, 47% yield)

When purified this compound, eluent was linear gradient of MeCN in water without TFA.

^{1}H NMR (CD_3OD, 500 MHz) δ 7.40-7.22 (m, 10H), 6.38 (d, *J* = 5.7 Hz, 1H), 4.83-4.70 (m, 3H), 4.64-4.52 (m, 2H), 4.19 (t, *J* = 5.2 Hz, 2H), 4.15-4.10 (m, 1H), 4.07 (m, 1H), 3.88 (dd, *J* = 8.0 Hz, 6.3 Hz, 1H); ^{13}C NMR (CD_3OD, 126 MHz) δ 145.6, 139.9, 129.4, 129.4, 129.3, 129.2, 129.0, 128.6, 125.3, 100.9, 78.0 (d, *J* = 8.4 Hz), 76.4, 75.6, 74.7, 71.3, 64.6 (d, *J* = 6.0 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.9; ESI-MS *m*/*z* 405.1 $[M–H]^–$; HRMS calcd for $[C_{20}H_{22}O_7P]^-$ requires *m*/*z* 405.1103; found 405.1104.

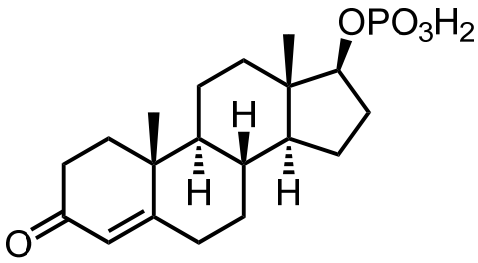
((2*R*,3*R*,4*S*,5*R*,6*S*)-3,4,5-Tris(benzyloxy)-6-(((2*R*,3*R*,4*S*,5*R*,6*S*)-3,4,5-tris(benzyloxy)-6-methoxytetrahydro-2*H*-pyran-2-yl)methoxy)tetrahydro-2*H*-pyran-2-yl)methyl dihydrogen phosphate (19):



General procedure A (38.0 mg, 0.0389 mmol, 78% yield)

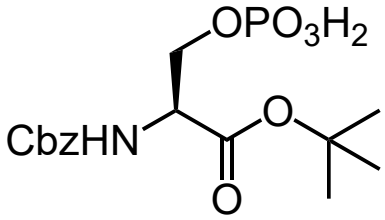
^{1}H NMR (CD_3CN, 400 MHz) δ 7.36-7.16 (m, 30H), 5.07 (d, *J* = 3.2 Hz, 1H), 4.89-4.50 (m, 13H), 4.20-4.00 (m, 2H), 3.90-3.60 (m, 8H), 3.50-3.44 (m, 1H) 3.34 (dd, *J* = 9.6 Hz, 3.7 Hz, 1H), 3.29 (s, 3H); ^{13}C NMR (CD_3CN, 101 MHz) δ 140.0, 139.8, 139.6, 139.5, 139.5, 139.4, 129.2, 129.2, 129.1, 129.1, 129.1, 128.8, 128.8, 128.7, 128.6, 128.6, 128.6, 128.5, 128.4, 128.4, 128.4, 128.3, 128.3, 128.2, 98.4, 97.5, 82.4, 81.7, 81.1, 81.0, 78.4, 77.9, 75.6 (d, *J* = 5.8 Hz), 75.4, 75.3, 73.0, 72.7, 71.0, 70.5, 70.4, 66.7, 66.2 (d, *J* = 5.8 Hz), 55.3; ^{31}P NMR (CD_3CN, 162 MHz) δ 0.9; HRMS calcd for $[C_{55}H_{60}O_{14}P]^-$ requires *m*/*z* 975.3721; found 975.3689.

(8*R*,9*S*,10*R*,13*S*,14*S*,17*S*)-10,13-Dimethyl-3-oxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-17-yl dihydrogen phosphate (20):



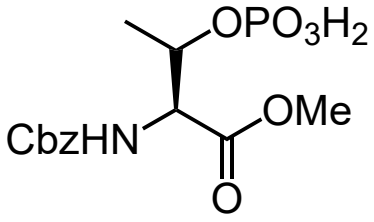
General procedure A (24.3 mg, 0.0660 mmol, 66% yield)
^{1}H NMR (CD_3OD, 500 MHz) δ 5.70 (s, 1H), 4.13 (q, *J* = 8.0 Hz, 1H), 2.53-2.43 (m, 2H), 2.33-2.25 (m, 2H), 2.19-2.10 (m, 1H), 2.08 (dq, *J* = 13.7 Hz, 2.9 Hz, 1H), 1.95 (dt, *J* = 13.2 Hz, 3.4 Hz, 1H), 1.92-1.85 (m, 1H), 1.76-1.59 (m, 5H), 1.48 (dq, *J* = 12.6 Hz, 3.4 Hz, 1H), 1.45-1.34 (m, 1H), 1.24 (s, 3H), 1.17 (dt, *J* = 13.2 Hz, 4.0 Hz, 1H), 1.08-0.94 (m, 3H), 0.87 (s, 3H); ^{13}C NMR (CD_3OD, 126 MHz) δ 202.6, 175.4, 124.1, 86.3, 55.3, 51.1, 44.0, 44.0, 40.0, 37.5, 36.7 (d, *J* = 3.6 Hz), 34.7, 33.8, 32.7, 29.6, 24.2, 21.6, 17.7, 11.9; ^{31}P NMR (CD_3OD, 162 MHz) δ –0.1; ESI-MS *m/z* 367.2 $[M–H]^–$; HRMS calcd for $[C_{19}H_{28}O_5P]^–$ requires *m/z* 367.1674; found 367.1680.

***tert*-Butyl *N*-((benzyloxy)carbonyl)-*O*-phosphono-*L*-serinate (21):**



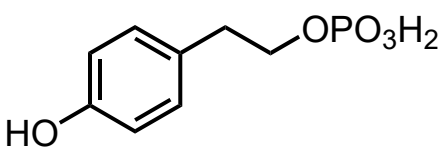
General procedure S (29.1 mg, 0.0775 mmol, 77% yield)
^{1}H NMR (CD_3OD, 500 MHz) δ 7.38-7.26 (m, 5H), 5.10 (s, 2H), 4.38-4.34 (m, 1H), 4.30-4.18 (m, 2H), 1.46 (s, 9H); ^{13}C NMR (CD_3OD, 126 MHz) δ 169.9, 158.4, 138.1, 129.5, 129.0, 128.9, 83.6, 67.8, 67.3 (d, *J* = 5.8 Hz), 56.6 (d, *J* = 9.7 Hz), 28.2; ^{31}P NMR (CD_3OD, 162 MHz) δ –0.2; ESI-MS *m/z* 374.2 $[M–H]^–$; HRMS calcd for $[C_{15}H_{21}NO_8P]^–$ requires *m/z* 374.1005; found 374.1003.

Methyl *N*-((benzyloxy)carbonyl)-*O*-phosphono-*L*-allothreoninate (22):



General procedure A (27.0 mg, 0.0778mmol, 78% yield)
^{1}H NMR (CD_3CN, 400 MHz) δ 7.40-7.25 (m, 5H), 6.25-6.05 (brs, 1H), 5.09 (s, 2H), 4.90-4.77 (brs, 1H), 4.42-4.30 (brs, 1H), 3.74 (s, 3H), 1.36 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (CD_3OD, 126 MHz) δ 171.7, 159.1, 138.1, 129.5, 129.1, 128.8, 75.0 (d, *J* = 3.9 Hz), 67.9, 60.1 (d, *J* = 7.7 Hz), 53.0, 18.8; ^{31}P NMR (CD_3OD, 162 MHz) δ –1.0; ESI-MS *m/z* 346.1 $[M–H]^–$; HRMS calcd for $[C_{13}H_{17}NO_8P]^–$ requires *m/z* 346.0692; found 346.0692.

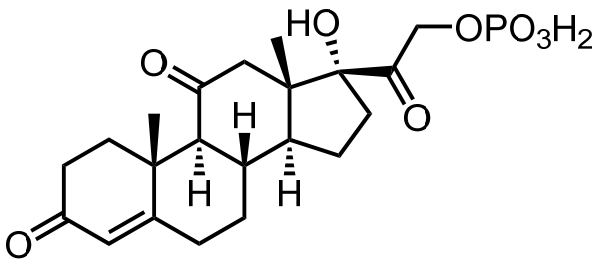
4-Hydroxyphenethyl dihydrogen phosphate (25):



General procedure A (12.9 mg, 0.0595 mmol, 60% yield)
^{1}H NMR (CD_3OD, 500 MHz) δ 7.06 (d, *J* = 8.6 Hz, 2H), 6.70 (d, *J* = 8.6 Hz, 1H), 4.07 (q, *J* = 7.4 Hz, 2H), 2.86 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (CD_3OD, 126 MHz) δ 157.1, 131.0, 129.7, 116.2, 68.7 (d, *J* =

5.8 Hz), 37.0 (d, J = 7.7 Hz); ^{31}P NMR (CD_3OD, 162 MHz) δ 1.1; ^{1}H-coupled ^{31}P NMR (DMSO-d_6, 162 MHz) δ –1.0 (t, J = 7.5 Hz); ESI-MS *m/z* 217.1 $[M–H]^–$; HRMS calcd for $[C_8H_{10}O_5P]^–$ requires *m/z* 217.0266; found 217.0265.

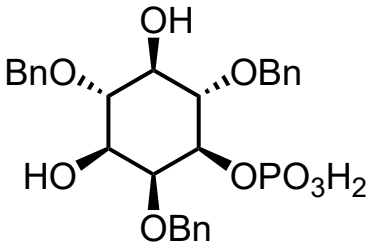
2-((8*S*,9*S*,10*R*,13*S*,14*S*,17*R*)-17-Hydroxy-10,13-dimethyl-3,11-dioxo-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-17-yl)-2-oxoethyl dihydrogen phosphate (26):



General procedure C (19.3 mg, 0.0439 mmol, 88% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 5.71 (s, 1H), 4.99 (dd, J = 18.3 Hz, 10.3 Hz, 1H), 4.69 (dd, J = 18.3 Hz, 8.0 Hz, 1H), 2.97 (d, J = 12.6 Hz, 1H), 2.75-2.67 (m, 2H), 2.57-2.41 (m, 3H), 2.36-2.29 (m, 1H), 2.23 (dt, J = 16.6 Hz, 3.4 Hz, 1H), 2.11 (dd, J = 12.6 Hz, 6.9 Hz, 2H), 2.06-1.85 (m, 4H), 1.46 (m, 2H), 1.42 (s, 3H), 1.32 (m, 1H), 0.62 (s, 3H); ^{13}C NMR (CD_3OD, 126 MHz) δ 212.2, 207.4 (d, J = 6.0 Hz), 202.7, 173.1, 124.7, 89.6, 70.8 (d, J = 4.8 Hz), 63.4, 52.4, 51.3, 50.9, 39.6, 37.8, 35.6, 35.2, 34.4, 33.5, 33.4, 24.0, 17.6, 16.0; ^{31}P NMR (CD_3OD, 162 MHz) δ 0.2; ESI-MS *m/z* 439.1 $[M–H]^–$; HRMS calcd for $[C_{21}H_{28}O_8P]^–$ requires *m/z* 439.1527; found 439.1523.

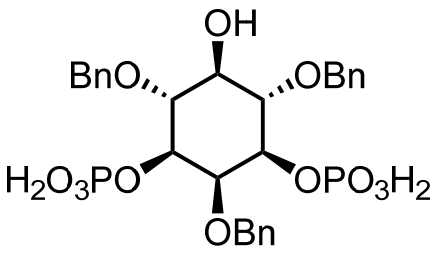
2,4,6-Tris(benzyloxy)-3,5-dihydroxycyclohexyl dihydrogen phosphate (27, rac):



General procedure A (24.3 mg, 0.0458 mmol, 46% yield)

^{1}H NMR (CD_3OD, 400 MHz) δ 7.51-7.20 (m, 15H), 4.90-4.73 (m, 6H), 4.25-4.22 (m, 2H), 3.84 (t, J = 9.6 Hz, 1H), 3.67 (t, J = 10.1 Hz, 1H), 3.59 (dd, J = 10.1 Hz, 2.7 Hz, 1H), 3.49 (t, J = 9.2 Hz, 1H); ^{13}C NMR (CD_3OD, 126 MHz) δ 140.5, 140.5, 140.2, 129.6, 129.2, 129.2, 129.1, 129.1, 129.0, 128.9, 128.5, 128.4, 83.3, 81.8 (d, J = 3.6 Hz), 81.7, 79.4, 79.3, 76.7, 76.1 (d, J = 7.2 Hz), 76.1 (d, J = 6.0 Hz), 72.9; ^{31}P NMR (CD_3OD, 162 MHz) δ –0.8; ESI-MS *m/z* 529.2 $[M–H]^–$; HRMS calcd for $[C_{27}H_{30}O_9P]^–$ requires *m/z* 529.1633; found 529.1623.

2,4,6-Tris(benzyloxy)-5-hydroxycyclohexane-1,3-diyl bis(dihydrogen phosphate)

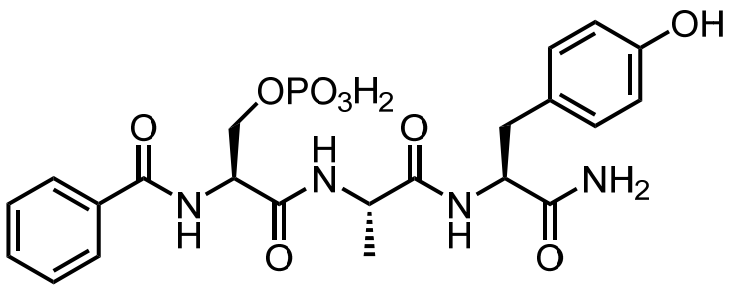


General procedure A (5.2 mg, 0.00848 mmol, 8% yield)

^{1}H NMR (CD_3OD, 400 MHz) δ 7.53-7.20 (m, 15H), 4.95-4.74 (m, 6H), 4.55 (t, J = 2.7 Hz, 1H), 4.27 (ddd, J = 9.5 Hz, 8.7 Hz, 2.3 H, 2H), 3.83 (t, J = 9.5 Hz, 2H), 3.50 (t, J = 9.5 Hz, 1H); ^{13}C NMR (CD_3OD, 126 MHz) δ 140.4, 140.1, 129.5, 129.1, 129.1, 128.8, 128.4, 128.4, 81.5 (d, J = 7.2 Hz), 80.1, 78.5 (d, J = 6.0 Hz), 76.9, 76.2, 75.4;

^{31}P NMR (CD_3OD, 162 MHz) δ −1.0; ESI-MS *m/z* 609.1 $[M–H]^–$; HRMS calcd for $[C_{27}H_{31}O_{12}P_2]^–$ requires *m/z* 609.1296; found 609.1294.

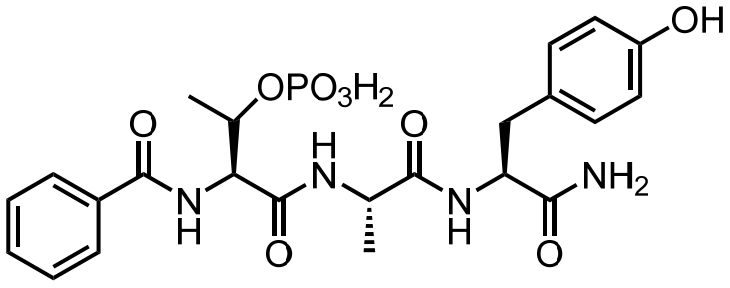
(*S*)-3-(((*S*)-1-(((*S*)-1-Amino-3-(4-hydroxyphenyl)-1-oxopropan-2-yl)amino)-1-oxopropan-2-yl)amino)-2-benzamido-3-oxopropyl dihydrogen phosphate (28):



General procedure D (14.2 mg, 0.0272 mmol, 75% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.64 (d, *J* = 8.6 Hz, 2H), 4.73 (t, *J* = 4.9 Hz, 1H), 4.48 (dd, *J* = 9.2 Hz, 5.5 Hz, 1H), 4.37 (dd, *J* = 8.6 Hz, 4.9 Hz, 2H), 4.24 (q, *J* = 7.2 Hz, 1H), 3.12 (dd, *J* = 13.7 Hz, 5.5 Hz, 1H), 2.91 (dd, *J* = 13.7 Hz, 9.2 Hz, 1H), 1.24 (d, *J* = 7.2 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.7; ^{1}H-coupled ^{31}P NMR (DMSO-d_6, 162 MHz) δ 0.0 (t, *J* = 2.5 Hz); ESI-MS *m/z* 521.2 $[M–H]^–$; HRMS calcd for $[C_{22}H_{26}N_4O_9P]^–$ requires *m/z* 521.1433; found 521.1427; Retention time (LC/MS): 7.4 min.

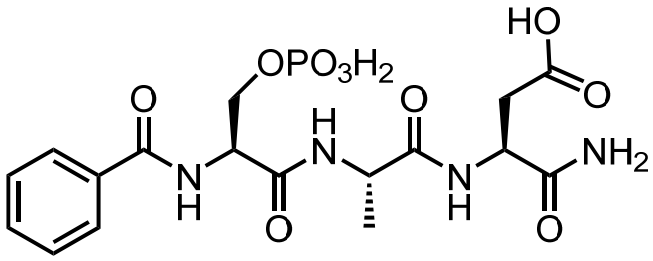
(2*S*,3*S*)-4-(((*S*)-1-(((*S*)-1-Amino-3-(4-hydroxyphenyl)-1-oxopropan-2-yl)amino)-1-oxopropan-2-yl)amino)-3-benzamido-4-oxobutan-2-yl dihydrogen phosphate (29):



General procedure C (4.8 mg, 0.00898 mmol, 57% yield)

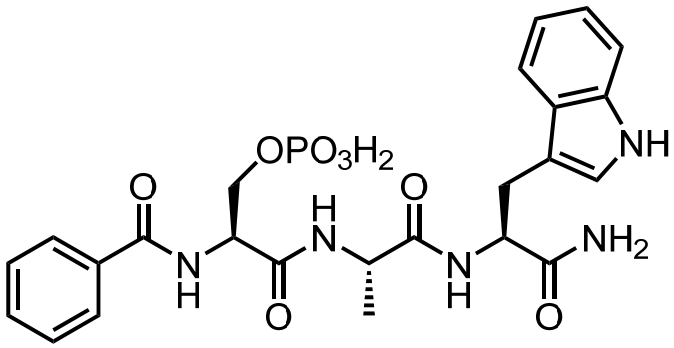
^{1}H NMR (CD_3OD, 500 MHz) δ 7.95 (d, *J* = 6.9 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.01 (t, *J* = 8.6 Hz, 2H), 6.62 (d, *J* = 8.6 Hz, 2H), 4.55-4.44 (m, 3H), 4.21 (q, *J* = 6.6 Hz, 1H), 3.10 (dd, *J* = 14.6 Hz, 6.3 Hz, 1H), 2.92 (dd, *J* = 14.6 Hz, 9.7 Hz, 1H), 1.41 (d, *J* = 6.6 Hz, 3H), 1.25 (d, *J* = 7.4 Hz, 3H); ^{31}P NMR (CD_3SOCD_3, 162 MHz) δ 1.2; ^{1}H-coupled ^{31}P NMR (DMSO-d_6, 162 MHz) δ 0.4 (d, *J* = 9.8 Hz); ESI-MS *m/z* 535.2 $[M–H]^–$; HRMS calcd for $[C_{23}H_{28}N_4O_9P]^–$ requires *m/z* 535.1599; found 535.1598; Retention time (LC/MS): 6.0 min.

(*S*)-4-Amino-3-((*S*)-2-((*S*)-2-benzamido-3-(phosphonooxy)propanamido)propanamido)-4-oxobutanoic acid (30):



General procedure C (7.9 mg, 0.0167 mmol, 71% yield) ^{1}H NMR (CD_3OD, 500 MHz) δ 7.91 (d, *J* = 8.6 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 2H), 4.73 (m, 2H), 4.44 (q, *J* = 6.6 Hz, 1H), 4.40-4.34 (m, 2H), 2.86-2.81 (m, 2H), 1.39 (d, *J* = 6.6 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.8; ESI-MS *m/z* 474.1 $[M-H]^-$; HRMS calcd for $[C_{17}H_{22}N_4O_{10}P]^-$ requires *m/z* 473.1079; found 473.1079; Retention time (LC/MS): 5.8 min.

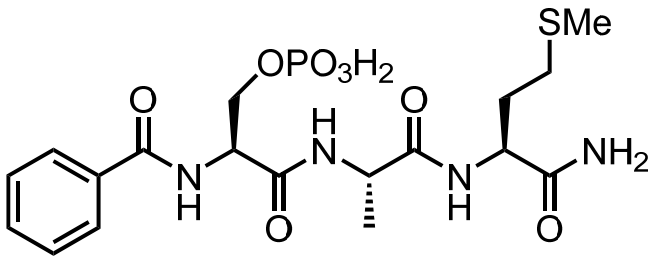
(*S*)-3-(((*S*)-1-(((*S*)-1-Amino-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl)amino)-1-oxopropan-2-yl)amino)-2-benzamido-3-oxopropyl dihydrogen phosphate (31):



General procedure C (8.0 mg, 0.0146 mmol, 76% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.6 Hz, 1H), 7.10-7.04 (m, 2H), 6.97 (t, *J* = 7.7 Hz, 1H), 4.72 (t, *J* = 5.2 Hz, 1H), 4.64 (dd, *J* = 8.8 Hz, 5.2 Hz, 1H), 4.35 (dd, *J* = 8.0 Hz, 5.2 Hz, 2H), 4.25 (q, *J* = 7.2 Hz, 1H), 3.36 (dd, *J* = 14.9 Hz, 5.2 Hz, 1H), 3.22 (dd, *J* = 14.9 Hz, 8.8 Hz, 1H), 1.21 (d, *J* = 7.2 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.7; ESI-MS *m/z* 544.2 $[M-H]^-$; HRMS calcd for $[C_{24}H_{27}N_5O_8P]^-$ requires *m/z* 544.1603; found 544.1602; Retention time (LC/MS): 6.4 min.

(*S*)-3-(((*S*)-1-(((*S*)-1-Amino-4-(methylthio)-1-oxobutan-2-yl)amino)-1-oxopropan-2-yl)amino)-2-benzamido-3-oxopropyl dihydrogen phosphate (32):

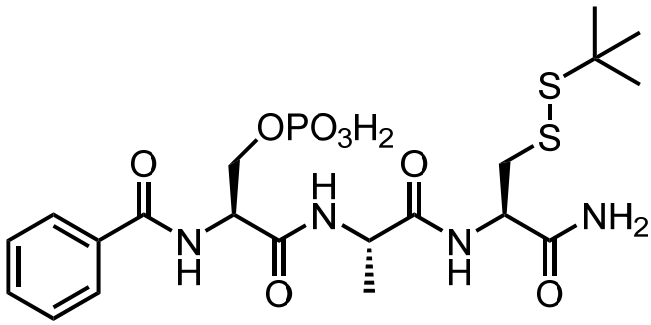


General procedure D (14.1 mg, 0.0288 mmol, 81% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.93 (d, *J* = 7.4 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 2H), 4.74 (t, *J* = 5.2 Hz, 1H), 4.44 (dd, *J* = 9.7 Hz, 4.6 Hz, 1H), 4.38 (dd, *J* = 8.0 Hz, 5.2 Hz, 2H), 4.33 (q, *J* = 6.9 Hz, 1H), 2.62-2.44 (m, 2H), 2.18-2.08 (m, 1H), 2.07 (s, 3H), 2.06-1.98 (m, 1H), 1.40 (d, *J* = 6.9 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.6; ESI-MS *m/z* 489.1 $[M-H]^-$; HRMS calcd for $[C_{24}H_{27}N_5O_8P]^-$

requires *m/z* 489.1214; found 489.1206; Retention time (LC/MS): 6.0 min.

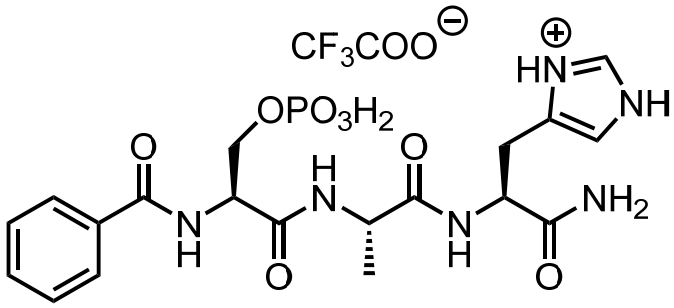
(*S*)-3-(((*S*)-1-(((*R*)-1-Amino-3-(*tert*-butyldisulfaneyl)-1-oxopropan-2-yl)amino)-1-oxopropan-2-yl)amino)-2-benzamido-3-oxopropyl dihydrogen phosphate (33):



General procedure C (12.0 mg, 0.0217 mmol, 77% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.94 (d, *J* = 6.9 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 4.73 (t, *J* = 5.2 Hz, 1H), 4.57 (dd, *J* = 9.7 Hz, 5.2 Hz, 1H), 4.39 (dd, *J* = 8.6 Hz, 5.2 Hz, 2H), 4.32 (q, *J* = 6.9 Hz, 1H), 3.25 (dd, *J* = 13.7 Hz, 5.2 Hz, 1H), 3.09 (dd, *J* = 13.7 Hz, 9.7 Hz, 1H), 1.41 (d, *J* = 6.9 Hz, 3H), 1.32 (s, 9H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.7; ESI-MS *m/z* 549.1 $[M-H]^-$; HRMS calcd for $[C_{20}H_{30}N_4O_8PS_2]^-$ requires *m/z* 549.1248; found 549.1259; Retention time (LC/MS): 7.1 min.

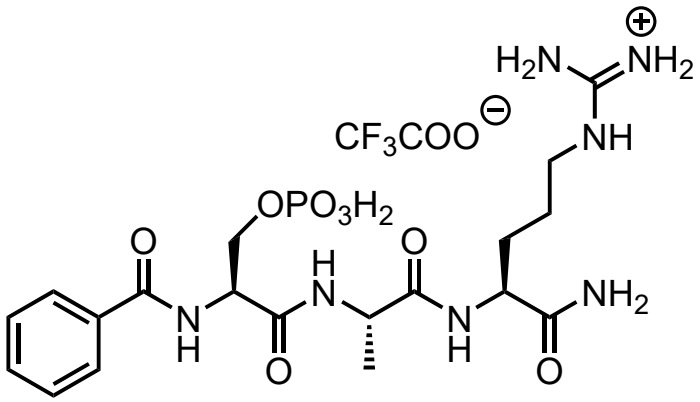
4-((*S*)-3-Amino-2-((*S*)-2-((*S*)-2-benzamido-3-(phosphonooxy)propanamido)propanamido)-3-oxopropyl)-1*H*-imidazol-3-ium trifluoroacetate (34):



General procedure C (9.2 mg, 0.0150 mmol, 85% yield)

^{1}H NMR (D_2O, 500 MHz) δ 8.42 (s, 1H), 7.69 (d, *J* = 7.4 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.11 (s, 1H), 4.70-4.50 (m, 2H), 4.21-4.08 (m, 3H), 3.18 (dd, *J* = 15.8 Hz, 6.3 Hz, 1H), 3.03 (dd, *J* = 15.8 Hz, 9.7 Hz, 1H), 1.20 (d, *J* = 6.9 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ –0.5; ESI-MS *m/z* 495.1 $[M-H]^-$; HRMS calcd for $[C_{19}H_{24}N_6O_8P]^-$ requires *m/z* 495.1399; found 495.1398; Retention time (LC/MS): 6.3 min.

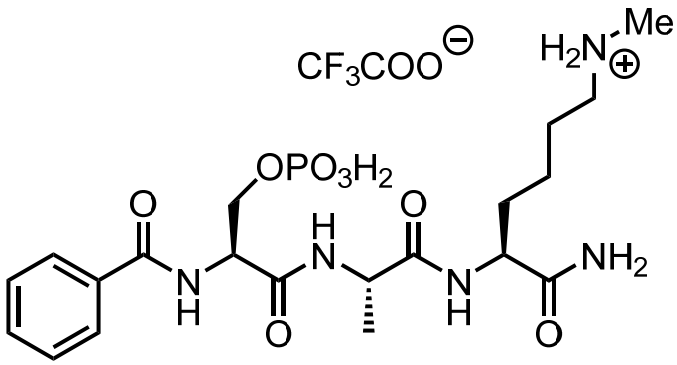
(3*S*,6*S*,9*S*)-14-Amino-9-carbamoyl-6-methyl-1,4,7-trioxo-1-phenyl-3-((phosphonooxy)methyl)-2,5,8,13-tetraazatetradecan-14-iminium trifluoroacetate (35):



General procedure C (6.4 mg, 0.0102 mmol, 76% yield)

^{1}H NMR (D_2O, 500 MHz) δ 7.70 (d, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 2H), 4.50 (m, 1H), 4.23 (q, *J* = 7.2 Hz, 1H), 4.17-4.10 (m, 3H), 2.99 (m, 2H), 1.80-1.68 (m, 1H), 1.68-1.58 (m, 1H), 1.54-1.40 (m, 2H), 1.26 (d, *J* = 7.2 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.3; ESI-MS *m/z* 514.2 $[M-H]^-$; HRMS calcd for $[C_{19}H_{29}N_7O_8P]^-$ requires *m/z* 514.1821; found 514.1811; Retention time (LC/MS): 6.3 min.

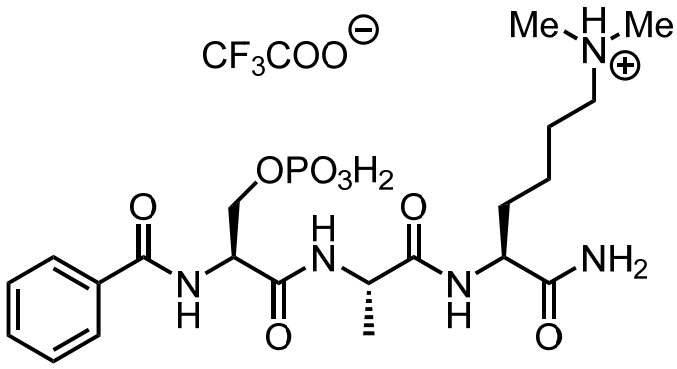
(*S*)-6-Amino-5-((*S*)-2-((*S*)-2-benzamido-3-(phosphonooxy)propanamido)propanamido)-*N*-methyl-6-oxohexan-1-aminium trifluoroacetate (36):



General procedure C (3.06 mg, 0.00936 mmol, 22% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.92 (d, *J* = 6.9 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 4.67 (t, *J* = 4.0 Hz, 1H), 4.42 (dd, *J* = 10.3 Hz, 4.0 Hz, 1H), 4.38-4.26 (m, 3H), 3.00-2.90 (m, 2H), 2.63 (s, 3H), 1.92-1.70 (m, 3H), 1.66-1.55 (m, 1H), 1.55-1.34 (m, 2H), 1.42 (d, *J* = 7.4 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 1.4; ESI-MS *m/z* 500.2 $[M-H]^-$; HRMS calcd for $[C_{20}H_{31}N_5O_8P]^-$ requires *m/z* 500.1916; found 500.1896; Retention time (LC/MS): 5.7 min.

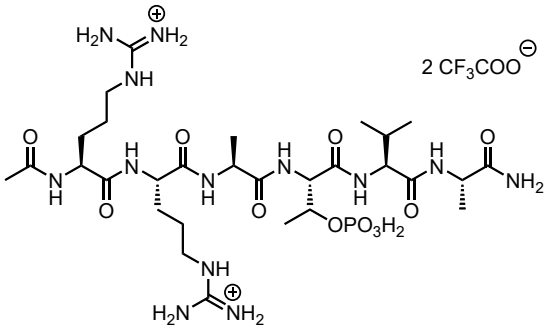
(*S*)-6-Amino-5-((*S*)-2-((*S*)-2-benzamido-3-(phosphonooxy)propanamido)propanamido)-*N*,*N*-dimethyl-6-oxohexan-1-aminium trifluoroacetate (37):



General procedure C (15.0 mg, 0.0239 mmol, 56% yield)

^{1}H NMR (CD_3OD, 500 MHz) δ 7.90 (d, *J* = 6.9 Hz, 2H), 7.56 (t, *J* = 6.9 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 4.74 (t, *J* = 4.6 Hz, 1H), 4.42-4.32 (m, 4H), 3.14-3.00 (m, 2H), 2.82 (s, 6H), 1.94-1.60 (m, 4H), 1.46 (m, 2H), 1.41 (d, *J* = 7.4 Hz, 3H); ^{31}P NMR (CD_3OD, 162 MHz) δ 0.7; ESI-MS *m/z* 514.2 $[M-H]^-$; HRMS calcd for $[C_{21}H_{33}N_5O_8P]^-$ requires *m/z* 514.2072; found 514.2064; Retention time (LC/MS): 5.8 min.

(6*S*,9*S*,12*S*,15*S*,18*S*,21*S*)-6-Acetamido-1,22-diamino-9-(3-((amino(iminio)methyl)amino)propyl)-18-isopropyl-12,21-dimethyl-7,10,13,16,19,22-hexaoxo-15-((*S*)-1-(phosphonooxy)ethyl)-2,8,11,14,17,20-hexaazadocosan-1-iminium trifluoroacetate (38):

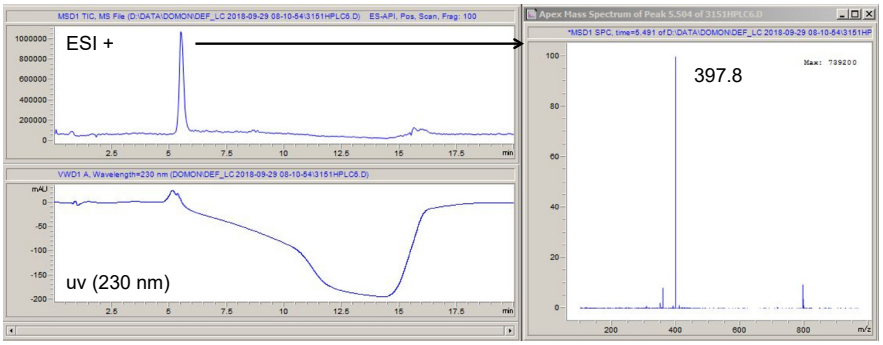


General procedure D (4.5 mg, 0.00436 mmol, 54% yield) The conditions for preparative HPLC were as follows: [2% acetonitrile for 3 min, followed by a linear gradient of 2–100% acetonitrile over 60 min. YMC-Triart C18, 230 nm]

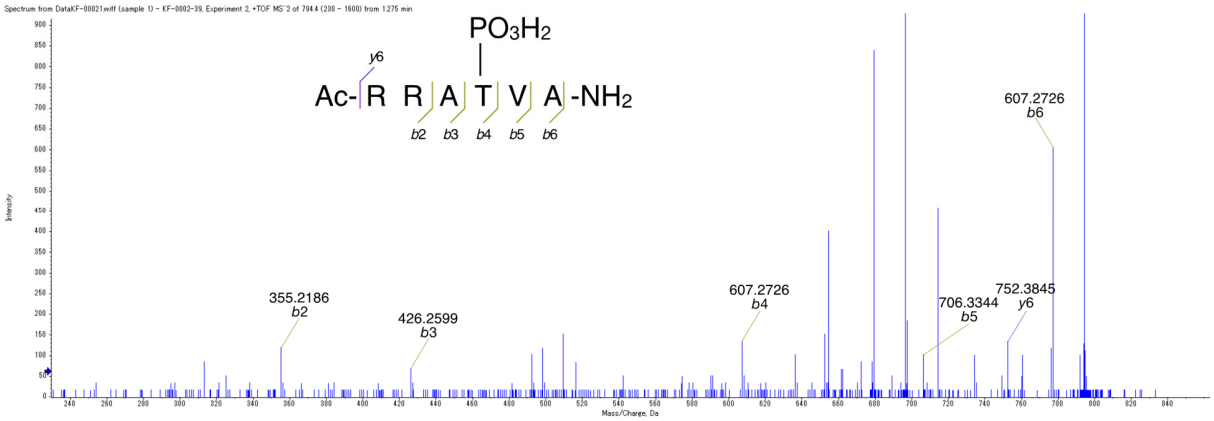
ESI-MS *m*/z 397.8 $[M+2H]^{2+}$; HRMS calcd for $[C_{21}H_{33}N_5O_8P]^-$ requires *m*/*z* 792.3887; found 792.3891;

Retention time (LC/MS): 5.5 min.

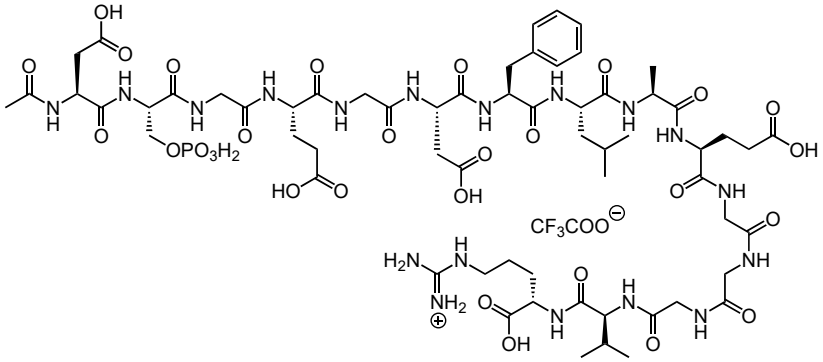
LC-MS chart of purified **38**



LC–MS/MS analysis of the phosphorylation position

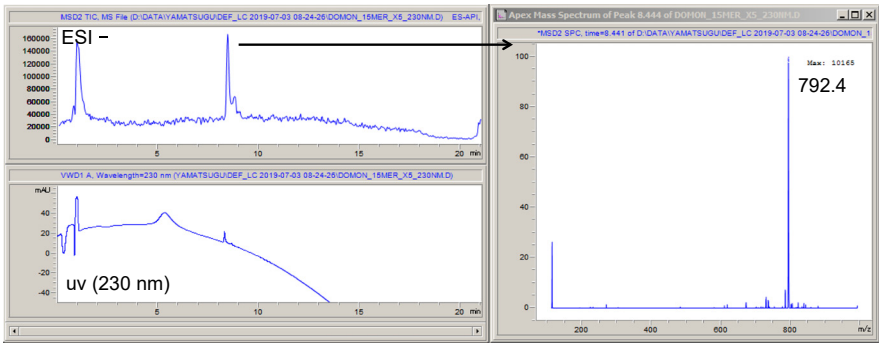


(6*S*,9*S*,21*S*,24*S*,27*S*,30*S*,33*S*,39*S*,45*S*,48*S*)-1-Amino-30-benzyl-6-carboxy-21,39-bis(2-carboxyethyl)-33,48-bis(carboxymethyl)-27-isobutyl-9-isopropyl-24-methyl-8,11,14,17,20,23,26,29,32,35,38,41,44,47,50-pentadecaoxo-45-((phosphonooxy)methyl)-2,7,10,13,16,19,22,25,28,31,34,37,40,43,46,49-hexadecaazahenpentacontan-1-iminium trifluoroacetate (39):

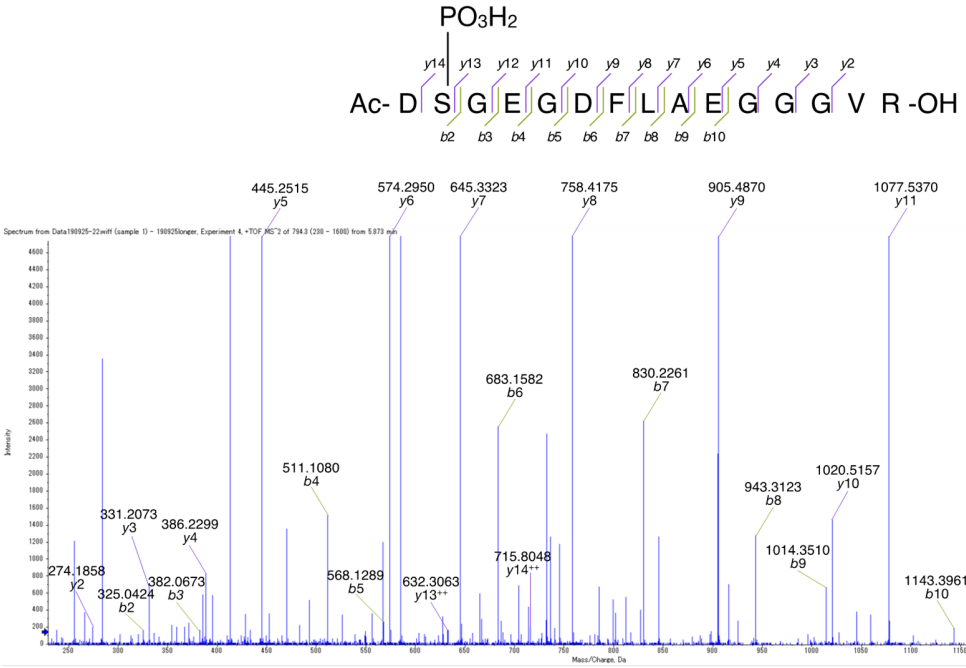


General procedure E (2.52 mg, 0.00148 mmol, 59% yield) ESI-MS *m*/z 792.4 $[M–2H]^{2–}$; HRMS calcd for $[C_{21}H_{33}N_5O_8P]^–$ requires *m*/*z* 1585.6177; found 1585.6213; Retention time (LC/MS): 8.3 min.

LC-MS chart of purified **39**



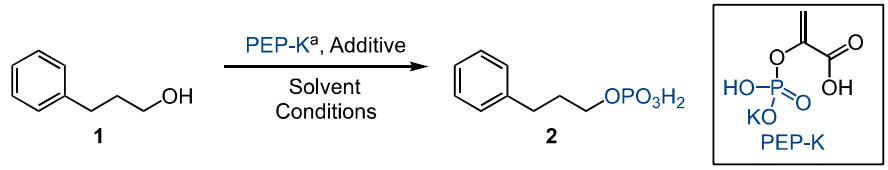
LC–MS/MS analysis of the phosphorylation position



Computational Details

All the calculations were carried out at the density functional theory (DFT) with the dispersion corrected[1] B3LYP-D3 functional,[2] including the solvation effect by the polarized continuum model (PCM)[3] with a dielectric constant of 37.219 (for DMF). The reaction pathways were searched using an automated reaction path search method, called the artificial force-induced reaction (AFIR) method.[4,5,6] First, the initial orientations between the target molecules were determined randomly, from which the AFIR calculations were applied. At this stage, the basis set (BS1); 6-311G(d,p) for S and P,[7] and 6-31G(d) for others,[8,9] were used. Next, the obtained approximate local minima and transition states were fully reoptimized without any restrictions. The geometry optimization and frequency calculations were carried out using the BS1 basis set. All the transition states were confirmed by the frequency and the intrinsic reaction coordinate (IRC)[10] calculations. The Gibbs free energies were evaluated using the Gibbs free energy correction terms at 373.15 K and 1 atm. These values were further corrected by an adjustment for the 1 atm to 1 M standard-state concentration change of $RT\ln(24.5\times373.15/298.15)$, 2.54 kcal mol^{-1}.[11,12] These free energy contributions were added to the single point electronic energies computed with the diffused basis set (BS2); 6-311+G(d,p) for S and P, and 6-31+G(d,p) for others. The geometry optimizations, frequency calculations, IRC calculations, and AFIR calculations were performed via the global reaction route mapping (GRRM) program,[13] using the energies and energy derivatives computed by the Gaussian09 program.[14]

Table S1. Complete list of reaction conditions for optimization of the phosphorylation of 3-phenyl-1-propanol (1)



Entry	PEP-K (equiv.)	Additive	pK_{a1}[b]	Solvent	Conditions	NMR yield
1	1.5	-	-	MeCN (0.10 M)	80 °C, 12 h	0%
2	1.5	Tetrazole (20 mol%)	4.90	MeCN (0.10 M)	80 °C, 12 h	0%
3	1.5	AcOH (20 mol%)	4.76	MeCN (0.10 M)	80 °C, 12 h	0%
4	1.5	Benzoic acid (20 mol%)	4.21	MeCN (0.10 M)	80 °C, 12 h	0%
5	1.5	2-Chlorobenzoic acid (20 mol%)	2.89	MeCN (0.10 M)	80 °C, 12 h	0%
6	1.5	H_3PO_4 (20 mol%)	2.12	MeCN (0.10 M)	80 °C, 12 h	4%
7	1.5	NBu_4HSO_4 (20 mol%)	1.99	MeCN (0.10 M)	80 °C, 12 h	35%
8	1.5	10-Camphorsulfonic acid (20 mol%)	1.20	MeCN (0.10 M)	80 °C, 12 h	6%
9	1.5	TFA (20 mol%)	−0.25	MeCN (0.10 M)	80 °C, 12 h	2%
10	1.5	TsOH (20 mol%)	−2.80	MeCN (0.10 M)	80 °C, 12 h	9%
11	1.5	NBu_4BF_4 (20 mol%)	-	MeCN (0.10 M)	80 °C, 12 h	0%
12	1.5	NBu_4PF_6 (20 mol%)	-	MeCN (0.10 M)	80 °C, 12 h	0%
13	1.5	NBu_4Br (20 mol%)	-	MeCN (0.10 M)	80 °C, 12 h	0%
14	1.5	NBu_4HSO_4 (20 mol%)	1.99	DMSO (0.10 M)	80 °C, 12 h	10%
15	1.5	NBu_4HSO_4 (20 mol%)	1.99	NMP (0.10 M)	80 °C, 12 h	9%
16	1.5	NBu_4HSO_4 (20 mol%)	1.99	1,4-Dioxane (0.10 M)	80 °C, 12 h	13%
17	1.5	NBu_4HSO_4 (20 mol%)	1.99	Toluene (0.10 M)	80 °C, 12 h	17%
18	1.5	NBu_4HSO_4 (20 mol%)	1.99	1,2-Dichroloethane (0.10 M)	80 °C, 12 h	33%
19	1.5	NBu_4HSO_4 (20 mol%)	1.99	DMA (0.10 M)	80 °C, 12 h	19%
20	1.5	NBu_4HSO_4 (20 mol%)	1.99	DMF (0.10 M)	80 °C, 12 h	43%
21	3.0	NBu_4HSO_4 (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	80%
22	3.0	$NaHSO_4$ (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	38%
23	3.0	$KHSO_4$ (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	33%
24	3.0	NMe_4HSO_4 (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	49%
25	3.0	$NOct_3MeHSO_4$ (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	51%
26	3.0	PBu_4HSO_4 (30 mol%)	1.99	DMF (0.20 M)	80 °C, 24 h	45%
27	4.5	NBu_4HSO_4 (30 mol%)	1.99	DMF (0.20 M)	100 °C, 6 h	88%

[a]The value of pK_{a1} of PEP-H is less than 2. [b]Values in water.

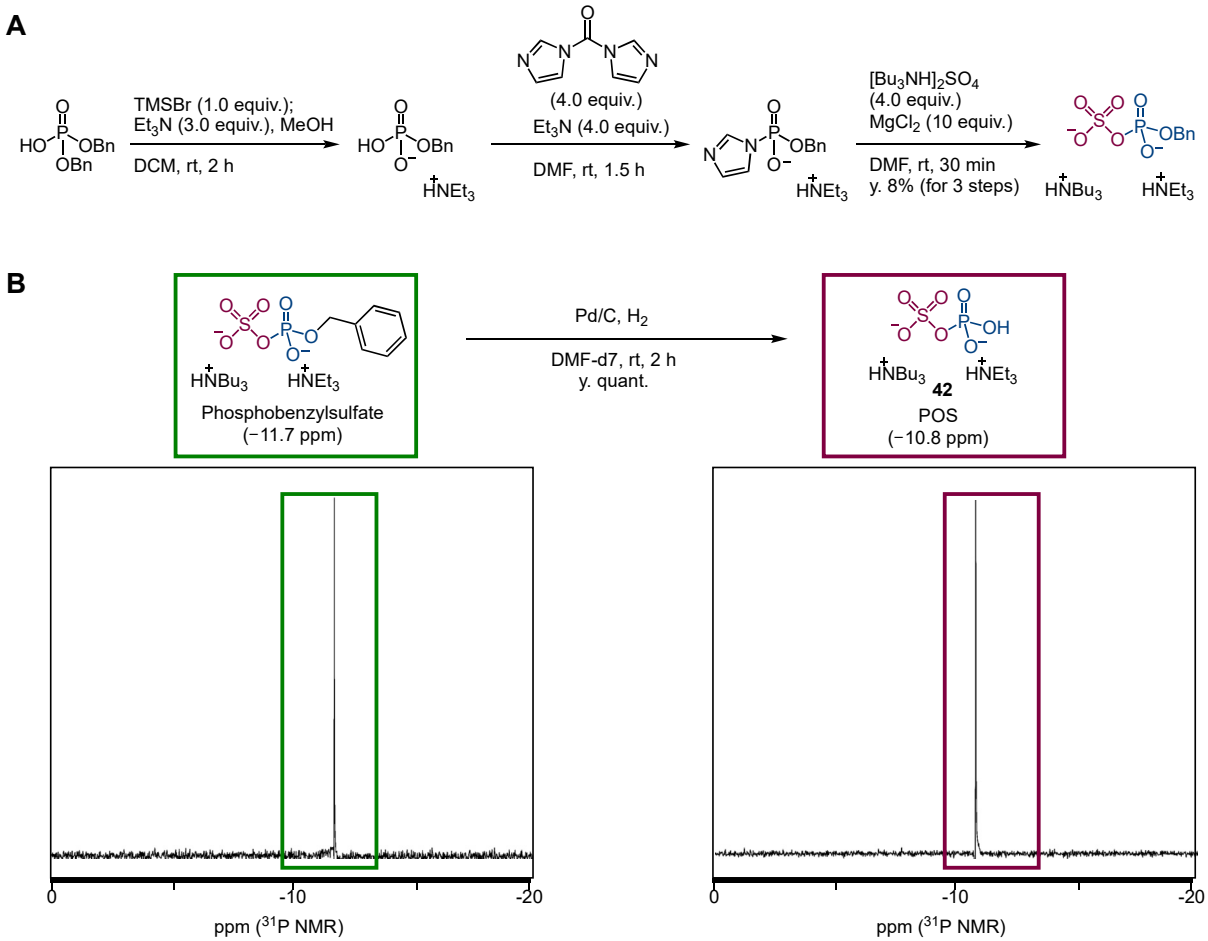


Figure S1. Synthesis of *O*-benzyl phosphosulfate (A) and ^{31}P NMR change in hydrogenolysis of *O*-benzyl phosphosulfate to prepare POS (42) (B).

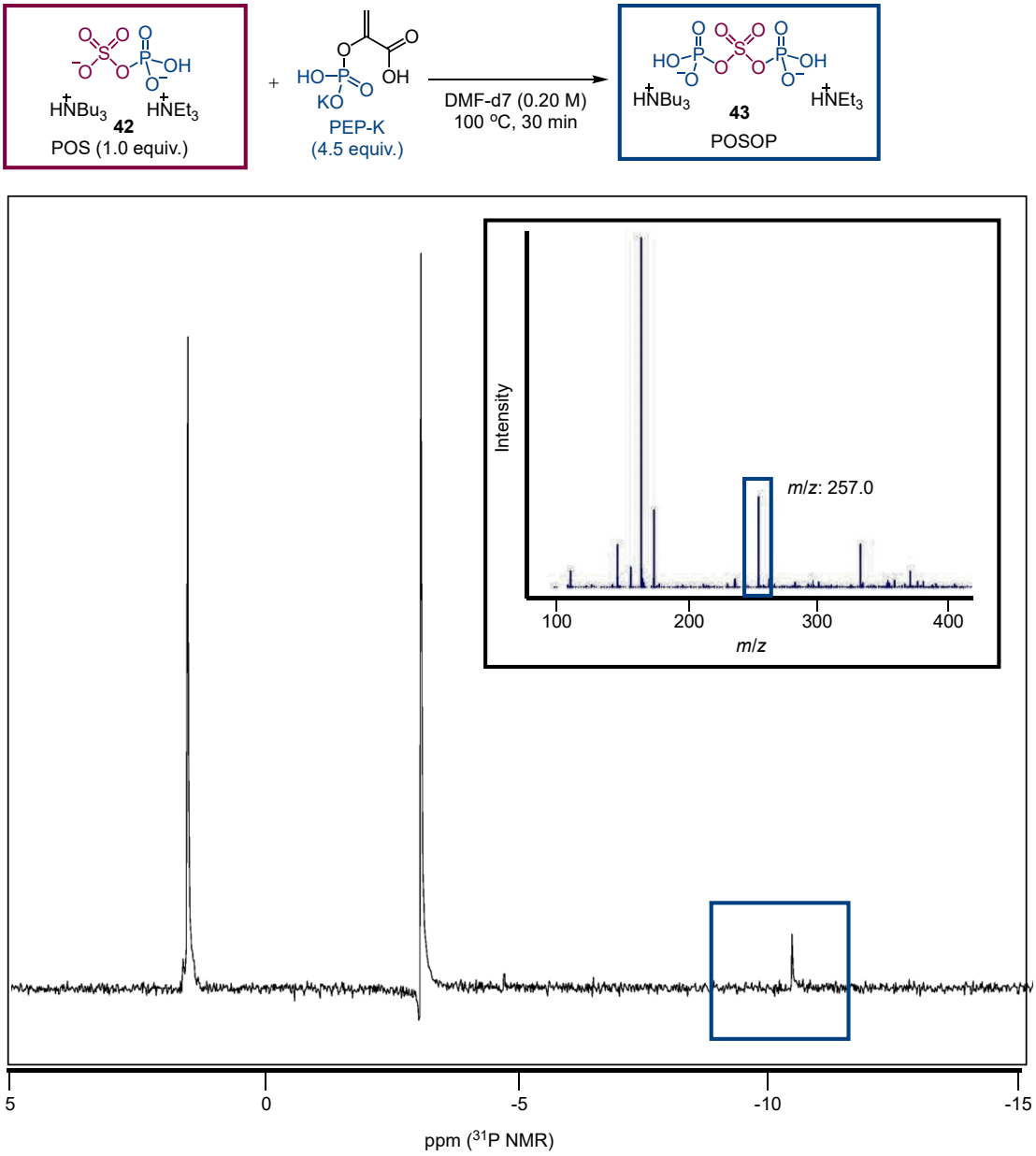


Figure S2. A ^{31}P NMR spectrum and a MS spectrum (inset) after the reaction between POS (42) and PEP-K at 100 °C for 30 min. A peak at 1.5 ppm is phosphoric acid and a peak at –3.0 ppm is PEP-K. A peak at –10.2 ppm is considered to be POSOP (**43**). The MS spectrum showed a peak of *m*/*z* 257.0 corresponding to POSOP (**43**).

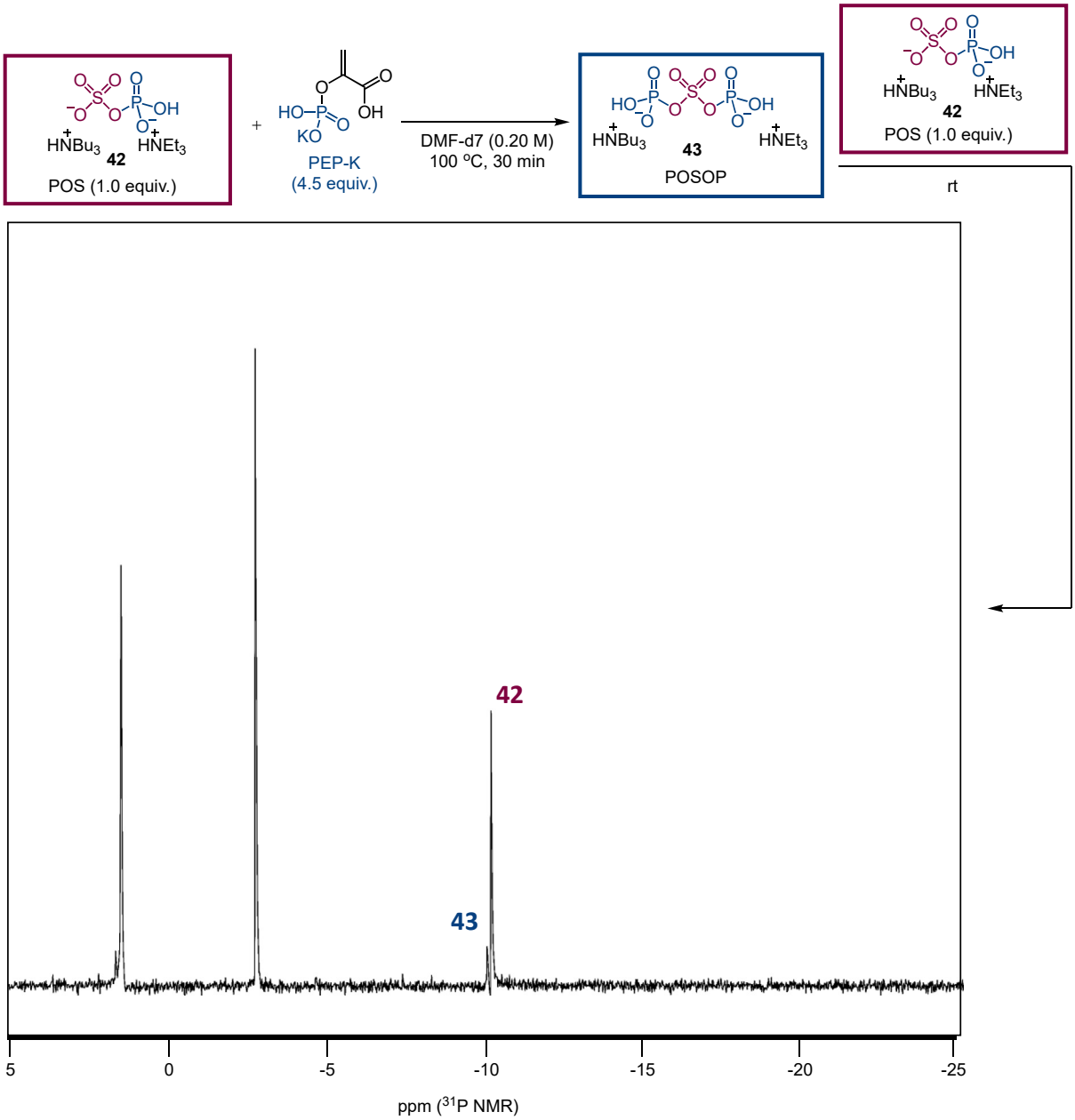


Figure S3. A ^{31}P NMR spectrum just after the further addition of POS (42) to the reaction mixture obtained in Fig. S2. In addition to the peak of POSOP (**43**) at −10.0 ppm, a new peak corresponding to POS (**42**) appeared at −10.1 ppm.

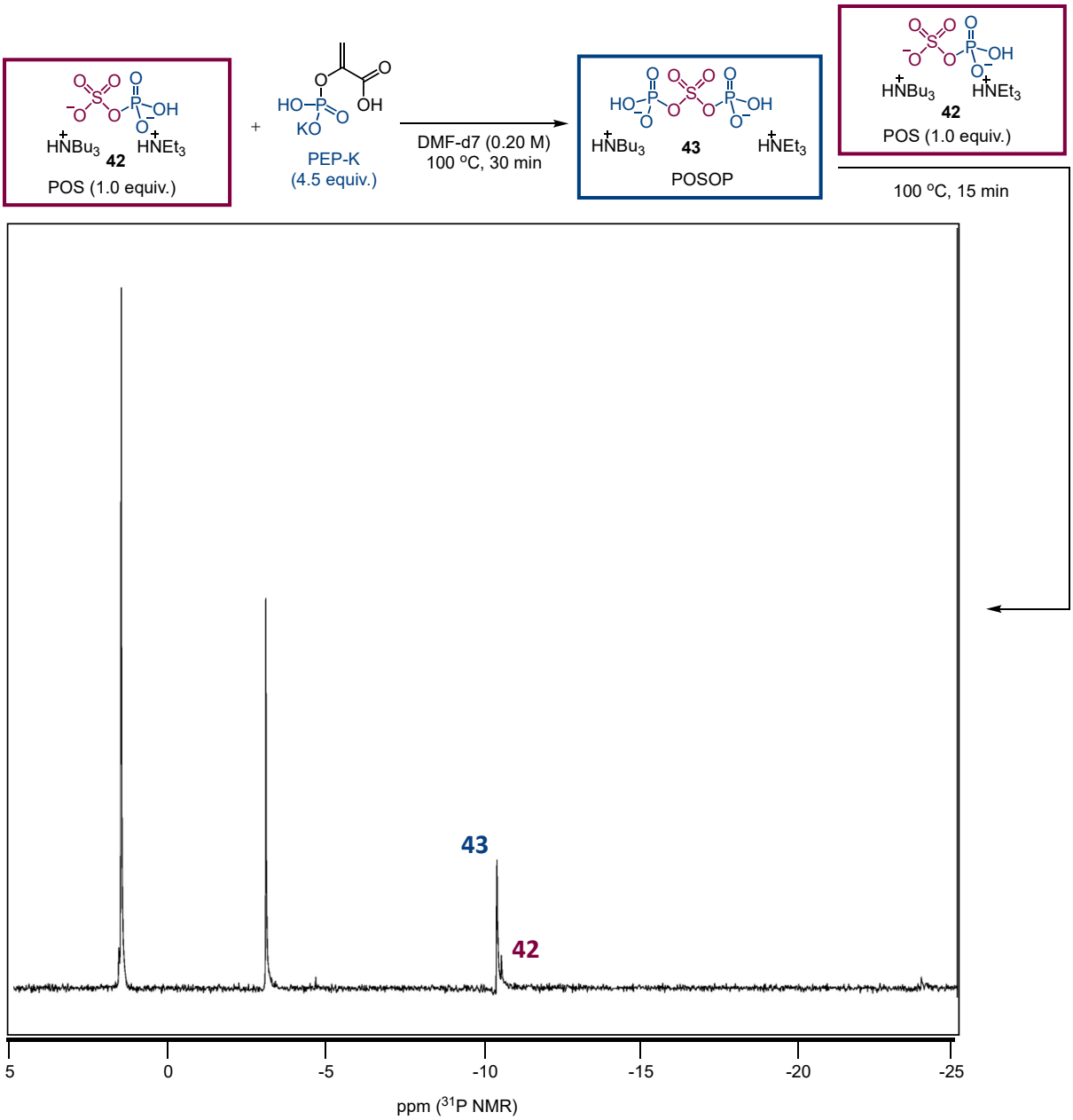


Figure S4. A ^{31}P NMR spectrum after heating the reaction mixture obtained in Fig. S3 at 100 °C for 15 min. The peak at −10.5 ppm corresponding to POS (**42**) decreased and the peak at −10.4 ppm corresponding to POSOP (**43**) increased.

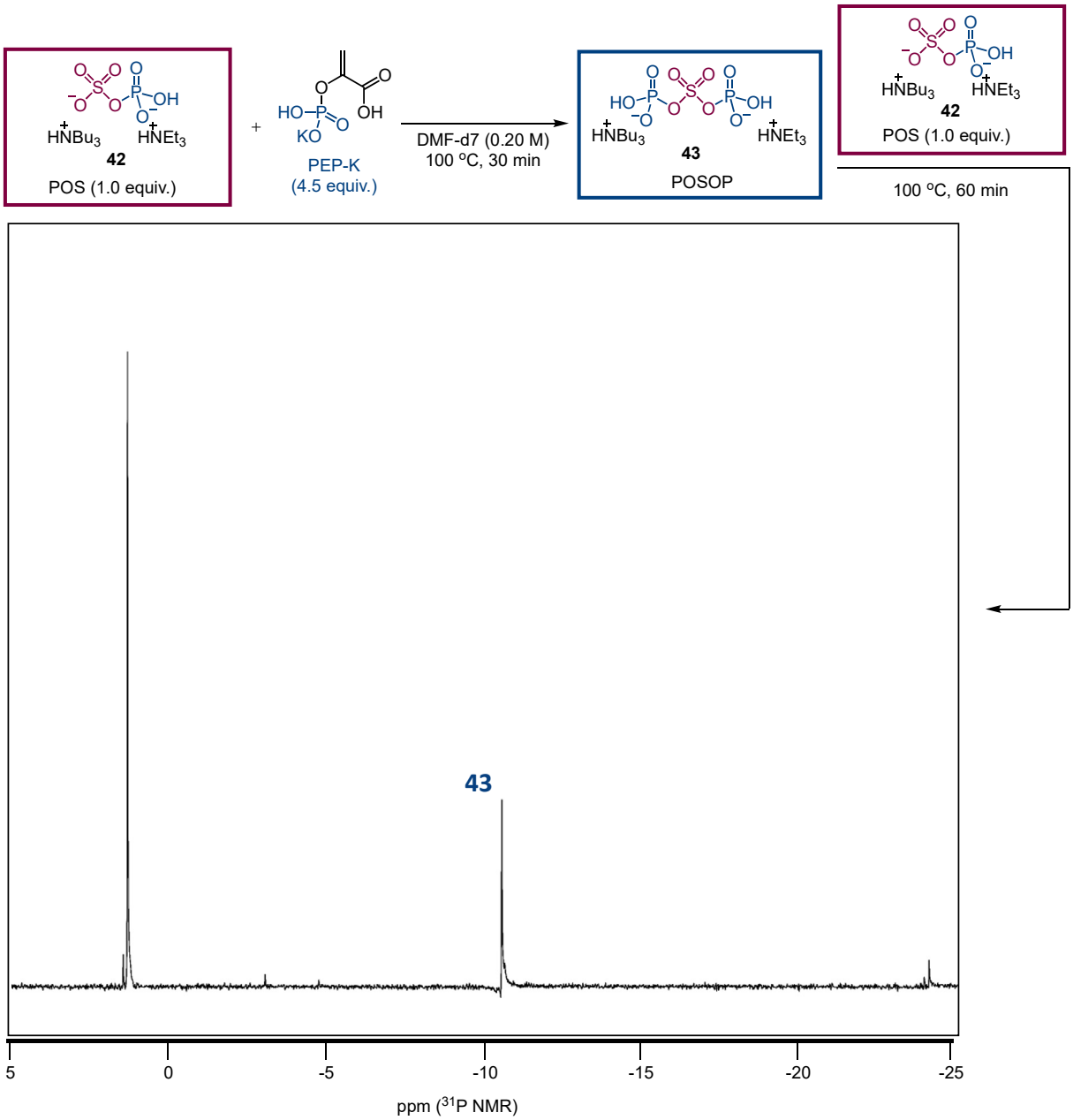


Figure S5. A ^{31}P NMR spectrum after heating the reaction mixture obtained in Fig. S4 at 100 °C for additional 45 min (total 60 min after Figure S3). The peak corresponding POS (**42**) disappeared completely. The experiments in Figures S2-S5 showed that peaks of POS (**42**) and POSOP (**43**) appeared in very close chemical shifts, but those are different.

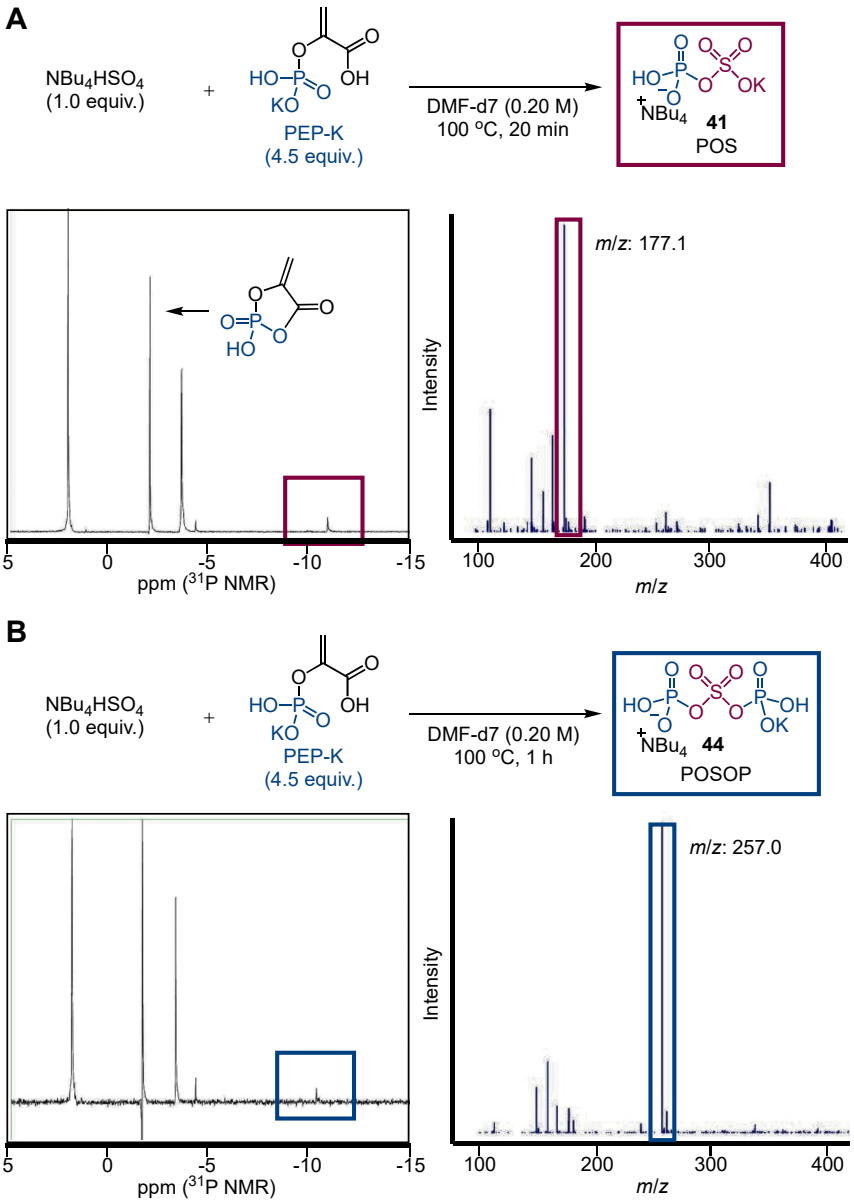


Figure S6. ^{31}P NMR (left) and MS (right) spectra of the reaction between TBAHS and PEP-K. (**A**) After 20 min. A peak at 1.6 ppm is phosphoric acid. A peak at –2.4 ppm matched with that of the cyclic acyl phosphate generated from PEP cyclohexylammonium salt and *N*,*N*'-dicyclohexylcarbodiimide.[15] A peak at –4.8 ppm is PEP-K. A peak at –11.4 ppm is considered to be POS (**41**). The MS spectrum showed a peak of *m*/*z* 177.1 corresponding to POS (**41**). (**B**) After 1 h. A peak at –10.8 ppm is considered to be POSOP (**44**). The MS spectrum showed a peak of *m*/*z* 257.0 corresponding to POSOP (**44**).

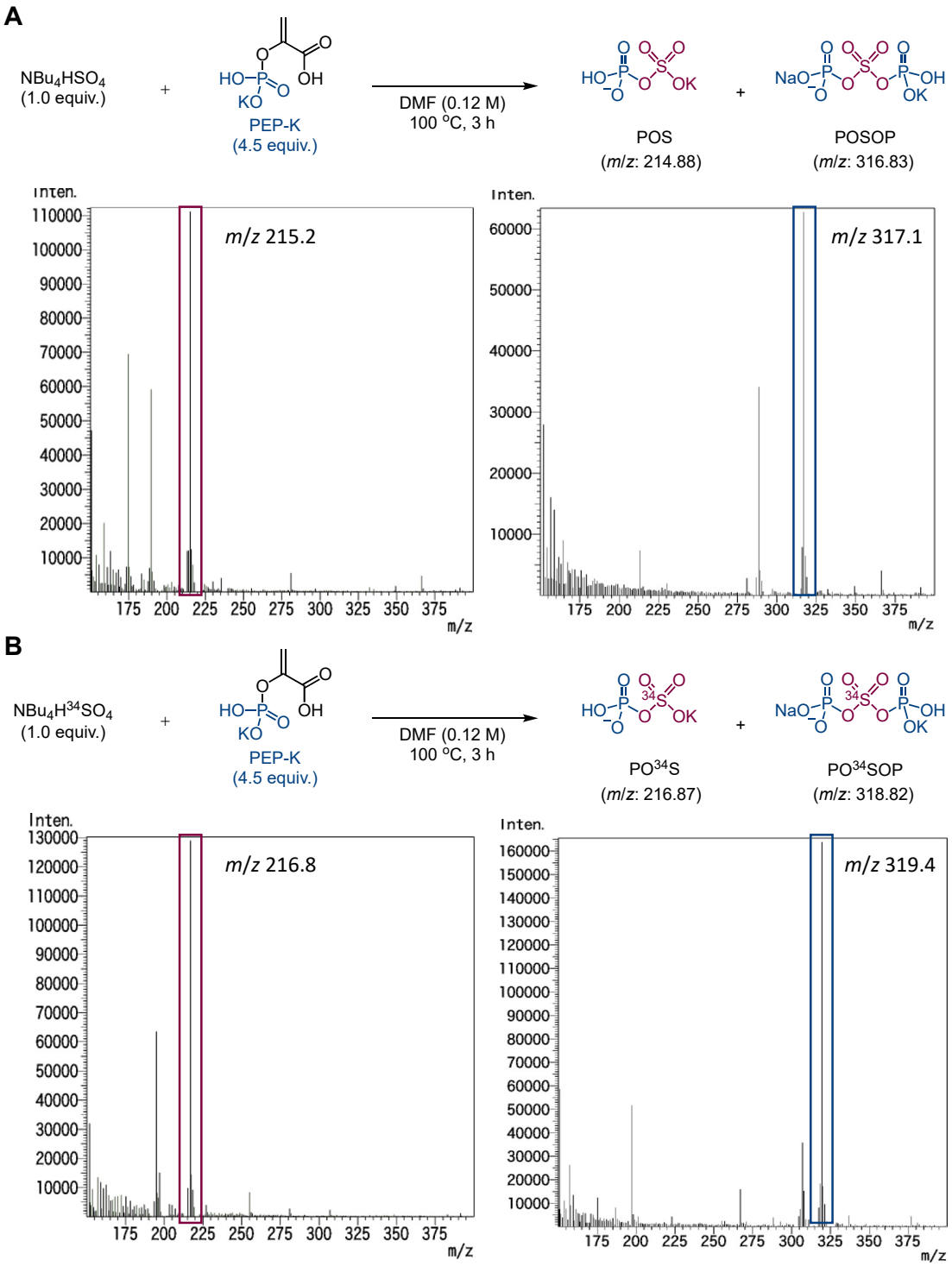


Figure S7. MS analyses of POS and POSOS using ^{34}S-labeled TBAHS. MS charts of the reaction using ^{32}S-TBAHS (**A**) and ^{34}S-TBAHS (**B**). The reaction mixtures were analyzed by LC-MS using an isocratic elution of acetonitrile over 3 min with a flow rate of 1 mL/min.

Detailed Gibbs free energy profiles and geometries

In Figures S8–S14, compounds with the same number of atoms are connected with solid lines. Dot lines are used to connect compounds with different number of atoms.

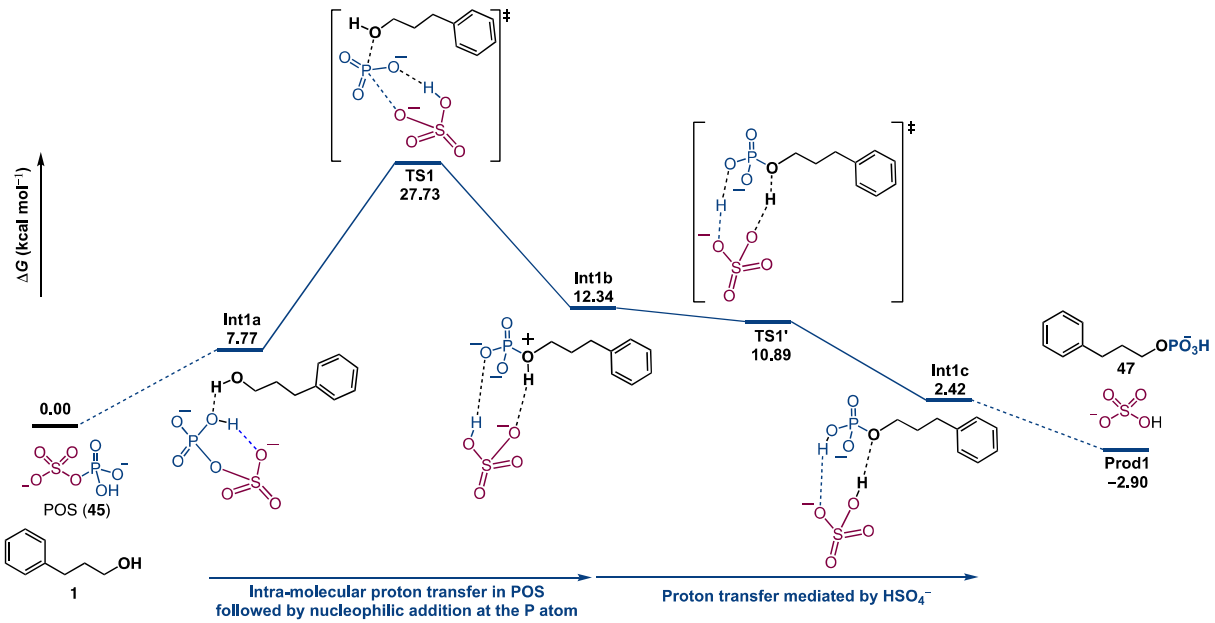


Figure S8. Gibbs free energy profile (in kcal mol^{-1}) of phosphorylation of alcohol (ROH) by POS. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POS **45**. Intramolecular proton transfer from the phosphate moiety to the sulfate moiety in POS **45** occurs prior to **TS1**, followed by nucleophilic addition at the P atom (**Int1a**–**Int1b**). Then, the proton in ROH migrates to the phosphate moiety through the mediation by the eliminated HSO_4^- group (**Int1b**–**Int1c**).

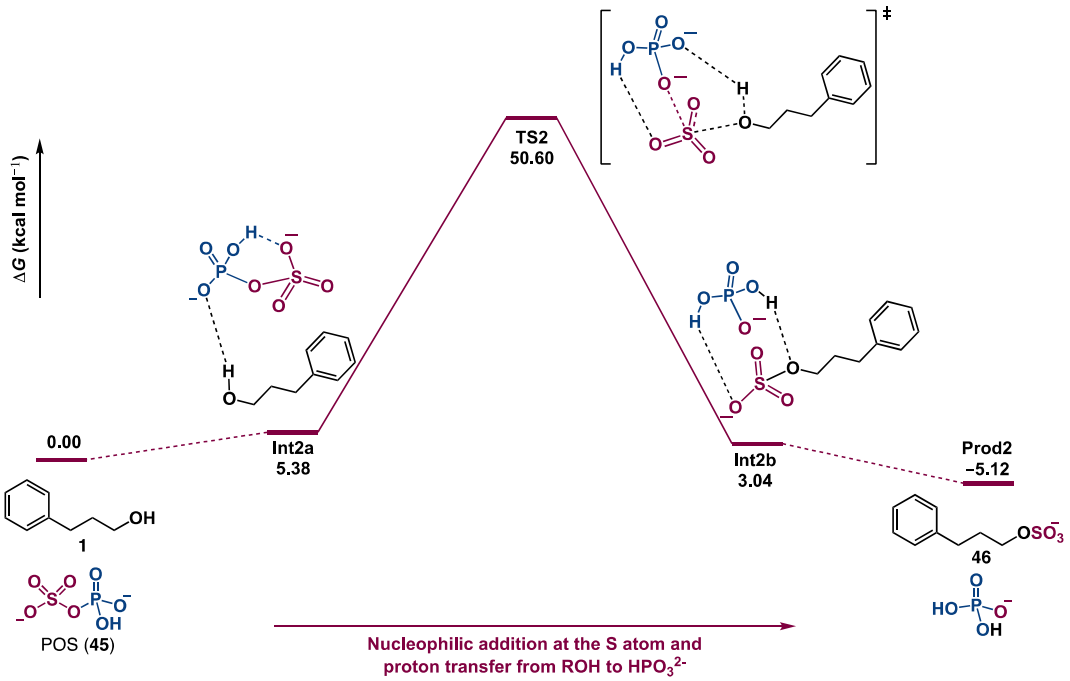


Figure S9. Gibbs free energy profile (in kcal mol^{-1}) of sulfation of alcohol (ROH) by POS. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POS **45**. Nucleophilic addition at the S atom and proton transfer from ROH to the phosphate moiety proceed concertedly (**Int2a**–**Int2b**).

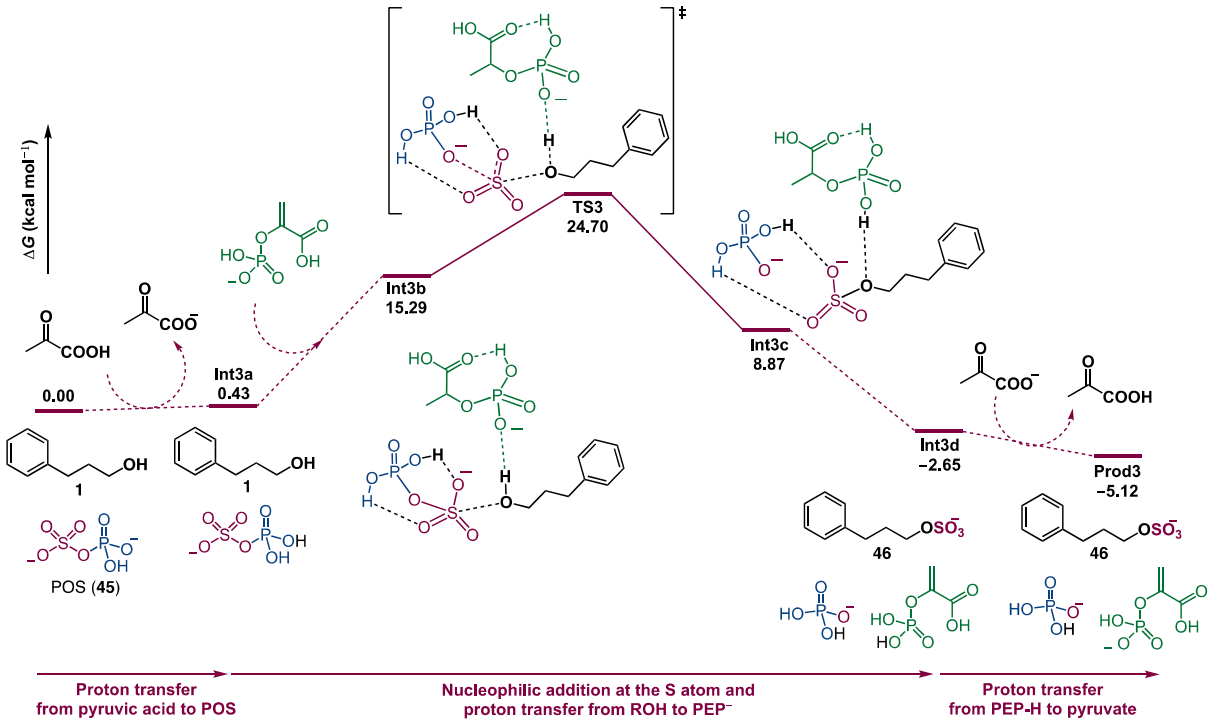


Figure S10. Gibbs free energy profile (in kcal mol^{-1}) of sulfation of alcohol (ROH) by POS mediated by PEP-H. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POS **45** + pyruvic acid + PEP^{-}. POS **45** abstracts the proton from pyruvic acid prior to **Int3a**, then nucleophilic addition at the S atom and proton transfer from ROH to PEP occur concertedly (**Int3b**–**Int3c**). Finally, the proton transfers from PEP-H to pyruvate (**Int3d**–**Prod3**).

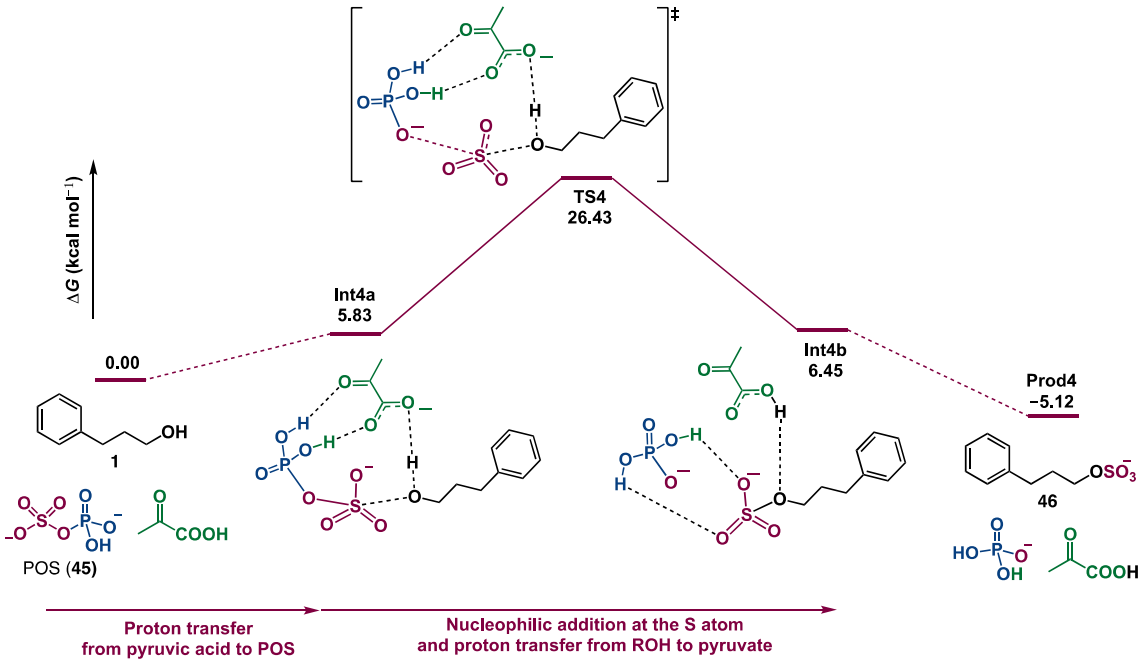


Figure S11. Gibbs free energy profile (in kcal mol^{-1}) of sulfation of alcohol (ROH) by POS mediated by pyruvic acid. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POS **45** + pyruvic acid. Proton transfer from pyruvic acid to POS **45** occurs prior to **Int4a**, followed by nucleophilic addition at the S atom and proton transfer from ROH to pyruvate (**Int4a**–**Int4b**).

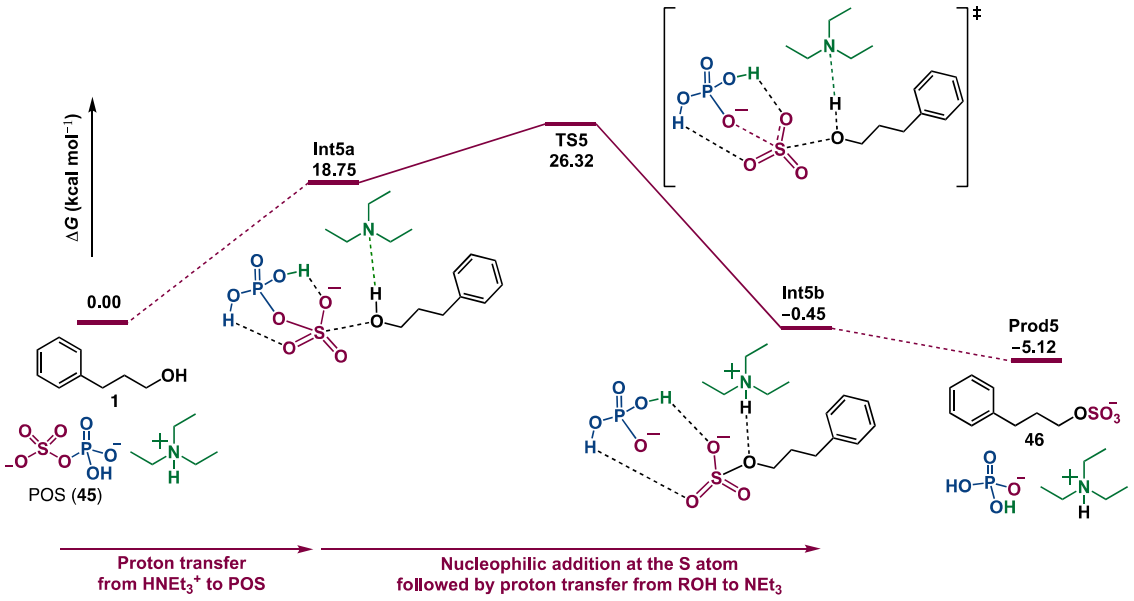


Figure S12. Gibbs free energy profile (in kcal mol^{-1}) of sulfation of alcohol (ROH) by POS mediated by $HNEt_3^+$. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POS **45** + $HNEt_3^+$. Proton transfer from $HNEt_3^+$ to POS **45** proceeds prior to **Int5a**, followed by nucleophilic addition at the S atom and proton transfer from ROH to NEt_3 (**Int5a**–**Int5b**).

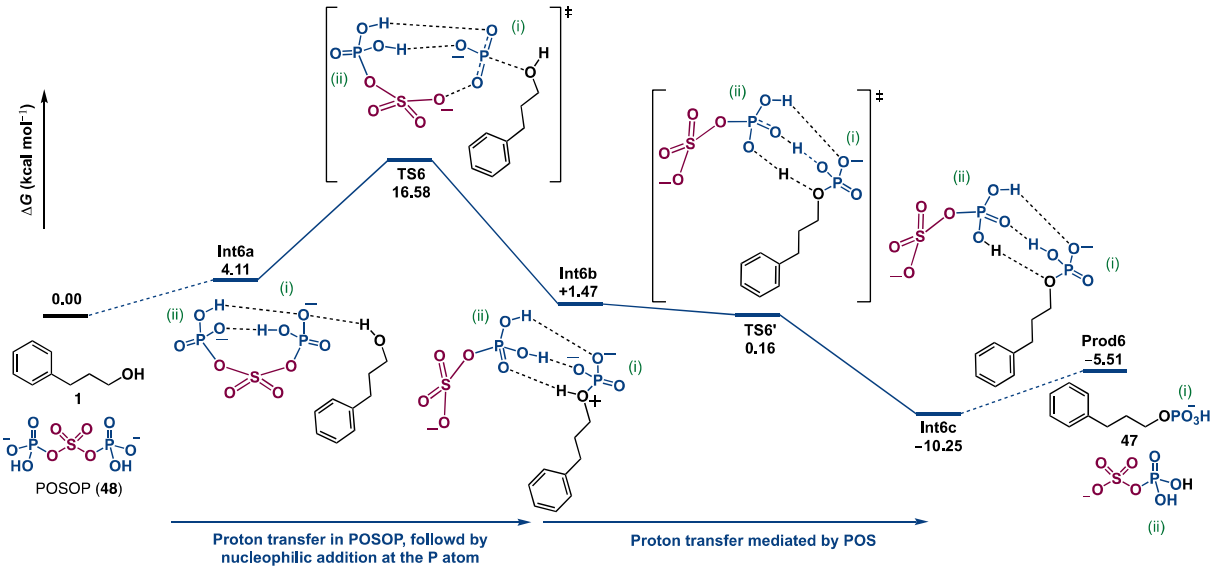


Figure S13. Gibbs free energy profile (in kcal mol^{-1}) of phosphorylation of alcohol by POSOP. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POSOP **48.** Intramolecular proton transfer from the phosphate moiety (i) to the other phosphate moiety (ii) in POSOP **48** takes place prior to **TS6**, followed by nucleophilic addition of ROH at the P atom (**Int6a**–**Int6b**). Then, proton transfer from ROH to the phosphate moiety (ii) and that from (ii) to (i) take place concertedly (**Int6b**–**Int6c**). Namely, the leaving protonated POS mediates the proton transfer from ROH to the phosphate moiety (i).

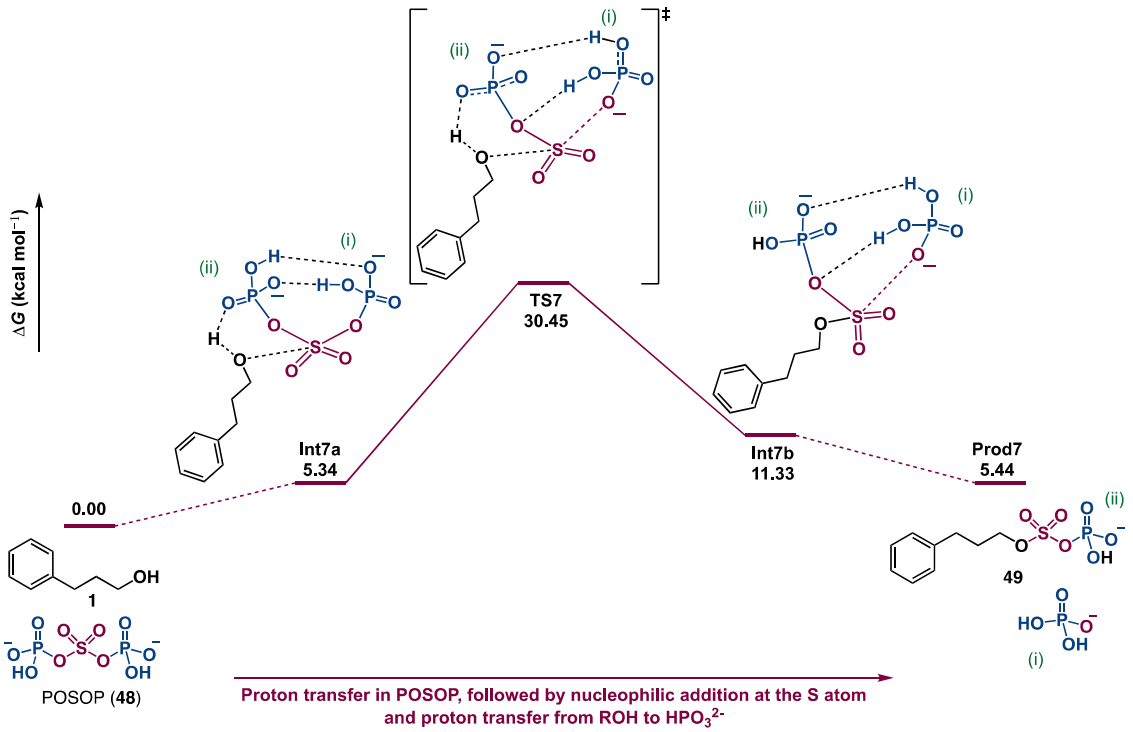


Figure S14. Gibbs free energy profile (in kcal mol^{-1}) of sulfation of alcohol (ROH) by POSOP. The reference of the relative Gibbs free energy (ΔG = 0.0) is ROH **1** + POSOP **48.** The leaving phosphate moiety (i) abstracts a proton from the other phosphate moiety (ii) in POSOP (**48**) (prior to **TS7**). Then, the nucleophilic addition of ROH at the S atom and the proton transfer from ROH to the phosphate moiety (ii) proceed concertedly (**Int7a**–**Int7b**). Namely, the phosphate moiety (ii) mediates the proton transfer from ROH to the leaving phosphate (i).

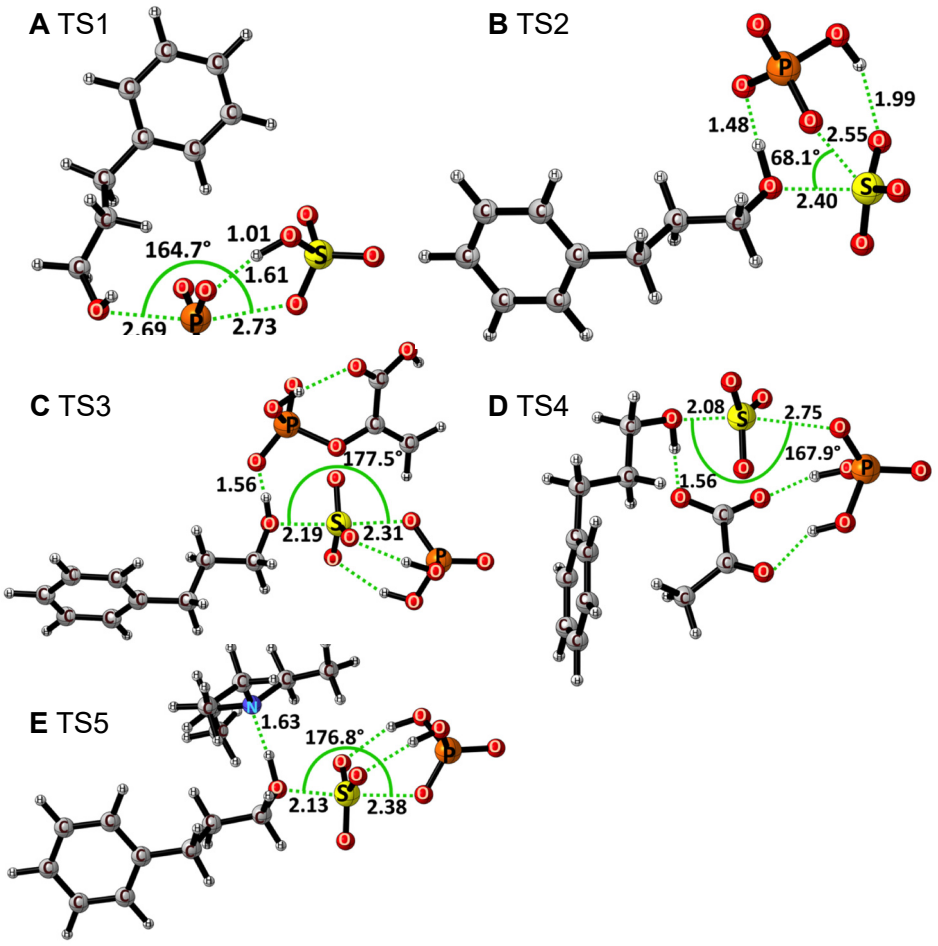


Figure S15. Geometries of TSs for phosphorylation and sulfation by POS. Geometries of TSs for phosphorylation by POS (**A**), sulfation by POS without proton-transfer mediators (**B**), with pyruvic acid (**C**), with PEP (**D**), and with $HNEt_3^+$ (**E**) are shown, respectively. The bond distances are in Å. The Gibbs free energy differences are shown in Figures S8-S12.

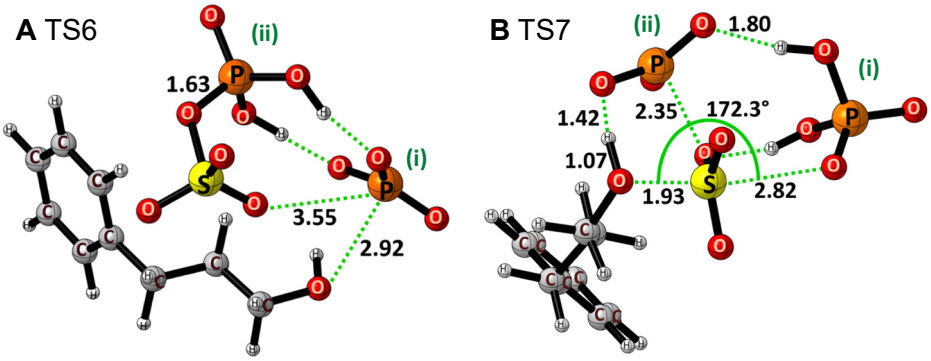


Figure S16. Geometries of the TSs for phosphorylation (A) and sulfation (B) by POSOP. Phosphorylation is shown in **A**, and sulfation is shown in **B**. The bond distances are in Å. The Gibbs free energy differences are shown in Figures S13-S14. (i) and (ii) are the same labels as shown in Figures S13 and S14.

Table S2. Bond orders/distances (in Å) of POS 45 and POSOP 48.

	POS **45**	POSOP **48**
P–O bond	0.56 [a)] / 1.71 [b)]	0.48 [a)] / 1.77 [b)]
S–O bond	0.67 [a)] / 1.66 [b)]	0.79 [a)] / 1.59 [b)]

[a,b]The corresponding O–P and O–S bonds are shown in red below.

POS **POSOP**

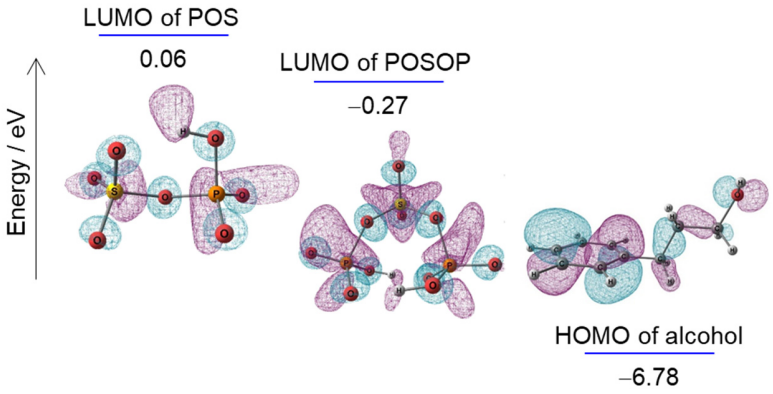


Figure S17. The frontier orbitals and their energy levels (in eV) of POS 45, POSOP 48, and 3-phenyl-1-propanol (1).

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Cartesian Coordinates of the Critical Points

The electronic energies and Gibbs free energies at 373.15 K and 1atm (without the correction terms of 2.54 kcal mol^{-1}) are shown in atomic unit. The Cartesian coordinates are in Å.

3-phenylpropan-1-ol (ROH: 1)
Electronic Energy = -425.455530641 / Gibbs Free Energy =-425.313460688

C	-1.293725518814	0.779219337764	-0.279277580828
H	-0.391236683292	0.984053517740	-0.872795520465
H	-1.475798251712	1.667203821243	0.339132877728
C	-1.041120314383	-0.444494894670	0.622517491073
H	-0.875449150039	-1.327428766692	-0.008596485742
H	-1.943359652073	-0.643757225986	1.215387399426
C	0.143370325407	-0.241627079621	1.541821912015
C	-0.019796559901	0.348151377347	2.803686820269
C	1.437709981998	-0.593666900101	1.132543626694
C	1.078421220543	0.579674770277	3.635384601895
H	-1.017867862508	0.625254955527	3.136606794265
C	2.539604005995	-0.364291811149	1.959970460779
H	1.580983430421	-1.054034854859	0.157183332383
C	2.363426003904	0.223953981186	3.215687094403
H	0.930251653759	1.034018531675	4.611715226574
H	3.534340779738	-0.647978896192	1.625839774816
H	3.218805534966	0.400317105962	3.862321452731
C	-2.480392530797	0.576951280269	-1.221311609601
H	-2.315404079210	-0.316017609569	-1.846363717953
H	-3.394943335882	0.403137654909	-0.642553391094
O	-2.746512029024	1.725203023433	-2.026601881118
H	-1.961814549106	1.880072551504	-2.576836628226

POS ($PO_3SO_4^{2-}$: 45)
Electronic Energy = -1267.18519708 / Gibbs Free Energy =-1267.18981843

O	-1.295814526079	-0.615525198368	0.509808060592
P	-1.251019065406	1.000125935985	-0.040942530416
S	-0.513029847620	-1.871381349582	-0.241415867087
O	-0.335959787596	-2.832404385037	0.861622730193
O	0.768797407749	-1.289490928148	-0.739774632775
O	-1.400768049383	-2.336040567292	-1.322175010839
O	-1.714871329476	1.039119480246	-1.466687449919
O	-1.940878879818	1.777735661468	1.035943228476
O	0.358359210983	1.280555053625	0.063138928746
H	0.814247556649	0.484884557096	-0.300831806968

Protonated POS ($HPO_3SO_4^-$)
Electronic Energy = -1267.63859747 / Gibbs Free Energy =-1267.63205134

P	1.460956834798	0.029154522616	0.134902994698
S	-1.457894957143	-0.045626101343	-0.006932517070
O	2.605913575312	-0.018725233552	1.060647383293
O	1.451560994748	-1.174555764666	-0.921903467407
H	0.526650123683	-1.417319216046	-1.174165476140
O	-1.309778900432	-1.196628747875	-0.925521768609
O	-2.454739776590	-0.182924602091	1.045294577080
O	-1.392358792389	1.270188186069	-0.681041531699
O	0.019910018188	-0.085012554743	0.891167702918
O	1.369747187750	1.400229012279	-0.688642669737
H	0.429789482080	1.635345259351	-0.886260857320

$ROSO_3^-$: 46
Electronic Energy = -1048.87351623 / Gibbs Free Energy =-1048.73668369

C	-1.339944506743	0.667265379706	-0.299489178867
H	-0.483303300179	0.501823243379	-0.965031437428
H	-1.264255370440	1.698891676781	0.068232713574

C	-1.270060769532	-0.311843740453	0.888139608657
H	-1.365324771357	-1.333845719990	0.505600182012
H	-2.132895823583	-0.133886406659	1.543451401612
C	0.014429832104	-0.165137912529	1.672634861163
C	0.108384024665	0.747006517237	2.734037737762
C	1.155963546524	-0.902198245876	1.324986253171
C	1.307342694607	0.918533096043	3.430156376200
H	-0.768552414359	1.325137186788	3.018150934637
C	2.357902333213	-0.734417464149	2.016977226374
H	1.099357828220	-1.615695580440	0.505537106909
C	2.437683119124	0.177609877859	3.073264587230
H	1.357898969293	1.627479694040	4.252679196318
H	3.230121618894	-1.318303106175	1.734146739441
H	3.370701220522	0.307389556439	3.615143338452
C	-2.628767760319	0.542099171288	-1.098436007583
H	-3.502624772330	0.671741417846	-0.447276110820
H	-2.673072775337	1.291576864693	-1.897525216167
O	-2.660929926549	-0.776474958267	-1.681823994678
S	-4.094036776487	-1.186930308775	-2.432215574097
O	-5.116400053094	-1.167843682035	-1.363959656690
O	-4.301708940622	-0.156764519738	-3.472805128900
O	-3.764614896244	-2.528117027015	-2.946490418283

$ROPO_3H^-$: 47

Electronic Energy = -992.789285324 / Gibbs Free Energy =-992.644165603

C	-0.423949876064	-0.843242365958	0.755922142714
H	-0.629852990966	0.040259483238	1.373591888735
H	-0.814593298205	-0.629328447408	-0.247065352486
C	-1.150452594366	-2.067925995529	1.343811410257
H	-0.748142609921	-2.279800628002	2.342874681053
H	-0.933013654405	-2.946161804901	0.721768601445
C	-2.646220346118	-1.855906645104	1.426543191015
C	-3.234915504775	-1.323835667547	2.582639467948
C	-3.471459338037	-2.141330002486	0.328888544205
C	-4.609963165502	-1.083481596480	2.642767147891
H	-2.608816520153	-1.098698228274	3.443499955107
C	-4.846649842766	-1.902803467505	0.383148316446
H	-3.030204797777	-2.556498076829	-0.574871170435
C	-5.421229675874	-1.372204221724	1.541875937215
H	-5.047512865664	-0.674094774026	3.549732620351
H	-5.469506984630	-2.134206246524	-0.477177474121
H	-6.491347673826	-1.188487550957	1.587322206158
C	1.081095992771	-1.054462840823	0.671533599593
H	1.503174349359	-1.244538328909	1.667311453035
H	1.311183829578	-1.923198679671	0.038304560971
O	1.673940196089	0.122403274146	0.109056826337
P	3.311013146244	0.130384753750	-0.125183817592
O	4.010721499265	-0.381418946926	1.099272551983
O	3.480717615055	-1.058065838540	-1.269842926445
H	3.137260976288	-0.737434626571	-2.120065507425
O	3.613984974403	1.467028629545	-0.736442513942

POSOP ($(HPO_3)_2SO_4^{2-}$: 48)

Electronic Energy = -1834.96655558 / Gibbs Free Energy =-1834.9539787

O	-0.964298502768	-0.510663050984	0.095498394899
P	-2.510858522320	-1.010098058175	0.768398223570
O	-2.304304423642	-2.409684861191	1.292056237603
O	-2.869124167733	0.128889076490	1.652000286176
O	-3.401147955071	-1.006893495191	-0.560958633918
H	-3.274857790231	-1.852426688363	-1.102101259698
S	0.171058236295	-1.443223786524	-0.525707639068
O	1.084281982194	-0.539563687433	-1.206953191122
O	0.701230240046	-2.336066505682	0.491639797468
O	-0.579096666693	-2.253154543267	-1.664906727057

P	-1.526698830284	-3.750768387977	-1.692257453043
O	-2.923908167144	-3.215139573599	-1.896389005478
O	-0.853600071603	-4.605436877163	-2.702920853697
O	-1.314231922596	-4.319178985075	-0.216419749818
H	-1.696235118462	-3.675169105876	0.459754083189

Protonated POSOP ($H(HPO_3)_2SO_4^-$)

Electronic Energy = -1835.39913704 / Gibbs Free Energy =-1835.3773535

O	-1.529048800565	0.778808877735	-0.220693073102
P	-1.743276519288	-0.810603099459	0.223664833334
O	-1.085333123300	-1.100854876013	1.522060387105
O	-1.292404355801	-1.645414290911	-1.020788238059
H	-0.259931962040	-1.808638022179	-1.013033427020
S	-0.108724499966	1.612927861416	-0.047990662803
O	-0.271935077241	2.748684151709	-0.926937348153
O	0.130443526126	1.801450801298	1.366573993814
O	0.924417669400	0.632067298906	-0.704079704280
P	1.920754436065	-0.741505571523	-0.105233356058
O	1.215921564704	-1.888619824101	-0.792703896365
O	3.315724330681	-0.357011110323	-0.403389738657
O	1.622618855154	-0.709028818335	1.462565542741
H	0.675727279155	-0.925264991244	1.667775504088
O	-3.324221283029	-0.896458765477	0.282926381452
H	-3.768414950050	-0.895358021505	-0.584753798029

$ROSO_3PO_3H^-$: 49

Electronic Energy = -1616.63677101 / Gibbs Free Energy =-1616.48400844

O	2.815301447172	-0.038027973862	-0.561078427213
P	3.241495259773	-0.863917505804	0.967188850455
S	1.860590671689	1.219600645335	-0.649632559391
O	1.128137457841	1.377458634800	0.606128431431
O	0.856301749483	0.747093569683	-1.811574588900
O	2.568502567025	2.355290455244	-1.205796297018
C	-1.351046998038	0.041571936840	-0.973396788465
H	-1.194196745025	0.623754885951	-0.060014417109
H	-1.836808645138	0.698535875269	-1.704284800644
C	-2.256963649621	-1.168493243507	-0.669695311474
H	-1.748299664002	-1.822885151656	0.050005669921
H	-2.402216882768	-1.754219155680	-1.586183072961
C	-3.596516307264	-0.737145410526	-0.113596663845
C	-4.687261653971	-0.505186332746	-0.963036772125
C	-3.759278050799	-0.513609981860	1.261264060288
C	-5.910530829193	-0.062310235696	-0.453628028289
H	-4.576629851952	-0.675674620313	-2.031808822720
C	-4.979979703254	-0.070746824144	1.775533543192
H	-2.921776540541	-0.691091339519	1.932733465767
C	-6.060797167259	0.156593984607	0.918538356350
H	-6.746099301594	0.108337273453	-1.127531473882
H	-5.088091379426	0.093183456212	2.844580838390
H	-7.012279614860	0.498319393758	1.317023865335
C	-0.004701786600	-0.409799134368	-1.514014742979
H	0.514238863936	-1.072827205694	-0.815980105012
H	-0.096597439218	-0.918207023252	-2.475777063340
O	3.830830152687	0.188090927325	1.840896778646
O	3.944986234137	-2.075256699997	0.474073992217
O	1.740784586893	-1.284591473354	1.442868226328
H	1.243275119888	-0.485802146499	1.702182877070

HSO_4^-

Electronic Energy = -699.852686245 / Gibbs Free Energy =-699.863727569

O	-0.979754187228	-0.438125139331	0.797270117584
O	-1.561651524229	1.967276762607	0.828123910568
O	0.026403386478	1.100522558545	-0.878441212429
O	-2.333705662084	0.529639166460	-1.073129447383

H	-3.127116954526	0.303766964716	-0.553082641497
S	-1.101762818412	0.815529677001	0.024205193156

$H_2PO_4^-$

Electronic Energy = -643.771744966 / Gibbs Free Energy =-643.774758683

O	-2.711384848174	1.530638797457	-2.171487122279
O	-4.092744520192	2.496262942332	-4.107207237778
H	-3.805545036764	3.298815875505	-3.641786926024
P	-3.815859453293	1.183994837320	-3.132640398524
O	-3.776511279083	-0.009261586924	-4.036987001093
O	-5.229153652645	1.089527477143	-2.268326838476
H	-5.084530439851	1.504023657165	-1.402307225824

PEP^-

Electronic Energy = -909.749353511 / Gibbs Free Energy =-909.7110822

C	0.986299629657	1.004718245410	-0.113912068489
C	2.264934554899	0.223613210351	-0.277550039101
O	3.321140173334	0.614073636327	0.455683414282
H	3.041239725211	1.246209667729	1.141373783330
O	2.395889035773	-0.691704659133	-1.073630120993
O	-0.168767834466	0.356795267264	-0.411625319762
C	1.003703237900	2.318648777049	0.153133120653
H	0.075843204342	2.877938344158	0.202450091816
H	1.930401634886	2.869272750665	0.269866680885
P	-0.478697534709	-1.195417156455	0.239230845578
O	0.462644658787	-1.356268239056	1.397359377707
O	-1.962124222633	-1.293308394216	0.368794605426
O	-0.019116025252	-2.105349364938	-1.038789519823
H	0.884383862276	-1.818553885151	-1.293327391510

PEP-H

Electronic Energy = -910.197377321 / Gibbs Free Energy =-910.150056356

C	-0.223567371120	-1.402195926277	0.497656050915
C	-0.793202466676	-2.363580729059	-0.489761589199
O	-0.029397682918	-3.439191479900	-0.679527559290
H	-0.457589724008	-4.002188709662	-1.354081317022
O	-1.855530869728	-2.191814119149	-1.078196971198
O	-1.070963360245	-0.374772712647	0.882840631678
C	0.984907289008	-1.529148377359	1.048394989086
H	1.343893934429	-0.793258585933	1.759215055674
H	1.620964949276	-2.368569985771	0.798084670443
P	-1.532455298459	0.870124183301	-0.073900128639
O	-1.786327700382	2.079997347547	0.726238141397
O	-0.390415449547	0.956654548468	-1.200967156963
O	-2.777589210984	0.323188046826	-0.886578539478
H	-2.661973278688	-0.649374729673	-1.060194735756
H	0.427008640033	1.387619139293	-0.892370681684

Pyruvate (CH_3COCOO^-)

Electronic Energy = -341.979953415 / Gibbs Free Energy =-341.961703762

C	0.816085483098	-0.234249868616	0.003728149777
O	0.903230107967	-1.490509440180	0.011140108535
O	1.725433686207	0.628658283166	0.000054321028
C	-0.659056335166	0.316909164641	-0.001535560315
C	-1.768813523195	-0.717383800577	-0.001445220634
H	-1.672438627493	-1.365001874169	0.876843257763
H	-2.748061051155	-0.230431850380	-0.006720845094
H	-1.666359012746	-1.372000140492	-0.873827169775
O	-0.903725727514	1.514405526610	-0.005200041283

Pyruvic acid ($CH_3COCOOH$)

Electronic Energy = -342.436347515 / Gibbs Free Energy =-342.404616803

C	-2.687406874957	0.686694642396	0.309518773293
O	-3.049209710068	-0.339291887288	0.840138866685

O	-3.467959855914	1.760536972044	0.163889708741
H	-2.929242770925	2.443488255804	-0.294781306389
C	-1.265474746272	0.889307161243	-0.273356081299
C	-0.317033149778	-0.261276488821	-0.158616537446
H	-0.738829523187	-1.136238943682	-0.666844769159
H	0.648646523427	0.000992774036	-0.592710866577
H	-0.200465115520	-0.538270363756	0.895464152052
O	-1.017082466811	1.968473448021	-0.784034909897

$HNEt_3^+$

Electronic Energy = -292.922599539 / Gibbs Free Energy =-292.744371097

N	0.003446190682	0.000513001261	-0.012691192804
C	-0.762566440684	-1.236197833832	0.431731715644
H	-0.070742886440	-2.076012183983	0.365250211322
H	-1.007231947487	-1.074625119146	1.484039411239
C	-1.997041976870	-1.494872487453	-0.420726919478
H	-1.728288547571	-1.663304467900	-1.469079118509
H	-2.485319008082	-2.400515504194	-0.049428385960
H	-2.724612321620	-0.680193891167	-0.369761243113
C	1.454231988378	-0.043803717288	0.442534297221
H	1.830614414329	0.978117422957	0.396849019114
H	1.430690602405	-0.354359299117	1.489383024850
C	2.306466083343	-0.963971196649	-0.419929323719
H	2.318826638767	-0.629639162559	-1.462831866805
H	3.333420455023	-0.932485714619	-0.044678598899
H	1.971439689700	-2.004277359191	-0.386417377361
C	-0.685491510670	1.280433966098	0.435374328471
H	-1.758747879796	1.098386782989	0.380244153706
H	-0.413708192369	1.414769981792	1.484822518493
C	-0.303232250272	2.477916354791	-0.423461886633
H	-0.838769661052	3.354503110060	-0.047553158009
H	0.766863134009	2.700569902975	-0.386333504516
H	-0.596595100286	2.326130343569	-1.467680942789
H	0.009090896568	0.000831780604	-1.038881311466

Int1a

Electronic Energy = -1692.65401854 / Gibbs Free Energy =-1692.48685781

C	1.382592031227	-0.833787398685	-1.292114792775
H	1.612479888906	-1.833695785977	-1.685002626967
H	2.327669918626	-0.294810803326	-1.185126078630
C	0.729054877683	-0.937933562532	0.097344256701
H	-0.170146751740	-1.566227716500	0.046083542671
H	0.408933640553	0.069551554268	0.390416172861
C	1.686977620831	-1.475057153238	1.138547687034
C	2.765089727773	-0.679028018393	1.561110998863
C	1.555612892254	-2.763555392082	1.672153907067
C	3.686175360879	-1.163415992379	2.490214724394
H	2.890403053329	0.317460834371	1.147172678943
C	2.475426938741	-3.250531553544	2.607642896944
H	0.726766033997	-3.392633074354	1.352851914197
C	3.544893485356	-2.451455260109	3.019782108347
H	4.514740702366	-0.527224223942	2.789619922111
H	2.355803894620	-4.253201089411	3.011414518933
H	4.261728627153	-2.829051385574	3.744915078725
C	0.519315169863	-0.065352874752	-2.293157272504
H	-0.399286277667	-0.621418158299	-2.522396863939
H	0.228308202890	0.892666611236	-1.837044865032
O	1.187177834528	0.147132971136	-3.535204121408
H	1.954616870047	0.717172096312	-3.322399859938
O	4.426565877349	3.128323747875	-0.708142527712
P	2.885763468642	2.843381385244	-1.367963720009
S	5.389457811739	1.948957121669	-0.029940668266
O	6.740453904210	2.503625776228	-0.219436389764
O	5.129441158874	0.725216247049	-0.844705699201

O	4.969862838015	1.827172210690	1.376198809235
O	2.017732172243	2.198626113435	-0.331279046001
O	2.504686439353	4.124758485703	-2.039273444039
O	3.311454971440	1.763773485558	-2.544186341152
H	3.962722008197	1.138204671670	-2.138335473671

TS1

Electronic Energy = -1692.62023556 / Gibbs Free Energy =-1692.45504314

C	0.999506072164	-0.743655156223	-1.215365917673
H	1.136658506275	-1.708298711308	-1.723621291287
H	1.978084339079	-0.264184857161	-1.164231579347
C	0.502347165114	-0.971769094299	0.224809627616
H	-0.375946058838	-1.629130352119	0.235518579801
H	0.185208720897	-0.002761637713	0.631162124450
C	1.600986929964	-1.533509866739	1.102904136394
C	2.707462299123	-0.726112856159	1.417178200522
C	1.572112095113	-2.847121638759	1.585575786829
C	3.757349875941	-1.220360539622	2.190638851968
H	2.750021180358	0.294659237065	1.044911426534
C	2.622224578902	-3.346919540954	2.364333703760
H	0.722879372333	-3.485410387050	1.349741485226
C	3.718221733166	-2.535713886697	2.668289979592
H	4.599163721720	-0.568834107878	2.407874454404
H	2.582489297972	-4.370113880278	2.730389315802
H	4.534976308910	-2.924966273460	3.271057921583
C	0.091835374830	0.171098063953	-2.039303675125
H	-0.767413722429	-0.379335973054	-2.449775602770
H	-0.285680092677	0.981374901148	-1.410132058554
O	0.799844350900	0.824506356538	-3.110290108283
H	1.542697529067	0.257599814426	-3.375531861863
O	4.786952713218	3.304521100870	-0.497727788741
P	2.610615475345	2.371258933040	-1.861528856464
S	5.597893911446	2.309543959066	0.263651172812
O	7.027583430999	2.667981558875	0.370779578360
O	5.597566498975	0.968777244602	-0.667352457151
O	4.984778622298	1.925707807791	1.556635686170
O	1.829473347224	2.280021994627	-0.592123672383
O	2.494463460010	3.552269965775	-2.770112231471
O	3.529754239029	1.233482980554	-2.261181891030
H	4.783688222625	1.016096917298	-1.266960025185

Int1b

Electronic Energy = -1692.6423495 / Gibbs Free Energy =-1692.4795784

C	1.226877721234	0.059924061996	-0.374683399150
H	1.384580991916	-0.681143698489	-1.165744353976
H	2.214020365770	0.351291724920	0.004891931400
C	0.391034422111	-0.565740700366	0.758509797946
H	-0.603978037454	-0.815284067393	0.367185011537
H	0.243287950364	0.173878517771	1.555605453431
C	1.044727581650	-1.808922019643	1.320167999422
C	1.852459571984	-1.749375921829	2.463983503487
C	0.889955383164	-3.044923662378	0.674831331154
C	2.487518899736	-2.893865067348	2.954022998873
H	1.982766770596	-0.798160958182	2.975672719879
C	1.521754817492	-4.191531892259	1.160301213050
H	0.266681671384	-3.105369406166	-0.214980286147
C	2.323763134764	-4.119638301371	2.303491065726
H	3.107187881210	-2.828012196851	3.844705655430
H	1.385535143718	-5.140997951039	0.648930595301
H	2.814031225384	-5.011439493508	2.684685230282
C	0.525115998106	1.268081252798	-0.973588349389
H	-0.454901590855	1.003461995276	-1.373716770860
H	0.411451440653	2.074940854081	-0.245430972017
O	1.329828802193	1.819780034139	-2.055811020587

H	1.531244409583	1.066595278442	-2.719783649519
O	1.747930426577	-0.170801269654	-3.656056182715
P	0.565553130364	3.312061211858	-3.053286219213
S	0.457883838194	-0.557873567369	-4.342470985992
O	0.609895600360	-1.770585389663	-5.164830382286
O	0.169758201271	0.630782264442	-5.384783210540
O	-0.670450342244	-0.600862246701	-3.386702599794
O	-0.889312127644	3.160795780484	-2.706952273080
O	1.362324937613	4.447377708308	-2.477445615597
O	1.007918224127	2.812161584636	-4.434555464952
H	0.488433595710	1.545930110072	-4.970480099894

TS1'

Electronic Energy = -1692.64268543 / Gibbs Free Energy =-1692.48187878

C	1.202635089259	-0.038246558247	-0.364438270404
H	1.422214448936	-0.796848491272	-1.124616159351
H	2.162114704333	0.310405401356	0.036563488753
C	0.359559645820	-0.666072735886	0.762570938818
H	-0.600850538467	-0.997010801841	0.346079827008
H	0.132614854658	0.098419857433	1.516522532145
C	1.067489690113	-1.835223210687	1.411534443171
C	1.812768585358	-1.666151989406	2.586473488197
C	1.028434303024	-3.107525871843	0.821863779938
C	2.500457480003	-2.738788147734	3.160475783594
H	1.851728581521	-0.685623629753	3.056147359521
C	1.713957380223	-4.182724914420	1.391014846008
H	0.453305877384	-3.253921748291	-0.090096795136
C	2.453112754373	-4.001538694776	2.564052395186
H	3.069900430643	-2.588314929955	4.074101402591
H	1.668587292118	-5.161988299104	0.921425261403
H	2.984976097949	-4.837699788162	3.010138860052
C	0.471983716961	1.121403530333	-1.021865382051
H	-0.482682793633	0.808788649306	-1.450055033052
H	0.300509860713	1.940893188744	-0.320431809902
O	1.298913345906	1.665405192144	-2.091984286832
H	1.442157157692	0.903449248291	-2.806963565733
O	1.563187065916	-0.216124973710	-3.734240919354
P	0.673441260487	3.227085573661	-2.964821484153
S	0.300818425511	-0.433198246643	-4.563507814087
O	0.475218826720	-1.570420830101	-5.487752298389
O	0.151373080112	0.865691377946	-5.446719767315
O	-0.887733746512	-0.541816318179	-3.684888722015
O	-0.804396264825	3.147237961147	-2.713772701447
O	1.508462434542	4.288394525408	-2.313659482696
O	1.148244237256	2.812563270535	-4.380975416889
H	0.598186928060	1.782885136889	-4.925896029266

Int1c

Electronic Energy = -1692.66229146 / Gibbs Free Energy =-1692.49537512

C	1.212085758584	0.336949627099	-0.379208830213
H	1.475038685771	-0.364040519765	-1.174656271595
H	2.145579747070	0.680885533570	0.084039691664
C	0.342508446480	-0.401705658089	0.654446293822
H	-0.630914251657	-0.615949667532	0.193519947791
H	0.150753416340	0.244992716892	1.519776493901
C	0.974387271500	-1.702557283144	1.101216288160
C	1.504738755604	-1.861343475217	2.387325413798
C	1.059016569046	-2.778976127488	0.201981537635
C	2.103641755689	-3.065195973225	2.773154735579
H	1.447083628445	-1.036238064216	3.094129656940
C	1.655567133657	-3.981443961426	0.583603625530
H	0.656640977205	-2.658734599153	-0.802094141428
C	2.180433535366	-4.129668224241	1.872437881748
H	2.507820280627	-3.169800008372	3.776969813351

H	1.710445121121	-4.805448641240	-0.123633458981
H	2.643903511715	-5.066584932806	2.170264572456
C	0.472978737641	1.510011349966	-1.005674580821
H	-0.499926044252	1.185832281781	-1.387118524378
H	0.302875877080	2.310412863519	-0.275019508278
O	1.266840536516	2.014224273065	-2.101286413259
H	1.693624175866	0.698856617891	-3.119764330960
O	1.850125595455	-0.111683969830	-3.683081642878
P	0.691786009341	3.344745677400	-2.973850273712
S	0.394789972265	-0.751230114915	-4.078043057005
O	0.755531483836	-1.789160704991	-5.058664057733
O	-0.385836664711	0.385391821584	-4.659064357712
O	-0.208011124078	-1.263240823827	-2.828576100217
O	-0.773237458724	3.489834725196	-2.669960723866
O	1.653581134280	4.478188136610	-2.766223029001
O	0.938410069444	2.770385453542	-4.479494620830
H	0.407845493339	1.947401503588	-4.629787875535

Int2a

Electronic Energy = -1692.65822584 / Gibbs Free Energy =-1692.49066393

C	2.409664376645	0.936208131933	0.127112003992
H	2.822201053035	0.489520904739	-0.782132290669
H	3.070042585566	0.643585671309	0.955504026949
C	0.992146943419	0.379624701536	0.351148685612
H	0.350271871247	0.753476429963	-0.456522987575
H	0.580816685916	0.765458320362	1.293672089372
C	0.945053464211	-1.133728105348	0.352095326352
C	0.566780372646	-1.855570943573	1.491781714408
C	1.289696808955	-1.848953656048	-0.808906849328
C	0.526747357066	-3.253897449007	1.480648931727
H	0.298200439177	-1.316890120505	2.398430826861
C	1.250935101392	-3.244133079403	-0.822046973337
H	1.606516362866	-1.304045752458	-1.694698541727
C	0.867663539220	-3.954122673799	0.321605698506
H	0.229169755636	-3.793088706159	2.376842935054
H	1.520500926604	-3.781150032750	-1.728617380312
H	0.836946113110	-5.040669140178	0.308262027856
C	2.421945097506	2.459498611921	-0.043846382710
H	1.608552679045	2.749978560162	-0.721785076270
H	2.238881889229	2.949715766243	0.922885502613
O	3.671500107588	2.941995174474	-0.530131430179
H	3.672400897624	2.742866104348	-1.496877451818
O	1.266704805887	1.027723040978	-2.903386865768
P	2.823255353950	1.043032718965	-3.566855776841
S	0.030772031454	2.064659588510	-3.299200596542
O	-1.135331271789	1.369152029274	-2.731688360656
O	0.047274053862	2.102477209648	-4.793094134109
O	0.332906645307	3.369587311007	-2.687296810071
O	3.476443906117	2.365247840863	-3.241270677236
O	3.444998937224	-0.244799577436	-3.124244907222
O	2.471183186450	0.956585101552	-5.157207635554
H	1.609254184595	1.417330639093	-5.313139489287

TS2

Electronic Energy = -1692.5804377 / Gibbs Free Energy =-1692.4185942

C	1.430648908828	-0.039806288894	-0.301672487359
H	2.228105474753	-0.542013940139	-0.864043647992
H	1.909821427588	0.495118521689	0.528535047330
C	0.446476913759	-1.088674909464	0.250368595604
H	-0.024922553632	-1.611038535507	-0.592591522463
H	-0.357743509586	-0.577153550616	0.795351927978
C	1.127088014347	-2.088482618160	1.158770921107
C	1.158639043422	-1.897403080232	2.547461770163
C	1.787542611336	-3.205197449182	0.624695125112

C	1.829600796518	-2.795550178369	3.381587432889
H	0.650406762672	-1.037003934345	2.977795735642
C	2.460043825080	-4.105978706963	1.453342442075
H	1.771629995553	-3.367984025317	-0.450961992403
C	2.483727615369	-3.903786518328	2.836658497168
H	1.838958567916	-2.631035810734	4.456119611959
H	2.962777220823	-4.966862788303	1.019945762675
H	3.004499764388	-4.604912628073	3.483417988294
C	0.743829221346	0.965050989644	-1.227200782706
H	0.264346828855	0.445573476303	-2.066387913192
H	-0.026332419395	1.524409422677	-0.681197940078
O	1.674837417329	1.913199945586	-1.729924023457
H	2.296201686806	1.401375524566	-2.395719393989
O	0.800018615895	1.307136765367	-4.292970912515
P	2.212414607226	0.794018989712	-4.676796197362
S	0.558697236411	3.544789023782	-3.089842090211
O	-0.619264752710	3.477468249303	-3.961438023025
O	1.836545679628	3.987494638735	-3.669302852048
O	0.233554559699	4.043294518867	-1.746049400160
O	3.092620628159	0.667473517147	-3.402577214938
O	2.228078600710	-0.412792455679	-5.593318235069
O	2.889016888246	2.041205176967	-5.569064174363
H	2.651577410686	2.862445724028	-5.098575299024

Int2b

Electronic Energy = -1692.66039709 / Gibbs Free Energy =-1692.49439445

C	1.151964613693	0.548082811513	-0.391055023355
H	1.784862618824	0.082857979663	-1.150074536287
H	1.801726367506	0.991625752391	0.373527343363
C	0.248442535345	-0.528490006760	0.238503988550
H	-0.468542426134	-0.867579383678	-0.521515940218
H	-0.338562816430	-0.096613790552	1.058427829143
C	1.045833600705	-1.715489755429	0.734426024299
C	1.234243203800	-1.955337350434	2.101093281601
C	1.641017588991	-2.591001510604	-0.188492859433
C	1.995440592904	-3.043446946289	2.540125901367
H	0.780118890662	-1.285547709516	2.828192325547
C	2.400970560386	-3.677996801623	0.244898454959
H	1.505431716945	-2.408750054023	-1.252497243520
C	2.580861377628	-3.908722569684	1.613242432756
H	2.128716065106	-3.214233291848	3.605426958266
H	2.851722613738	-4.346807887577	-0.483937765782
H	3.171170731339	-4.755998653356	1.952031986873
C	0.330288003799	1.624017083698	-1.080792020368
H	-0.321157145395	1.173626007960	-1.831046863507
H	-0.270576985075	2.203614208312	-0.368846940730
O	1.262109849097	2.512756172292	-1.750088459008
H	2.644372405595	1.578138580357	-2.569889205893
O	1.081770751441	-0.305842043177	-3.573829080080
P	2.370912868253	0.166902422081	-4.203038102964
S	0.617745533711	3.679434555352	-2.771440147918
O	-0.700669424696	3.177630005321	-3.195185688087
O	1.638808393234	3.701006827603	-3.850842515665
O	0.586684174701	4.910168127885	-1.963863629056
O	3.249022960900	0.998997195559	-3.080924506990
O	3.304553804364	-0.814509812939	-4.855551490794
O	2.048624003801	1.351199387168	-5.303950291616
H	1.840664268971	2.196139348858	-4.841043745764

Int3b

Electronic Energy = -2602.86136214 / Gibbs Free Energy =-2602.6248202

C	-4.714653025801	-2.791679147741	4.231045222116
H	-4.055849213518	-3.370673775628	4.891485174453
H	-4.379123259148	-1.747297595645	4.281967780116

C	-6.169047215689	-2.895403628589	4.728871360629
H	-6.488002929517	-3.945241226826	4.685191197711
H	-6.822429233646	-2.338615057728	4.043721391648
C	-6.336160600825	-2.366280905265	6.135824201259
C	-6.634480124925	-1.014821311172	6.363835838781
C	-6.147841300760	-3.202526145020	7.246010840424
C	-6.742918705070	-0.511514895244	7.662448484004
H	-6.785250321501	-0.352793099100	5.513587493219
C	-6.255113666456	-2.704994108837	8.546990018033
H	-5.916992675664	-4.253740765225	7.086549138654
C	-6.553492509829	-1.356033740830	8.760052373514
H	-6.978764267808	0.538410256502	7.816957243471
H	-6.109089115322	-3.370987074919	9.393665339509
H	-6.640495077750	-0.967479207966	9.771241007150
C	-4.547911260566	-3.302335152734	2.798302710571
H	-4.891587070317	-4.344756091570	2.727928780362
H	-5.177534282750	-2.712611705294	2.118276773513
O	-3.212887570387	-3.177139223218	2.332015939848
H	-2.673163237824	-3.835241178419	2.831101185236
C	-1.219656539380	-8.200806528689	2.137683657224
C	0.098392470426	-8.816719705392	2.523695757883
O	0.867763675548	-9.299039750572	1.533025651665
H	0.528314851185	-9.008120356560	0.668112201315
O	0.470257831492	-8.937129285109	3.679931497061
O	-1.762724318865	-7.332108237679	3.033162928103
C	-1.899814547723	-8.603545229801	1.055697955603
H	-2.865834116022	-8.173530073703	0.827319608828
H	-1.529619886922	-9.388671216577	0.405752164146
P	-0.849682958368	-6.038910929193	3.644383042256
O	0.326337765592	-5.860949472532	2.733136956549
O	-1.832052278449	-4.939814176444	3.931729601527
O	-0.423789472297	-6.677825358608	5.085004844236
H	-0.035546631639	-7.561719399400	4.906659187494
P	-4.883649965199	-7.377983261904	-1.713633049527
S	-3.493822251651	-5.324202930513	-0.142362727193
O	-4.718534829628	-8.420758119192	-2.743169168338
O	-5.431985117934	-7.967215238156	-0.325537813956
H	-5.181968123291	-7.371443357495	0.422646392655
O	-4.106218636594	-5.988030267425	1.026570019463
O	-2.073571927544	-5.021686062622	-0.081275617695
O	-4.365216448467	-4.316395608394	-0.785611729097
O	-3.504003709332	-6.620996805550	-1.326061437512
O	-5.876524726190	-6.197703569543	-2.156834399373
H	-5.585417354777	-5.329219373040	-1.784501462335

TS3

Electronic Energy = -2602.84901783 / Gibbs Free Energy =-2602.60982884

C	-4.954361440444	-3.194750793064	4.206215991623
H	-4.135514913252	-3.487600934638	4.874567022726
H	-4.754562784664	-2.166628134980	3.880012977831
C	-6.292191411370	-3.250753398660	4.968842445295
H	-6.478777377760	-4.284152778213	5.289063357191
H	-7.107727777858	-2.977540057806	4.286911500111
C	-6.297204244296	-2.331534178732	6.170477881685
C	-6.776158664718	-1.017742016611	6.069285684776
C	-5.777548047890	-2.759656809321	7.400973533495
C	-6.739488117731	-0.153803349938	7.166750769047
H	-7.183423128709	-0.670798135927	5.121971319812
C	-5.738197128934	-1.900219301545	8.501209480903
H	-5.402984627350	-3.776715202391	7.495637375668
C	-6.219888832210	-0.592738458126	8.387642953052
H	-7.119204573114	0.860010925172	7.068871643939
H	-5.335000664839	-2.252118680254	9.447337337424
H	-6.192859600054	0.076609005314	9.243323352213

C	-4.952389486644	-4.114862689086	2.990532995378
H	-5.143609203642	-5.155170579764	3.281894710510
H	-5.718372384781	-3.816198815787	2.268175741187
O	-3.695311266560	-4.031949703212	2.300050649124
H	-2.994237734749	-4.465027974296	2.898544439634
C	-0.972686407047	-8.084431011482	1.850101712276
C	0.266197185151	-8.741239724292	2.393459635967
O	1.211011666368	-9.108985586760	1.511498194296
H	1.028280945500	-8.724403772546	0.636020190256
O	0.433365973117	-8.987901481007	3.577841981182
O	-1.699676434384	-7.348490575576	2.739204272248
C	-1.428899182505	-8.341184926553	0.616848594727
H	-2.341893919006	-7.892144600532	0.246386666888
H	-0.912973186949	-9.032689157501	-0.041115291122
P	-0.988535578770	-6.151345299094	3.686017937929
O	0.308350573835	-5.760340538120	3.050111574155
O	-2.081793921284	-5.148546190966	3.968067832733
O	-0.783506048849	-6.978166398333	5.075085015021
H	-0.330458876081	-7.819610366028	4.846500641384
P	-4.702733647546	-7.212736422576	-1.961669377384
S	-3.622565895477	-5.230194479927	0.472546899211
O	-4.664721002101	-7.996460200075	-3.230169888903
O	-5.221091141320	-8.196051151446	-0.760462010867
H	-4.989045686758	-7.779222964950	0.094745584807
O	-4.215111312369	-6.379047304019	1.159623284334
O	-2.186722242027	-5.036214780484	0.426654711344
O	-4.524940674686	-4.302222089492	-0.214060932766
O	-3.443755188858	-6.500290988836	-1.452860810924
O	-5.876403357970	-6.071111480109	-2.063657921761
H	-5.607563402570	-5.293154840458	-1.533667030068

Int3c

Electronic Energy = -2602.87333713 / Gibbs Free Energy =-2602.63505595

C	-5.075282817281	-3.220402571873	4.165151571302
H	-4.331942737097	-3.649904009295	4.847799264388
H	-4.725413844831	-2.217333917652	3.893901161515
C	-6.436581830637	-3.122254628135	4.881130645563
H	-6.782200131888	-4.131800371970	5.137234718370
H	-7.176369403286	-2.697358962634	4.190903169802
C	-6.348876726440	-2.274070290002	6.131235032041
C	-6.546468339576	-0.887157078424	6.071754648623
C	-6.016998279399	-2.850106816393	7.365772697484
C	-6.417272862967	-0.095095070663	7.215128053982
H	-6.804819768643	-0.426098652561	5.120822672426
C	-5.886811406230	-2.062632788737	8.512223290557
H	-5.860941030361	-3.925028686257	7.427405815715
C	-6.086613397677	-0.681069443634	8.440321713924
H	-6.577634157109	0.977983846425	7.149792581239
H	-5.632486827128	-2.527952560491	9.461038932343
H	-5.988137299510	-0.067017507603	9.331474248124
C	-5.161861128167	-4.076965464869	2.912153570182
H	-5.461324416757	-5.104429330945	3.143214979293
H	-5.864377524677	-3.654914342080	2.185458267879
O	-3.839503745235	-4.098318773882	2.311403751315
H	-2.685767803949	-4.797415951287	3.376994683208
C	-0.934496378289	-8.022236197852	1.771718445904
C	0.239610961794	-8.785952703881	2.304252033623
O	1.042986432955	-9.418361613269	1.439836602696
H	0.824683002931	-9.207078636192	0.516014318560
O	0.489269784582	-8.862147650448	3.499454819498
O	-1.635745512267	-7.315706638974	2.730816785408
C	-1.396373132974	-8.090777124376	0.520169555423
H	-2.261933833565	-7.526062921280	0.197366714966
H	-0.936743491874	-8.731415794148	-0.225175740303

P	-0.959176064664	-6.148134475875	3.656164240712
O	0.192432491792	-5.483071956410	3.005584839795
O	-2.204138284607	-5.280940840040	4.102265325159
O	-0.661664991445	-6.898312471483	5.039761859626
H	-0.204408425739	-7.742038060514	4.810494859845
P	-4.602497143767	-7.391139288447	-2.100834204835
S	-3.690882767016	-4.983948409409	0.879730573777
O	-5.091083430638	-8.260539462068	-3.222841295575
O	-5.007134383311	-8.155783889015	-0.699515346678
H	-4.726201613519	-7.592081376572	0.054332208359
O	-4.238182408337	-6.312562525600	1.233476008514
O	-2.242150578377	-4.907893414977	0.690511272663
O	-4.513618532803	-4.254871139822	-0.111873808539
O	-3.160860284854	-6.947542292673	-2.020350457892
O	-5.566740271514	-6.052717716653	-2.062766825196
H	-5.184631970721	-5.379318560711	-1.459093263971

Int4a

Electronic Energy = -2035.11012456 / Gibbs Free Energy =-2034.89051447

O	-0.323941856081	0.276416010447	0.944547191434
P	-0.245900473791	-1.349281930407	0.923773009089
S	-1.511836524173	1.212753998604	0.087974470233
O	-2.746887308392	0.439678306985	0.276724132594
O	-0.990373048267	1.260212426309	-1.282887538069
O	-1.439646843094	2.477457796811	0.832525205297
O	0.962199336514	-1.772091431402	1.671103067683
O	-1.586872266443	-1.894087210782	1.591572716456
O	-0.251092503869	-1.810410800380	-0.587462051226
H	-1.147062269698	-1.786986593600	-1.091370244768
C	-5.637029795223	1.850714550939	-0.481015999679
H	-5.205096177415	0.851713823030	-0.370601491825
H	-5.133629588721	2.485390768015	0.259439727019
C	-7.149374932205	1.807965175401	-0.196362650554
H	-7.651821311897	1.236475022141	-0.988257505005
H	-7.555763234798	2.828087694737	-0.241202428735
C	-7.459328568405	1.187453727467	1.148750620373
C	-7.204037860904	1.891050866558	2.335924818012
C	-7.961791975555	-0.117476785928	1.246327978236
C	-7.438078231272	1.306909674297	3.582210525148
H	-6.815740128108	2.905803674627	2.279361726110
C	-8.197356482269	-0.708313545293	2.491098828642
H	-8.172224209967	-0.676669227261	0.337866845175
C	-7.934751485562	0.002041514575	3.664837693320
H	-7.234032327417	1.870041745475	4.489415723925
H	-8.586886600350	-1.721969413419	2.541992909190
H	-8.116799522659	-0.454184338749	4.634225919032
C	-5.310881126830	2.361125424574	-1.885450281311
H	-5.862480025275	1.759709448183	-2.626912529712
H	-5.645481188573	3.401264069733	-1.997735550514
O	-3.917971762516	2.346140993299	-2.163802391729
H	-3.665724111858	1.399732826152	-2.199740926123
C	-3.488229473088	-1.305164813850	-1.881497573714
O	-4.045674095750	-0.425870360276	-2.572575003561
O	-2.328731585076	-1.787005520476	-2.025619146004
H	-2.395749220273	-1.886940896988	1.005376845127
C	-4.367686557695	-1.923125879473	-0.764015935686
C	-5.829972566313	-2.098217333211	-1.081692680999
H	-5.936704255090	-2.800400321452	-1.918829914558
H	-6.370260256945	-2.472709041929	-0.210057331618
H	-6.246994358057	-1.145171721508	-1.417344861018
O	-3.911636766706	-2.256561625731	0.325159938234

TS4

Electronic Energy = -2035.08000571 / Gibbs Free Energy =-2034.85769271

O	0.153792810290	0.360727880760	0.874670911614
P	0.277409778772	-1.150398926547	0.836307220880
S	-1.956615476741	1.408258524617	-0.552727782750
O	-2.632570398025	0.407962961280	0.256477915100
O	-1.126410162423	1.023182542776	-1.676888716671
O	-1.816483534864	2.749391330308	0.000599575027
O	1.546610858946	-1.775831574804	1.347509183309
O	-0.972891692162	-1.843072180578	1.650776077627
O	0.040382063714	-1.719430926467	-0.682624091101
H	-0.867497641794	-1.568205323009	-1.037328254563
C	-5.480765763807	1.699885526190	-0.206259899262
H	-5.734724381435	0.736933468263	-0.659699578398
H	-4.842062757982	1.483273293420	0.654929268338
C	-6.765674739546	2.408147162897	0.257433291454
H	-7.387448976869	2.639058312017	-0.618307318815
H	-6.514856528787	3.365288877596	0.731391721920
C	-7.539718533853	1.535411976235	1.222104406062
C	-7.494506481327	1.759729097628	2.603969657632
C	-8.272853971260	0.436549205996	0.746683599874
C	-8.163538237835	0.910831640458	3.490755405622
H	-6.929131681425	2.605794313853	2.988553155633
C	-8.940425143264	-0.415958157427	1.628074676438
H	-8.319303414385	0.250707123343	-0.324491561228
C	-8.887516481778	-0.180958290913	3.005761583946
H	-8.117620535884	1.103143249439	4.559625459351
H	-9.503469787870	-1.260978555440	1.240210461038
H	-9.407492040893	-0.842142922576	3.693709100792
C	-4.701834467267	2.518210417063	-1.229951201573
H	-5.343616392752	2.811135320023	-2.069696862511
H	-4.273396088930	3.423522661863	-0.792173689574
O	-3.581480160363	1.794529222541	-1.800256997224
H	-3.880027961461	0.842350937280	-2.050017848282
C	-3.597479557873	-1.477815072027	-1.572835147967
O	-4.384351535668	-0.633574556430	-2.112576869351
O	-2.436879745261	-1.771846732899	-1.912982068545
H	-1.804976984039	-1.860736599674	1.128836210505
C	-4.199880134746	-2.189479894642	-0.335669876690
C	-5.688782508641	-2.440117291418	-0.325554838114
H	-6.055180044544	-2.710295580921	-1.320138193909
H	-5.932062675099	-3.216622774545	0.404151231512
H	-6.201168747541	-1.514304704977	-0.034458851964
O	-3.498661508487	-2.489044061509	0.622165470017

Int4b

Electronic Energy = -2035.11275123 / Gibbs Free Energy =-2034.88953015

O	0.557930394771	-0.252927600308	1.668925950892
P	0.077286513047	-1.381996513312	0.791222936869
S	-2.356592307725	1.881056093410	-0.471385600967
O	-2.629615850308	1.098358875160	0.756256883765
O	-1.185561524007	1.409978522572	-1.236772063510
O	-2.455049164060	3.334860551542	-0.296099560624
O	0.631087720230	-2.770149582400	0.943378102427
O	-1.566085578287	-1.504016288366	0.933272663136
O	0.251844121411	-0.970535356659	-0.789725490043
H	-0.277735918497	-0.169862355608	-0.996245523720
C	-5.664407415214	1.673254511947	-0.154060655835
H	-5.787921416815	0.584510286050	-0.198246657991
H	-5.102035759069	1.892199731452	0.759078312730
C	-7.047607468514	2.349460670946	-0.090844136188
H	-7.600404745743	2.130806362388	-1.013676155708
H	-6.914179999920	3.438279206066	-0.050727770337
C	-7.844506064269	1.884087534091	1.108064878501
C	-7.708694831654	2.522095652696	2.349344684902
C	-8.697636332466	0.775253249922	1.016347669690

C	-8.407165399804	2.066448672623	3.469831991113
H	-7.050808752625	3.384290504612	2.435918569963
C	-9.398614301338	0.315364913182	2.133868152862
H	-8.814266804449	0.270309035055	0.059703786776
C	-9.255496678080	0.960304703097	3.365549441791
H	-8.291332546726	2.576517732522	4.422666396594
H	-10.058006293657	-0.543853914935	2.041773644459
H	-9.801817670983	0.605885886974	4.235504596211
C	-4.877457567625	2.146524343833	-1.371523585051
H	-5.412965748998	1.917380793887	-2.297374752676
H	-4.688767752930	3.223425042913	-1.334985184655
O	-3.603839474904	1.461833257360	-1.533689103652
H	-3.845446823703	-0.288080687773	-1.318858757918
C	-3.021453837119	-2.000179771846	-1.494999576050
O	-3.936326894560	-1.200344123480	-0.939419430686
O	-2.328050414552	-1.710336027899	-2.446397423555
H	-1.982453060876	-0.612972404290	0.911581434036
C	-2.959492079006	-3.382309596515	-0.801217276869
C	-3.888684412475	-3.629497041480	0.356382726588
H	-4.926892412052	-3.441210076776	0.061395079284
H	-3.774413873759	-4.657528107960	0.706679640131
H	-3.641124707109	-2.925742298098	1.156874878070
O	-2.171830422401	-4.201802121651	-1.230706370377

Int5a

Electronic Energy = -1985.57507104 / Gibbs Free Energy =-1985.2096902

O	0.906494463368	-2.295142163051	-1.730168986440
P	2.190409953906	-1.735882981090	-2.556000413650
S	-0.277312790154	-1.176382158971	-1.082988920468
O	-1.244242581229	-2.077005432957	-0.471488426339
O	-0.716478031575	-0.472084582685	-2.303810408198
O	0.549719177089	-0.377416516308	-0.154924610000
O	2.890868055917	-0.693052028239	-1.559168733525
O	3.103135425610	-2.797833876826	-3.017149682786
O	1.558367699798	-0.887779505867	-3.762389583166
H	0.664995265677	-0.545666757541	-3.510518710156
C	-4.196734114293	2.690456495605	0.296572595561
H	-4.092288601408	3.279040497183	-0.622256004442
H	-4.853185095464	1.845119779919	0.053269784849
C	-4.845488969752	3.565226109375	1.384908784541
H	-4.147799268632	4.368036604679	1.659123746165
H	-5.004875623330	2.963125287589	2.288829063018
C	-6.153710825290	4.165705021576	0.921042600261
C	-7.370018573023	3.501567289259	1.133446853122
C	-6.170373429751	5.377514254294	0.213867856722
C	-8.570764734598	4.031405299533	0.654012181076
H	-7.374508053310	2.561244428228	1.680686440400
C	-7.367596306190	5.911688674768	-0.267758463438
H	-5.234970543318	5.906308416068	0.042167474621
C	-8.573752075807	5.239434512503	-0.048984966426
H	-9.503613336294	3.502564914884	0.832352655729
H	-7.359191513199	6.853508927598	-0.810543166156
H	-9.506931315600	5.654378345981	-0.420408668094
C	-2.819013508442	2.158332923038	0.700521914096
H	-2.187120125752	2.994579026165	1.046874614521
H	-2.919594531604	1.469874001373	1.549361871334
O	-2.187544378021	1.438582485149	-0.344169040493
H	-1.935030474595	2.085125457708	-1.052749789792
N	-1.537058076339	3.276759139690	-2.498601330662
C	-2.715918640575	3.172517920800	-3.388624366168
H	-3.488383874200	3.838649791281	-2.994095671647
H	-2.463098505599	3.549745323308	-4.396976279793
C	-3.304954578177	1.763027827854	-3.483851454489
H	-3.553016948420	1.383393498608	-2.488959196179

H	-4.217216253249	1.790424700744	-4.090556411091
H	-2.615948783531	1.051762110631	-3.948614916521
C	-1.247493091229	4.696026334423	-2.195857029809
H	-0.244705886370	4.746923322263	-1.764987486598
H	-1.214716319777	5.279539155940	-3.134598652712
C	-2.215858606473	5.352979607792	-1.211191115401
H	-2.204681469977	4.833730697920	-0.248380599885
H	-1.911219549318	6.391692668682	-1.040462370596
H	-3.247372992337	5.371093283468	-1.576853517715
C	-0.355622561534	2.640776760525	-3.126625615419
H	-0.675938155059	1.676465271416	-3.521319367197
H	-0.011293399970	3.247073805268	-3.984916287450
C	0.794219413642	2.385854607747	-2.151350331318
H	1.561943173597	1.776794041415	-2.642000123287
H	1.275684730953	3.308203572973	-1.809725178962
H	0.432095270810	1.830995599065	-1.283376160818
H	2.240465957699	-0.343144161680	-0.900867396286

TS5

Electronic Energy = -1985.56328217 / Gibbs Free Energy =-1985.19762162

O	0.773775394420	-2.108021619431	-1.227138846058
P	2.116122144209	-1.773457081719	-1.880183429135
S	-0.874289631691	-0.395085708807	-1.198274880599
O	-1.776484815235	-1.295789028130	-0.506069599928
O	-0.812035349691	-0.388382244486	-2.659133153215
O	0.064508906320	0.423911237091	-0.425704602648
O	2.699924207776	-0.438668296752	-1.124586609100
O	3.205339786417	-2.790697085633	-1.953844912069
O	1.799792854124	-1.243128283137	-3.401609796592
H	0.886481207069	-0.893256199766	-3.423810934638
C	-4.087856250794	2.351284969740	-0.105432724916
H	-4.024595501545	3.144462309387	-0.858560323678
H	-4.832875621310	1.632635251710	-0.466748614024
C	-4.545727222060	2.963636495333	1.231412003182
H	-3.769563236501	3.651507942282	1.592798434421
H	-4.641374918541	2.170129695802	1.982857254409
C	-5.856299180451	3.704795432233	1.083126662497
C	-7.076692153807	3.087466521605	1.388672064197
C	-5.876022637227	5.014590783410	0.580699139150
C	-8.287158281969	3.759966159683	1.199279336104
H	-7.077678212535	2.071833009097	1.778421831925
C	-7.082573040609	5.690584590734	0.388934948125
H	-4.935811955840	5.506279433310	0.338938207280
C	-8.293970382738	5.064211316173	0.698068918904
H	-9.223443520822	3.265609909570	1.445178638729
H	-7.077421272412	6.706364926863	0.002077537279
H	-9.234049520263	5.589374407645	0.552041910413
C	-2.738042580674	1.652948523247	0.012226562146
H	-1.972816353870	2.314303289340	0.437889306098
H	-2.815319669374	0.771242222334	0.654458036269
O	-2.309054587277	1.181668165884	-1.276751215775
H	-1.905933568318	1.970140454947	-1.839116165628
N	-1.454325620812	3.140147403132	-2.878883774816
C	-2.716418028744	3.436502606270	-3.608718294199
H	-3.419287935735	3.859814647746	-2.887935378333
H	-2.527123784233	4.213439946530	-4.368660425363
C	-3.369813506932	2.214886969419	-4.257984490737
H	-3.471435958965	1.397806258477	-3.537251727461
H	-4.370281530354	2.491333081817	-4.607244902315
H	-2.807835937631	1.849553796017	-5.121963912030
C	-0.900955999746	4.374919001941	-2.264241104953
H	0.022209823793	4.095348663729	-1.753330513653
H	-0.627820156938	5.085873365196	-3.062736755176
C	-1.809222810028	5.069941598558	-1.249349674034

H	-2.086806126167	4.396362215347	-0.433369675199
H	-1.262633483319	5.911583109868	-0.810895236855
H	-2.724389452019	5.471150385855	-1.694129718817
C	-0.459217220044	2.536641441824	-3.811600629097
H	-0.870147842914	1.580496086626	-4.135427630874
H	-0.363214525816	3.179672119563	-4.702700484005
C	0.920003503036	2.286939303558	-3.199181810515
H	1.469231276802	1.578714548318	-3.827704063580
H	1.517495171635	3.200474550542	-3.123567270302
H	0.835181266335	1.842616008603	-2.205377784949
H	1.947056025477	0.043189035927	-0.727229322242

Int5b

Electronic Energy = -1985.60914888 / Gibbs Free Energy =-1985.2402816

O	1.335517792693	-2.709438561452	-1.443505248142
P	2.252296988568	-1.718903949901	-2.119823321684
S	-1.299380458326	-0.195332277848	-1.007300043985
O	-2.039163597932	-1.304769172425	-0.396452873144
O	-1.053452288595	-0.311529489460	-2.459893890913
O	-0.138063314497	0.286148955164	-0.220993992169
O	2.428887732097	-0.410490580880	-1.135339768328
O	3.626261747669	-2.104474356661	-2.585600357501
O	1.468934308949	-1.083919865250	-3.426929013147
H	0.553106948917	-0.850211605015	-3.161387613966
C	-4.122872895710	2.317707727313	0.052424548456
H	-3.972761313373	3.082806095937	-0.717996568577
H	-4.880964143098	1.626379805830	-0.332904710758
C	-4.625456418982	2.992205844074	1.342588444448
H	-3.843547915867	3.662453433674	1.723027057558
H	-4.791098391459	2.228009612938	2.112018750933
C	-5.898647084899	3.773678447593	1.102484099615
C	-7.153967483762	3.203683758613	1.353795861561
C	-5.845818276950	5.071924129861	0.573598137924
C	-8.328683331630	3.911661879177	1.086127780700
H	-7.210345222346	2.197768691903	1.764019625028
C	-7.016711361769	5.783224681977	0.303577097796
H	-4.877815266922	5.527907604861	0.375450062191
C	-8.263510872814	5.204280575820	0.559467006421
H	-9.293191632091	3.454511737808	1.291299011862
H	-6.956238894834	6.789765641656	-0.102183147711
H	-9.175739566447	5.757396494946	0.352743834125
C	-2.824628467554	1.559447201356	0.278668609669
H	-2.051733736085	2.186035910170	0.738222181766
H	-2.992138373575	0.686684986632	0.917481158861
O	-2.349647615184	1.115776365940	-1.018667152492
H	-1.483870945861	2.388113965403	-2.152671228003
N	-1.262641548626	3.032904437659	-2.933613637423
C	-2.540264227061	3.147418704692	-3.742818807898
H	-3.281287614257	3.590976805009	-3.077559293108
H	-2.334380105491	3.856091158604	-4.549415140805
C	-3.050867561346	1.809662812981	-4.268019339485
H	-3.080736464921	1.061728288952	-3.471902504673
H	-4.067281987199	1.960909690640	-4.643916784944
H	-2.444237793297	1.425449340819	-5.091431219535
C	-0.844779378726	4.368107645045	-2.351917089276
H	0.127942906072	4.210514603539	-1.888771578363
H	-0.716111189991	5.043741749781	-3.201438271438
C	-1.811872409113	4.930942935057	-1.317670896033
H	-1.938985667051	4.242908337255	-0.477016667456
H	-1.379376010783	5.855053430832	-0.922457200356
H	-2.792915030512	5.178509510988	-1.730289795349
C	-0.138415711707	2.393591031094	-3.731025889529
H	-0.523220397332	1.431005960080	-4.057332310020
H	0.022394077678	3.032701998930	-4.603129644282

C	1.131651579689	2.183724240916	-2.914474743322
H	1.734136819212	1.418978493619	-3.408999464798
H	1.727731706746	3.094788733932	-2.816861942878
H	0.902248747294	1.792375216590	-1.920193785948
H	1.560136810774	-0.185143302671	-0.737166314106

Int6a

Electronic Energy = -2260.44276572 / Gibbs Free Energy =-2260.25684432

C	-2.216647110223	-1.444476041189	-0.972851997617
H	-2.749647426928	-2.401307681984	-0.954755380352
H	-2.328889638164	-0.988187252045	0.020083115211
C	-2.848092747080	-0.539704573417	-2.047826690637
H	-2.742768835765	-1.038375378658	-3.018665744730
H	-2.286861849205	0.402835973550	-2.106147423838
C	-4.307197078008	-0.248581188207	-1.774831624112
C	-4.711444025407	0.964287119615	-1.199457842056
C	-5.288111263631	-1.212086544067	-2.058517150727
C	-6.057519307455	1.213611021986	-0.915171129793
H	-3.963771976525	1.722209611062	-0.973877144404
C	-6.632989918608	-0.967771433132	-1.773634568331
H	-5.000931400654	-2.162601645078	-2.497444285320
C	-7.024952694314	0.247021145038	-1.201825843031
H	-6.349303986618	2.162926482619	-0.472497127730
H	-7.375142736491	-1.729443352120	-2.000737185582
H	-8.072376020386	0.438414986922	-0.983078349565
C	-0.733887370746	-1.710414146553	-1.241793962686
H	-0.613061923004	-2.100222777794	-2.262860611304
H	-0.171521066190	-0.768634195685	-1.186124481619
O	-0.151825380037	-2.591260761586	-0.286973324190
H	-0.518812172606	-3.483529179200	-0.472457561778
O	-0.618491545398	-4.355400830496	-3.511016525449
P	-0.349709440001	-5.575341246275	-2.291286532805
O	-1.059236308803	-6.852110916209	-2.931757018077
O	1.127419389093	-5.714908147173	-2.271545697987
O	-1.114483047330	-5.081817668198	-1.076470194966
H	-2.751483071247	-4.902454395648	-0.826017051159
S	-1.961195155469	-3.976881767985	-4.293678839708
O	-1.739629262352	-2.637233593767	-4.812096001993
O	-2.308287575481	-5.039977811161	-5.222028407016
O	-3.051437632331	-3.841347850392	-3.151915454827
P	-4.132963174287	-5.048229735582	-2.449086751765
O	-3.739908811141	-4.757752695311	-0.922390901649
O	-5.508175408241	-4.576001460206	-2.753476185704
O	-3.626729546006	-6.391846738174	-2.908592310059
H	-2.067527538802	-6.761996391220	-2.919087394295

TS6

Electronic Energy = -2260.41553305 / Gibbs Free Energy =-2260.2369786

C	-1.731106217116	-1.557682338482	-1.308453833104
H	-2.261859923716	-2.490669577313	-1.516858136840
H	-1.826625418915	-1.350752478054	-0.232306167693
C	-2.389822840614	-0.422231717829	-2.113054614808
H	-2.299336081192	-0.658746610502	-3.179065467825
H	-1.852468189804	0.518037554316	-1.931121210429
C	-3.850789146827	-0.261756403024	-1.751180172765
C	-4.264205440573	0.684529542302	-0.803386491920
C	-4.818069592490	-1.103154741573	-2.324133392219
C	-5.608284208686	0.792585022996	-0.433802031700
H	-3.525599663615	1.343571292630	-0.350925343983
C	-6.160991381299	-0.998713023871	-1.956001738676
H	-4.510086156073	-1.839027238876	-3.060008155497
C	-6.562502519838	-0.050697502097	-1.008993227924
H	-5.908843407940	1.535524651792	0.301082431491
H	-6.896293226405	-1.657719202866	-2.411870897275

H	-7.608353701525	0.031350579604	-0.724321034523
C	-0.260649752225	-1.753741630994	-1.657461626126
H	-0.165474978528	-1.952172257810	-2.730271561619
H	0.312023404997	-0.843392224905	-1.423306441808
O	0.326856904070	-2.853765532463	-0.942536243182
H	-0.353875552498	-3.219021187055	-0.352769873200
O	-1.608750874108	-3.752838278190	-3.713314195959
P	-0.264964949629	-5.710974354707	-1.077587944410
O	-0.537709829705	-6.266342993234	-2.445520982874
O	1.050743447056	-5.891369577485	-0.418069468435
O	-1.406187842077	-5.046294337105	-0.344450941692
H	-2.792485887053	-4.746144793573	-1.127000898358
S	-2.633383081523	-3.569682513450	-4.752177141938
O	-2.994087443827	-2.178094828969	-5.057591060319
O	-2.495310507183	-4.444519036746	-5.925777651984
O	-4.088791065488	-4.130269516308	-4.010562146288
P	-4.145845168429	-5.259683650820	-2.839554718319
O	-3.702787694742	-4.529804184608	-1.500558886056
O	-5.524589591562	-5.802528753995	-2.788328166425
O	-3.058888753438	-6.363930905915	-3.185620566050
H	-2.094030898553	-6.180579934894	-2.957920438227

Int6b

Electronic Energy = -2260.43770976 / Gibbs Free Energy =-2260.26105014

C	-3.073084231496	-0.780857825379	-1.010842712080
H	-3.991169172632	-1.332434888315	-1.245624024150
H	-3.085463777846	-0.569875244143	0.065559161375
C	-3.042785592722	0.544573370596	-1.796508903565
H	-3.019411293613	0.325102837773	-2.871582711217
H	-2.115309583771	1.081629909595	-1.560632097522
C	-4.238691089973	1.413904395870	-1.473511971220
C	-4.192919841600	2.330870197965	-0.413734657534
C	-5.434107787638	1.284208899924	-2.194702650324
C	-5.311190140235	3.100053032828	-0.083035486176
H	-3.272303768564	2.443082547222	0.154936130678
C	-6.555214564142	2.050868439182	-1.868057839552
H	-5.484371174378	0.577153958487	-3.020054356336
C	-6.497193389040	2.962066487707	-0.809635973267
H	-5.255268097179	3.807972218824	0.739870360076
H	-7.471982987579	1.938621953543	-2.441136702423
H	-7.367398485964	3.561170666903	-0.555213907231
C	-1.868475269031	-1.647759437025	-1.336449346826
H	-1.847487364459	-1.948026804736	-2.385931326801
H	-0.923699426856	-1.154411498546	-1.087829639968
O	-1.946180319766	-2.895818459089	-0.583372444605
H	-1.911256058129	-2.663443086946	0.419338472816
O	-0.379540526709	-1.902765415960	6.367932822892
P	-0.533118619684	-4.142381403505	-0.915758116371
O	0.662963285585	-3.231447896216	-0.652525357278
O	-0.825732241361	-4.536702139984	-2.325258486245
O	-0.885852904238	-5.098467319286	0.217423616982
H	-0.530752050678	-4.707168804527	1.666320089769
S	-1.250493185983	-1.900002404466	5.189031156346
O	-2.159032526197	-3.046405192108	5.062304310605
O	-1.812490859324	-0.597594440304	4.816511877047
O	-0.035795632240	-2.177484422490	3.947148900792
P	-0.347106163101	-2.711768888998	2.477988745748
O	-0.286435725544	-4.292473197829	2.581976837002
O	-1.640196366159	-2.220151901056	1.871590604322
O	0.937093685617	-2.214146182812	1.692157016047
H	0.908277802875	-2.588458506426	0.727864809198

TS6'

Electronic Energy = -2260.43748288 / Gibbs Free Energy =-2260.26313317

C	-3.028816503787	-0.838448573817	-0.987949769482
H	-3.951441316595	-1.392592288547	-1.197272073008
H	-3.000536773123	-0.647206385320	0.091520171091
C	-3.038088166093	0.502247853266	-1.748171530671
H	-3.071100687746	0.306570253267	-2.827411745979
H	-2.098989656668	1.034141003981	-1.548784505693
C	-4.213790116834	1.364366105264	-1.342419027095
C	-4.121906866538	2.223597515413	-0.237925899726
C	-5.433740935454	1.285140160763	-2.028448748867
C	-5.219411015813	2.984319052415	0.171503817239
H	-3.181380226981	2.296336927352	0.304064919346
C	-6.534568429219	2.043977904857	-1.623081145141
H	-5.520069435872	0.624010340729	-2.888156700257
C	-6.430849713820	2.896520619620	-0.520465745222
H	-5.127767483688	3.646582648581	1.028498431978
H	-7.471272817009	1.971265645260	-2.169696059061
H	-7.285263584255	3.489177625004	-0.204807473684
C	-1.830301373970	-1.688857325390	-1.373584521138
H	-1.849689729303	-1.983713399638	-2.424541201996
H	-0.882002995838	-1.186187399530	-1.159719872085
O	-1.864259507039	-2.939581499203	-0.616609028896
H	-1.840688198080	-2.702132564445	0.412702391147
O	-0.525129673150	-1.643569778057	6.259083709060
P	-0.473733209539	-4.142301495845	-0.940680177710
O	0.729451101986	-3.209020610046	-0.657997146517
O	-0.692863750605	-4.511338619705	-2.367571564566
O	-0.787127952843	-5.114354248531	0.178830211968
H	-0.571739932786	-4.812427783386	1.787321417909
S	-1.344769522096	-1.724847138245	5.045412849928
O	-2.308176185971	-2.832490200569	5.000971491122
O	-1.826533056957	-0.442045852085	4.520302694355
O	-0.099764378376	-2.188744976420	3.902138359689
P	-0.367629856506	-2.799847444492	2.449256938063
O	-0.422185476600	-4.379807960969	2.690301138568
O	-1.644855556611	-2.300344332505	1.796750927064
O	0.923074775333	-2.452010441808	1.651861578628
H	0.865367896042	-2.804595048146	0.553672864812

Int6c

Electronic Energy = -2260.45797362 / Gibbs Free Energy =-2260.27973443

C	-2.937980426005	-0.830367104232	-1.038806367541
H	-3.875532728214	-1.395413813338	-1.107698270033
H	-2.809712705793	-0.545528166719	0.013116276925
C	-3.029103444231	0.440796519244	-1.904579820783
H	-3.146200630931	0.153052307064	-2.957163325612
H	-2.083782614237	0.993542737169	-1.828848777638
C	-4.179849487697	1.327802404281	-1.482057455054
C	-4.021630206864	2.258511576528	-0.444846292711
C	-5.440816495855	1.204189572249	-2.082089635233
C	-5.093498741306	3.045709319544	-0.017982322065
H	-3.048713914341	2.366551951493	0.030035529016
C	-6.516349379111	1.989435172653	-1.659297529000
H	-5.579388966052	0.487151616508	-2.888511554146
C	-6.345983519697	2.913535696255	-0.624780550818
H	-4.950053334819	3.763531339540	0.785540042177
H	-7.485571415488	1.881173147685	-2.139390708654
H	-7.180647195946	3.526853378887	-0.295967000524
C	-1.782914084880	-1.723283983116	-1.464071319671
H	-1.905322213592	-2.059893979480	-2.499833395533
H	-0.824414754679	-1.196540866117	-1.381640874983
O	-1.756721463587	-2.882625911492	-0.600749731264
H	-1.916340840622	-2.428968678625	1.068279790730
O	-0.443459197334	-1.828366035997	6.374438566263
P	-0.661628319526	-4.100035635500	-0.957419524847

O	0.747203439978	-3.297764899921	-0.907157803245
O	-0.881480521634	-4.607949855998	-2.342136498894
O	-0.797494512982	-5.024596595858	0.241086148301
H	-0.487232858750	-4.627327173231	1.707973799023
S	-1.334207263911	-1.904432473902	5.212471366225
O	-2.129163912702	-3.131640843436	5.094798112149
O	-2.024535730319	-0.660008732503	4.858235810944
O	-0.116361885270	-2.045036200473	3.941384346611
P	-0.302516215055	-2.625016590201	2.472938882412
O	-0.316032388888	-4.202883776324	2.630293230697
O	-1.772741445122	-2.176628743086	2.021386343359
O	0.770940596125	-2.121366578350	1.554273953118
H	0.868013062192	-2.850856929808	-0.026424050352

Int7a

Electronic Energy = -2260.43540016 / Gibbs Free Energy =-2260.25488877

C	-2.964027990533	-1.295564787674	-1.769634718932
H	-3.803328026650	-1.698690540500	-1.190616782936
H	-2.213065377243	-0.976289582943	-1.039400084541
C	-3.434301227844	-0.089826869004	-2.602805652643
H	-4.198206834560	-0.414650836428	-3.321573662087
H	-2.588697684817	0.292218271720	-3.191205382025
C	-3.986607546736	1.013414171265	-1.727466205021
C	-3.122489910087	1.920653680916	-1.095757879663
C	-5.362055490734	1.121854714834	-1.479390312916
C	-3.617195242847	2.909534538316	-0.243083551630
H	-2.051889816696	1.847416618196	-1.275432410890
C	-5.863104569487	2.109202763824	-0.626511623690
H	-6.045966199084	0.425219986717	-1.959749709081
C	-4.991645811572	3.007565854912	-0.005237320773
H	-2.930771483753	3.604335166690	0.234267847638
H	-6.933504532449	2.177468932762	-0.449428295002
H	-5.378930973415	3.777447552466	0.656837013935
C	-2.373763987043	-2.416342067810	-2.627130133036
H	-3.129961368610	-2.758445392739	-3.357186247407
H	-1.523466237809	-2.034636982441	-3.208012693843
O	-1.881584547140	-3.502552217857	-1.854080360059
H	-2.626446794153	-3.804665553036	-1.286962952578
O	-1.252190719039	-1.958374369333	3.197140566212
P	-2.193984426882	-2.763336486969	4.437867053040
O	-2.128451392851	-4.236974921551	4.116416932004
O	-1.637288795354	-2.193084617512	5.690802051134
O	-3.650427509297	-2.166165150193	4.137849115711
H	-4.143911769027	-2.673474185866	3.423478861773
S	-1.158459012407	-2.362170407550	1.652147529505
O	-0.716539045022	-1.159123854044	0.967629883609
O	-0.385608546199	-3.582942344643	1.496160316936
O	-2.677977071637	-2.590185882757	1.260197628422
P	-3.740816830152	-3.985617024153	1.206643877621
O	-4.813205190726	-3.552574914165	2.172945339076
O	-4.030556181138	-4.208569474072	-0.242718534410
O	-2.827895815221	-5.158445692596	1.777619493044
H	-2.520407019327	-4.929733942258	2.714285570173

TS7

Electronic Energy = -2260.39062638 / Gibbs Free Energy =-2260.21487389

C	-2.829311719038	-0.966296348826	-1.231086622333
H	-3.770357707914	-1.494613472375	-1.045268308000
H	-2.503550040537	-0.548261506540	-0.274316944897
C	-3.061069110890	0.174977309599	-2.240022436260
H	-3.393460180122	-0.247821020694	-3.196673436292
H	-2.110882325735	0.690034350653	-2.430830502768
C	-4.088550338262	1.159566978884	-1.724670980252
C	-3.701628498863	2.252142123783	-0.935987206608

C	-5.454063654328	0.965944953887	-1.976768100063
C	-4.653357497543	3.130836322304	-0.412992622039
H	-2.645533585286	2.414114941433	-0.730993762427
C	-6.409717941388	1.841726214735	-1.456241874878
H	-5.769324004806	0.121533529269	-2.586014002228
C	-6.011866495180	2.927958441056	-0.671643627234
H	-4.333952379828	3.973781034461	0.194344176691
H	-7.463695911674	1.676760379477	-1.664567715429
H	-6.753764389997	3.611080457844	-0.266901356077
C	-1.787372195398	-1.951357793306	-1.745181513079
H	-2.051548369184	-2.340766088548	-2.732942270349
H	-0.790607908497	-1.509630371630	-1.794226715747
O	-1.647163313757	-3.142449776936	-0.904575294487
H	-2.604639306394	-3.594385081994	-0.739256959741
O	-0.466566215282	-2.617171866464	3.661150830391
P	-1.620149069675	-2.825784875952	4.619363630555
O	-2.279536753693	-4.311725488449	4.409399800753
O	-1.423525770537	-2.639655197623	6.095555868047
O	-2.854625207024	-1.830710876287	4.145957512752
H	-2.786661839023	-1.717169887679	3.179789581462
S	-1.030935588360	-2.872986716778	0.906866176108
O	-0.070913203454	-1.807583667133	0.693884545778
O	-0.601703543829	-4.237889318260	1.126107457401
O	-2.354477714457	-2.464884589725	1.444737106193
P	-4.252721402738	-3.810849534611	1.137568225975
O	-5.219034399724	-2.713767064566	1.406065078967
O	-3.853178835526	-4.103390996267	-0.303988272709
O	-3.862633465398	-4.809296156300	2.181881312573
H	-2.773155400891	-4.401144609879	3.560079118925

Int7b

Electronic Energy = -2260.4239871 / Gibbs Free Energy =-2260.2453447

C	-2.692837405173	-0.796187506396	-1.184376864694
H	-3.599567473478	-1.407310008430	-1.250790050959
H	-2.548384528093	-0.556981420827	-0.126235736970
C	-2.872318543724	0.510404148357	-1.982431413108
H	-3.033786679604	0.270024924864	-3.040779405953
H	-1.947332484390	1.098790323371	-1.926132785623
C	-4.032901412616	1.324914257423	-1.453953802224
C	-3.854318004743	2.210331599694	-0.381394106116
C	-5.319058533823	1.173498127325	-1.990175943276
C	-4.932193082996	2.927469656358	0.142394351853
H	-2.861558675205	2.337473880644	0.045096717050
C	-6.400455520395	1.889332543801	-1.470493148427
H	-5.473044247598	0.489579366847	-2.822095437228
C	-6.210180996795	2.769262164232	-0.401552522153
H	-4.773723700112	3.610899710514	0.972548907517
H	-7.390053613023	1.760967721709	-1.901415138919
H	-7.049767909297	3.328046160785	0.003071152282
C	-1.503795236686	-1.589147811011	-1.709042280312
H	-1.585055798763	-1.768085402095	-2.782968027180
H	-0.553180890719	-1.090862710208	-1.500836634483
O	-1.433878888969	-2.956551166788	-1.174653612638
H	-2.954107511665	-5.486040975765	0.043514702979
O	-0.728799058338	-3.394729190040	4.081909045504
P	-1.811225459559	-2.524551773987	4.672551261954
O	-3.208884389891	-3.376637881159	4.773631831255
O	-1.625421986079	-1.828904355454	5.990672025483
O	-2.189814461719	-1.341779162537	3.574781778352
H	-2.124999236274	-1.706854194167	2.674655931238
S	-1.108150174050	-3.156256595481	0.385971448397
O	-0.179993644606	-2.132232480433	0.828375852988
O	-0.793845028692	-4.568944857297	0.516310300500
O	-2.497716653340	-2.827568027292	1.086264156463

P	-3.916571459324	-3.897505001579	1.162765678638
O	-5.047095987462	-2.976026985276	0.895357948918
O	-3.651307784598	-4.829426400957	-0.135593276552
O	-3.726598923498	-4.681465436392	2.424334597304
H	-3.371125135236	-3.885678938762	3.940688793842

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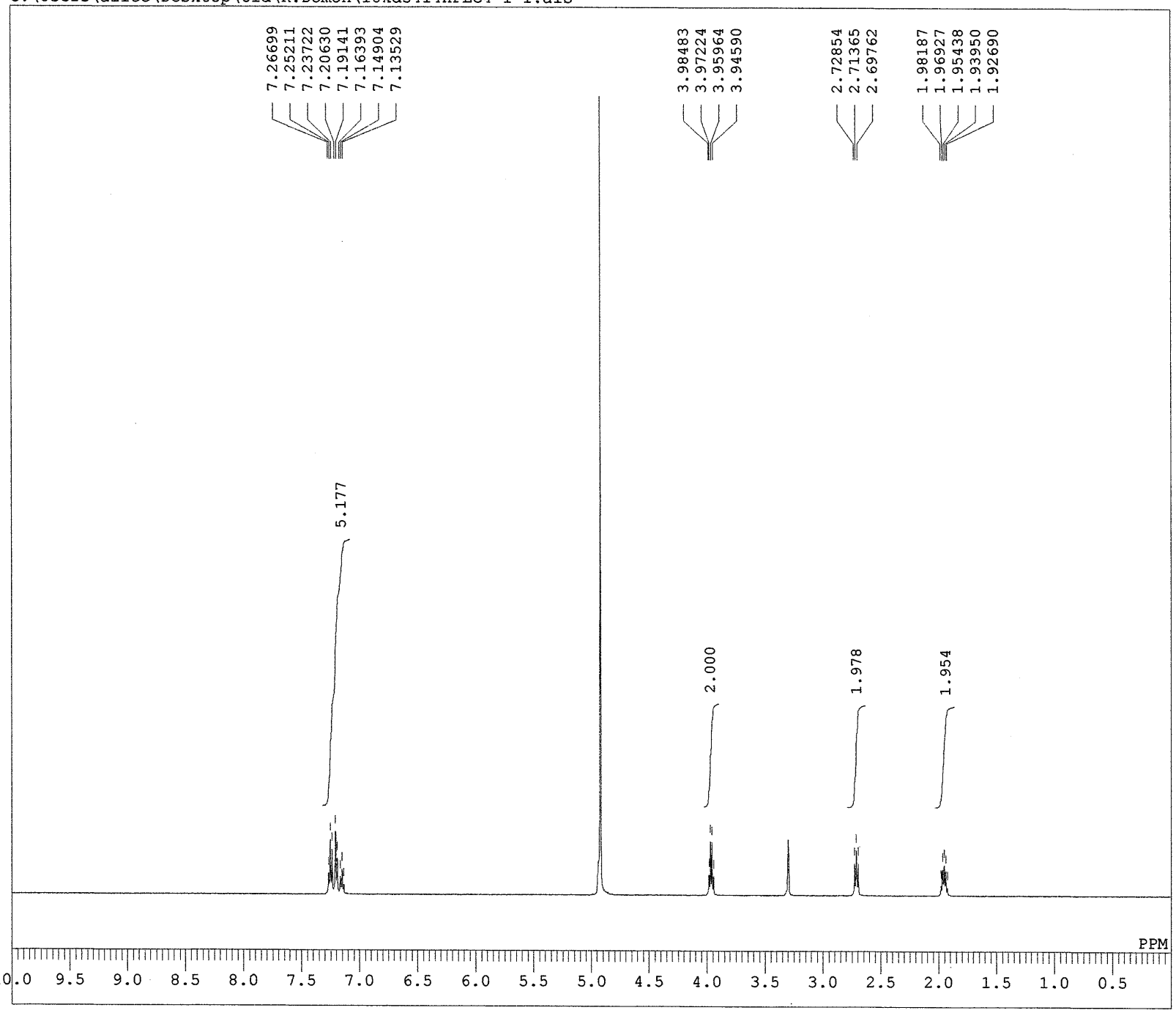

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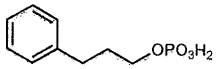
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	3
ACQTM	1.7459 sec
PD	6.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.3 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	38



2

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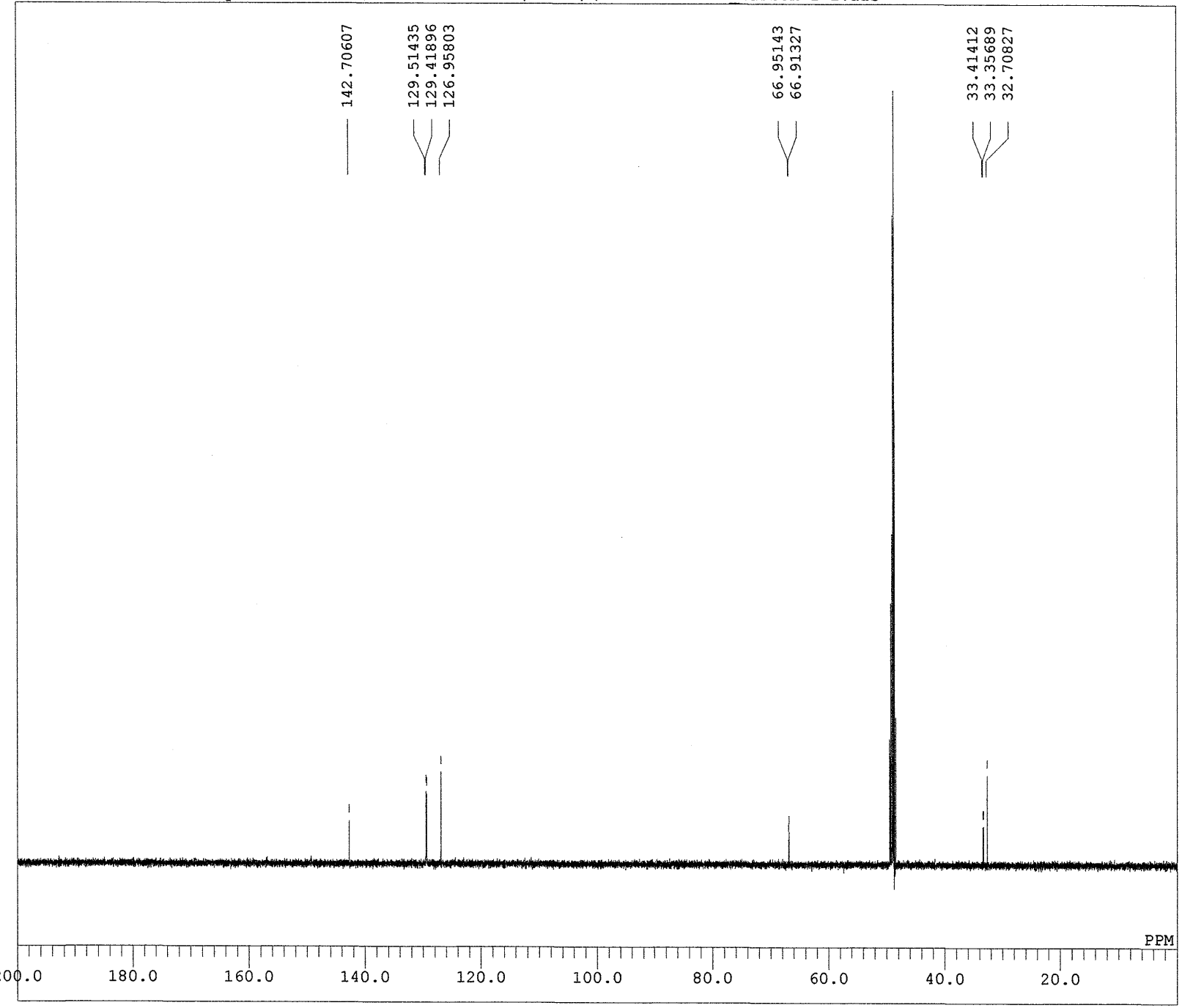

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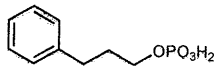
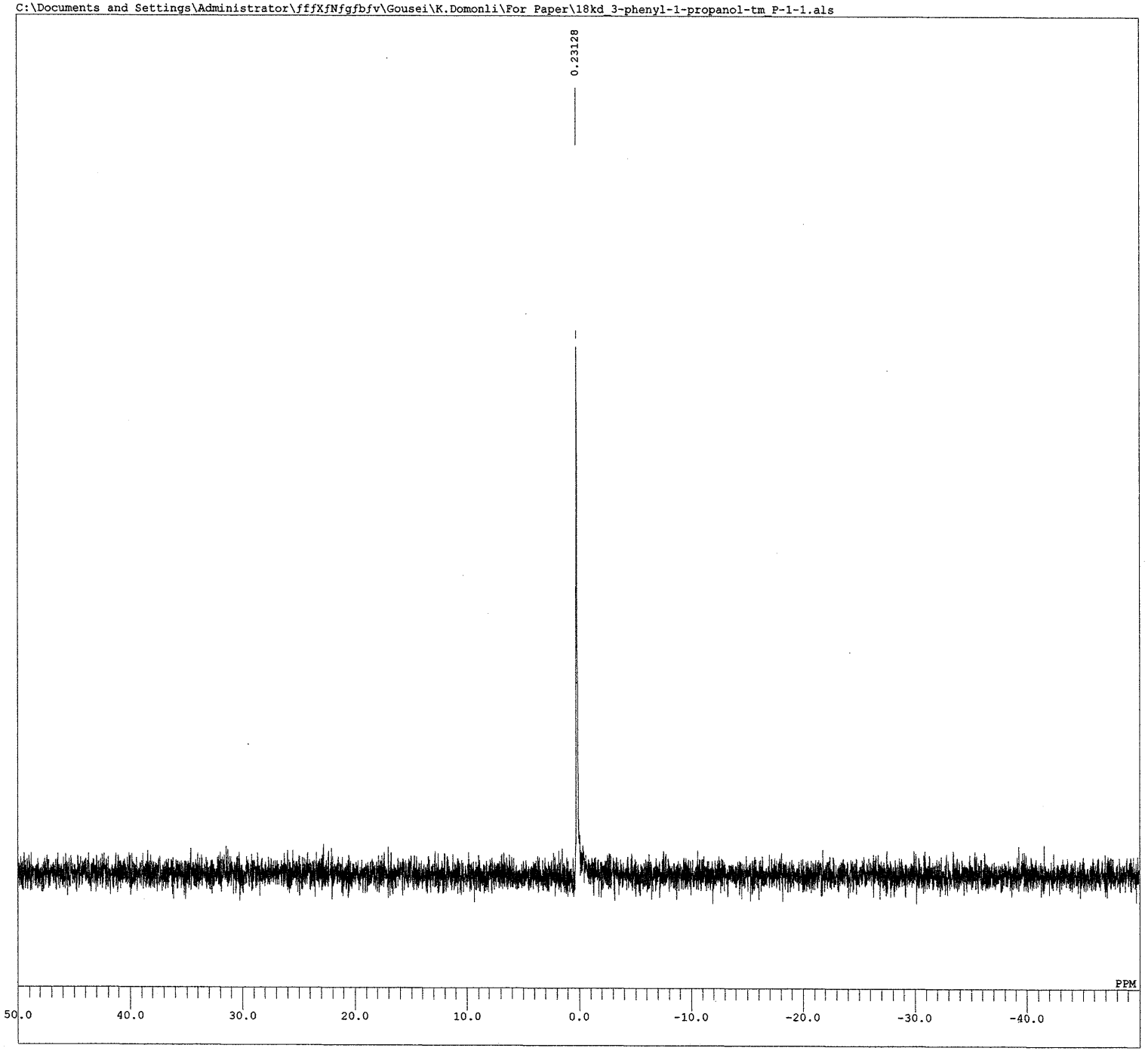
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	324
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

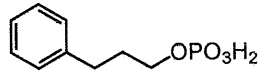


2

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd_3-phenyl-1-propanol-tm_P-1-1.als

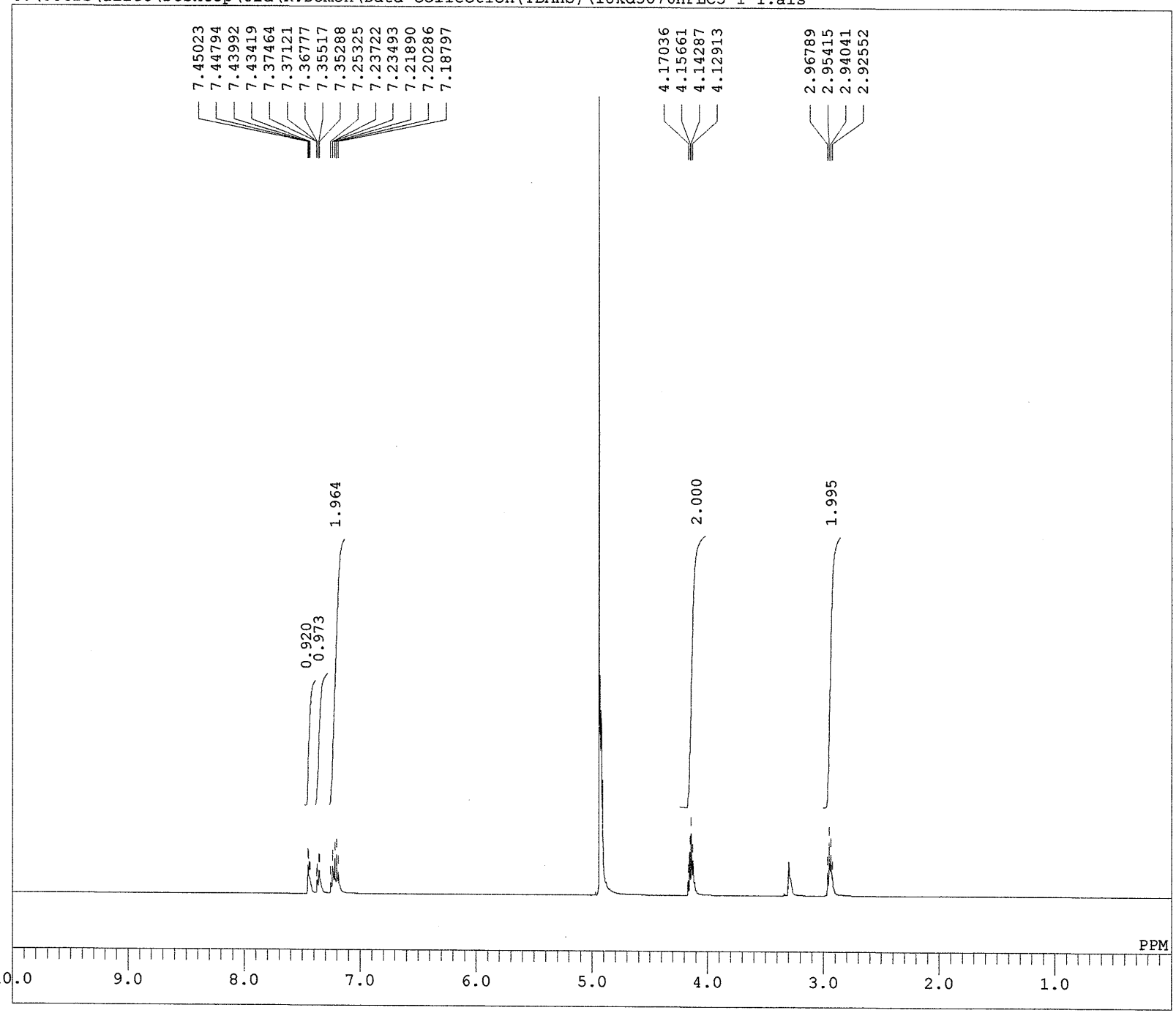


DFILE	18kd_3-phenyl-1-propanol-tm_P-1-1.als
COMNT	
DATIM	07-03-2019 04:58:29
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	9
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	20.0 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

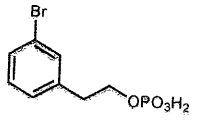


2

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3076HPLC3-1-1.als

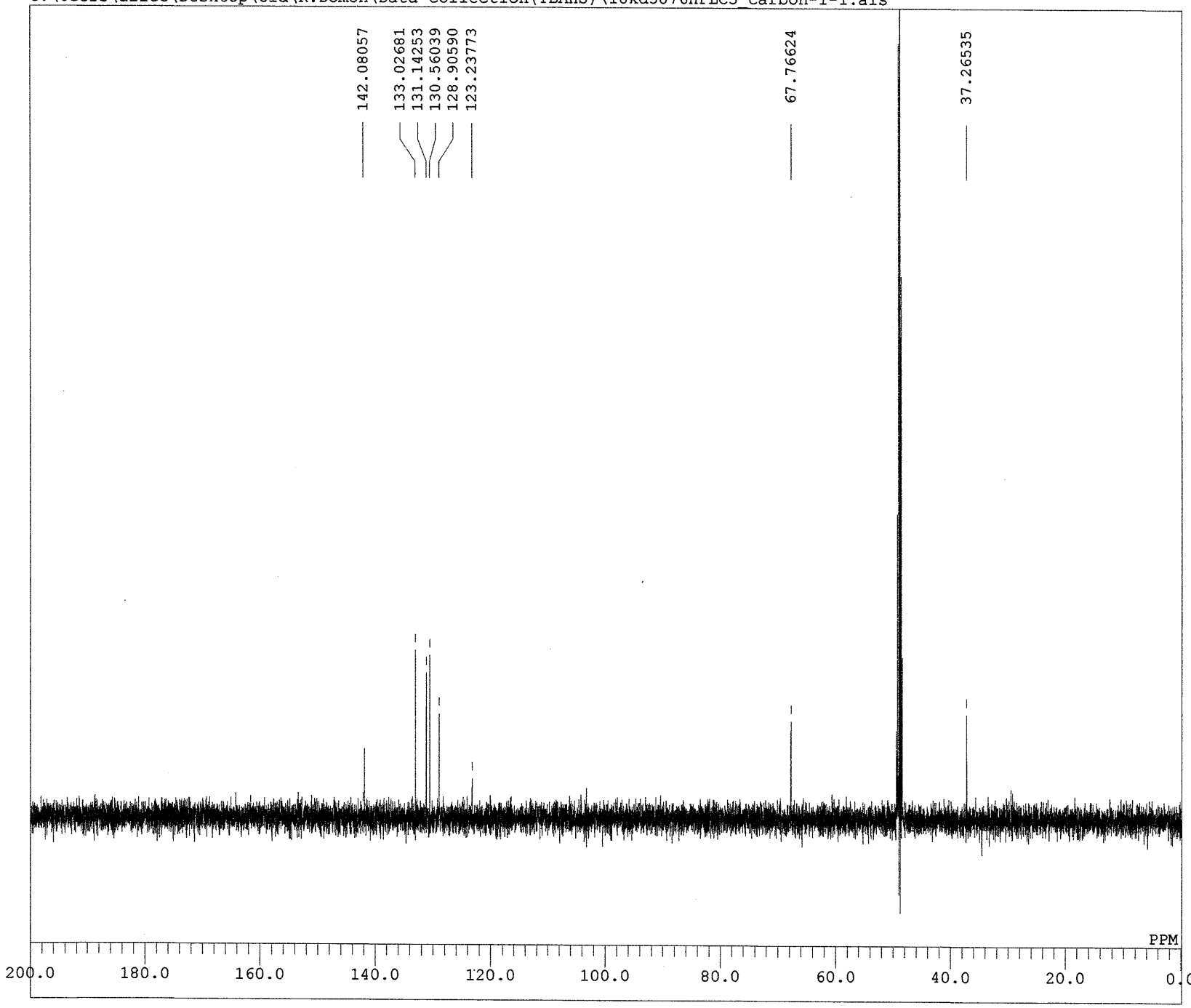


DFILE	18kd3076HPLC3-1-1.als
COMNT	
DATIM	2018-09-01 03:07:51
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

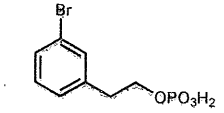


3

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3076HPLC3_carbon-1-1.als

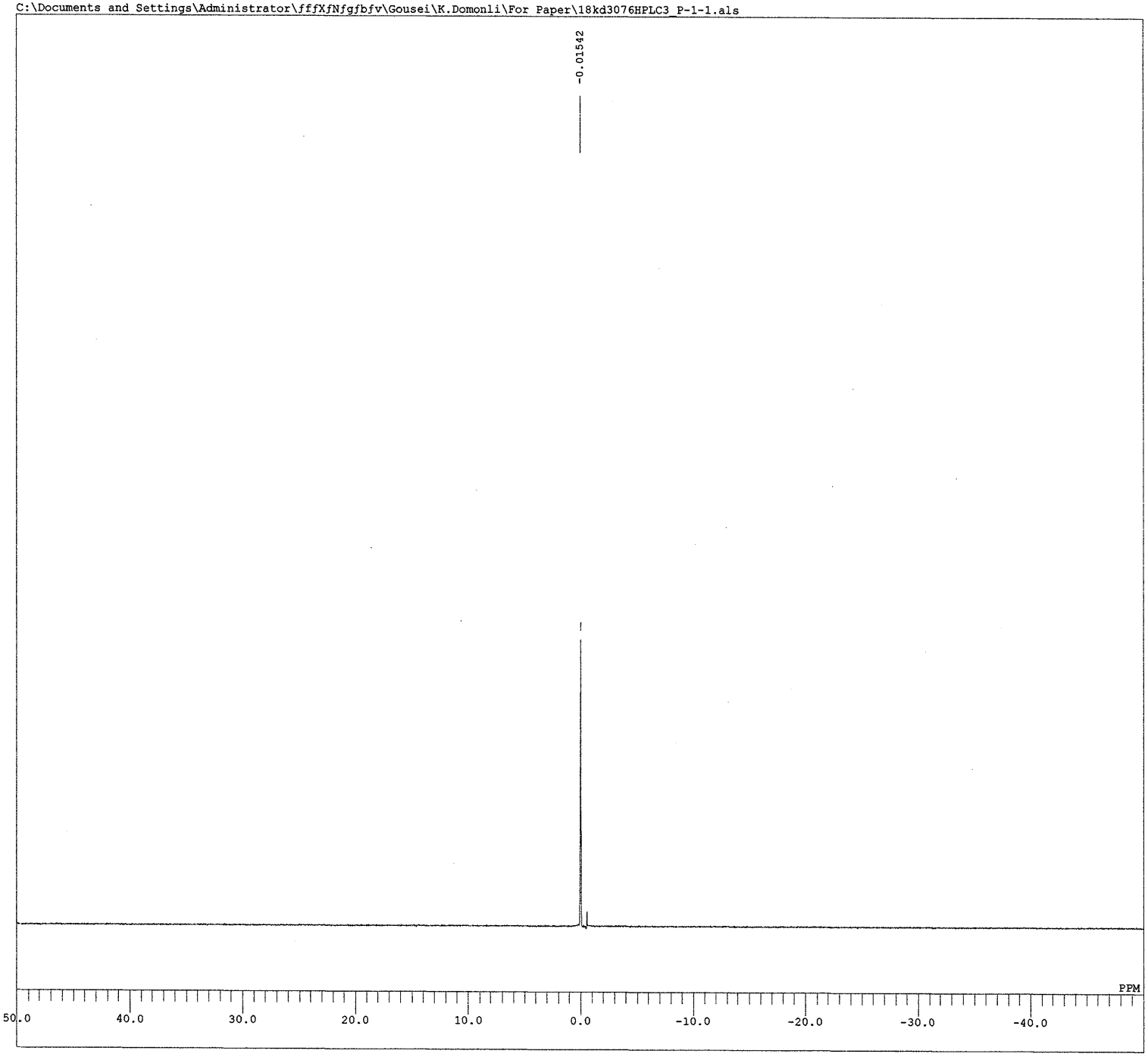


DFILE	18kd3076HPLC3_carbon-1-1.als
COMNT	
DATIM	2018-09-01 04:03:41
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	135
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	21.9 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

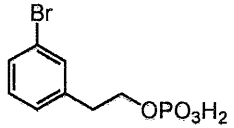


3

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3076HPLC3_P-1-1.als

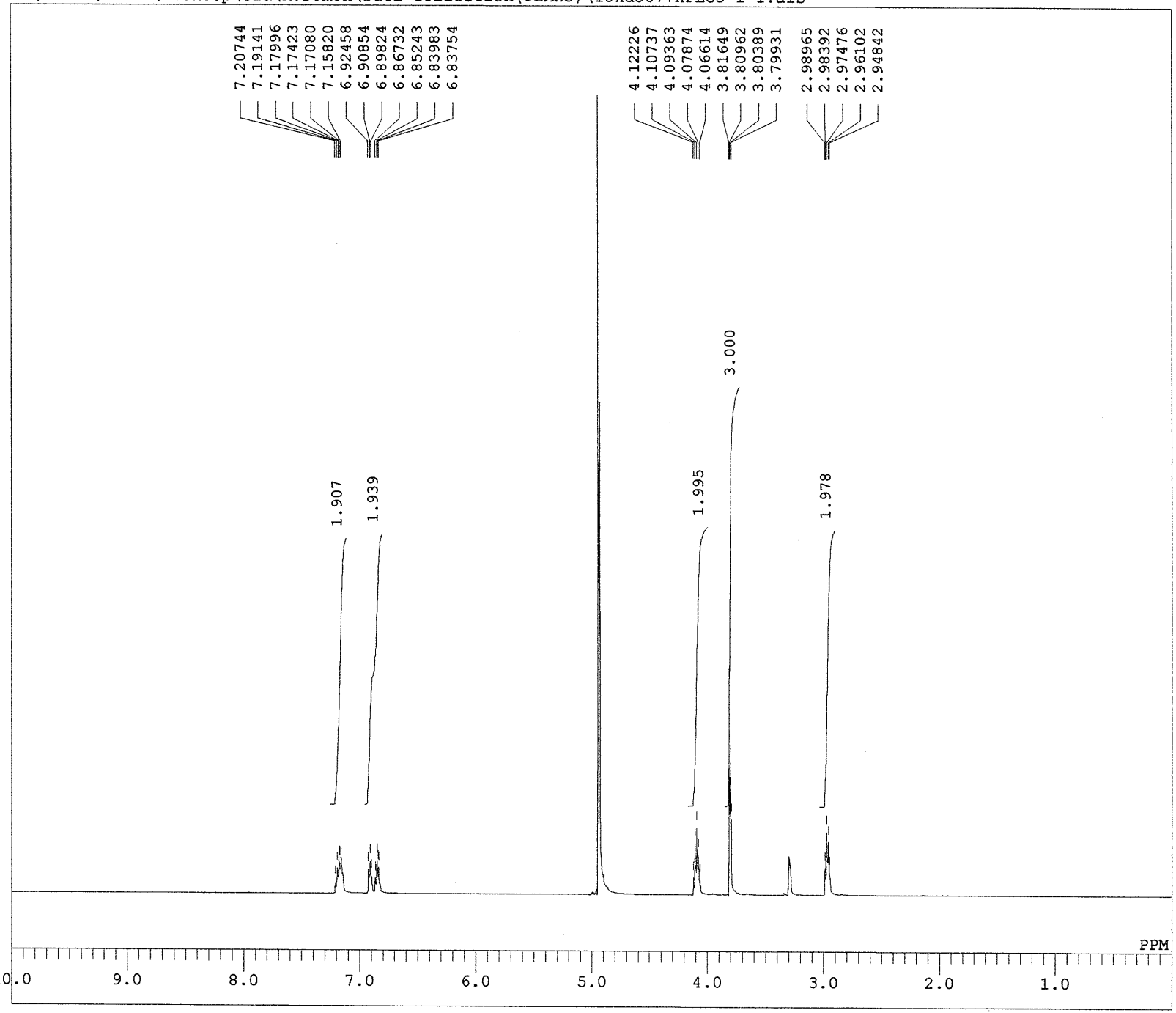



```
DFILE  18kd3076HPLC3_P-1-1.als
COMNT
DATIM  01-09-2018 04:50:03
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS           319
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.6 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

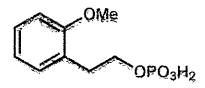


3

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3077HPLC3-1-1.als

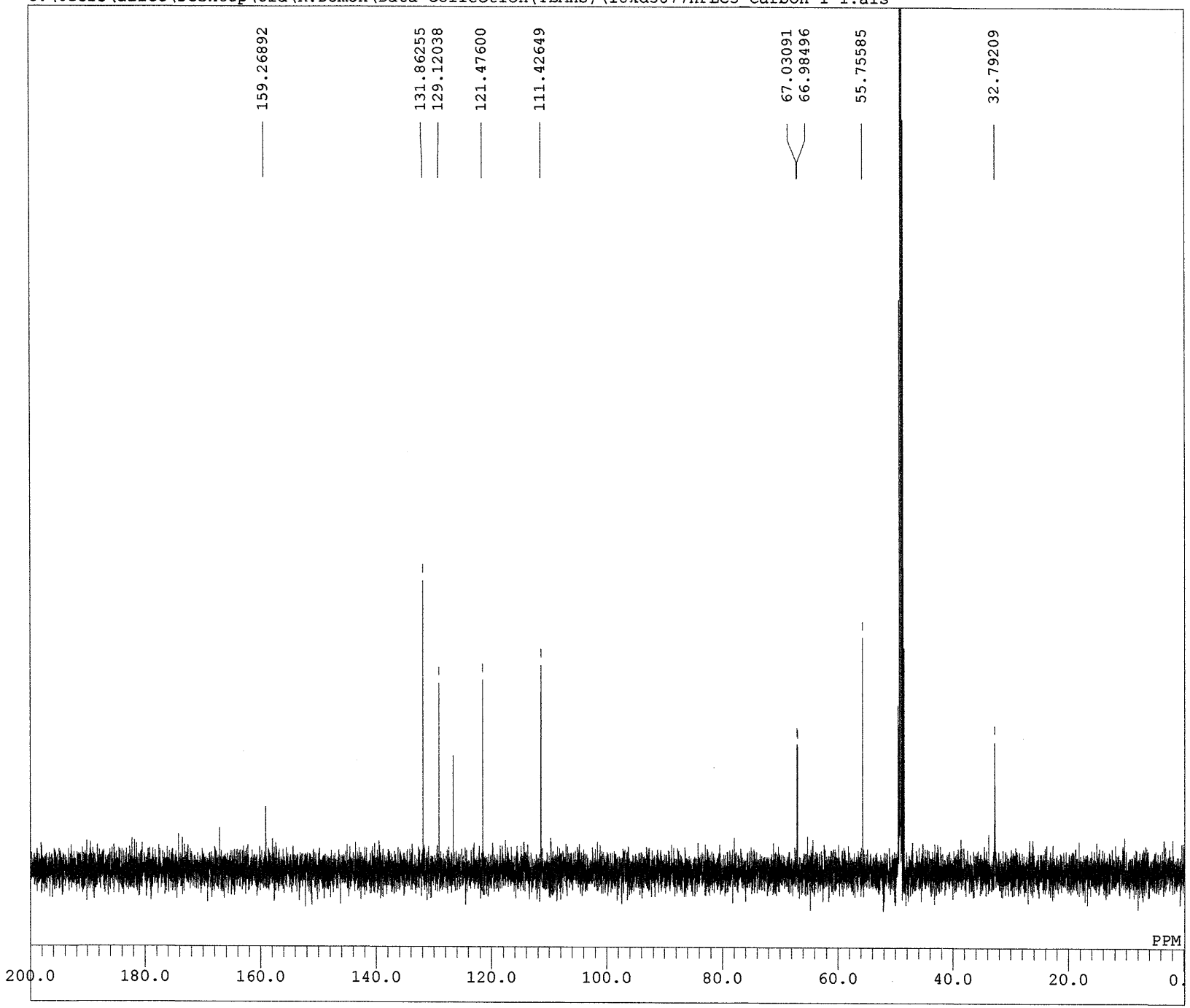


DFILE	18kd3077HPLC3-1-1.als
COMNT	
DATIM	2018-09-01 03:10:45
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

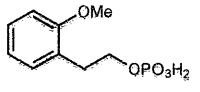


4

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3077HPLC3_carbon-1-1.als

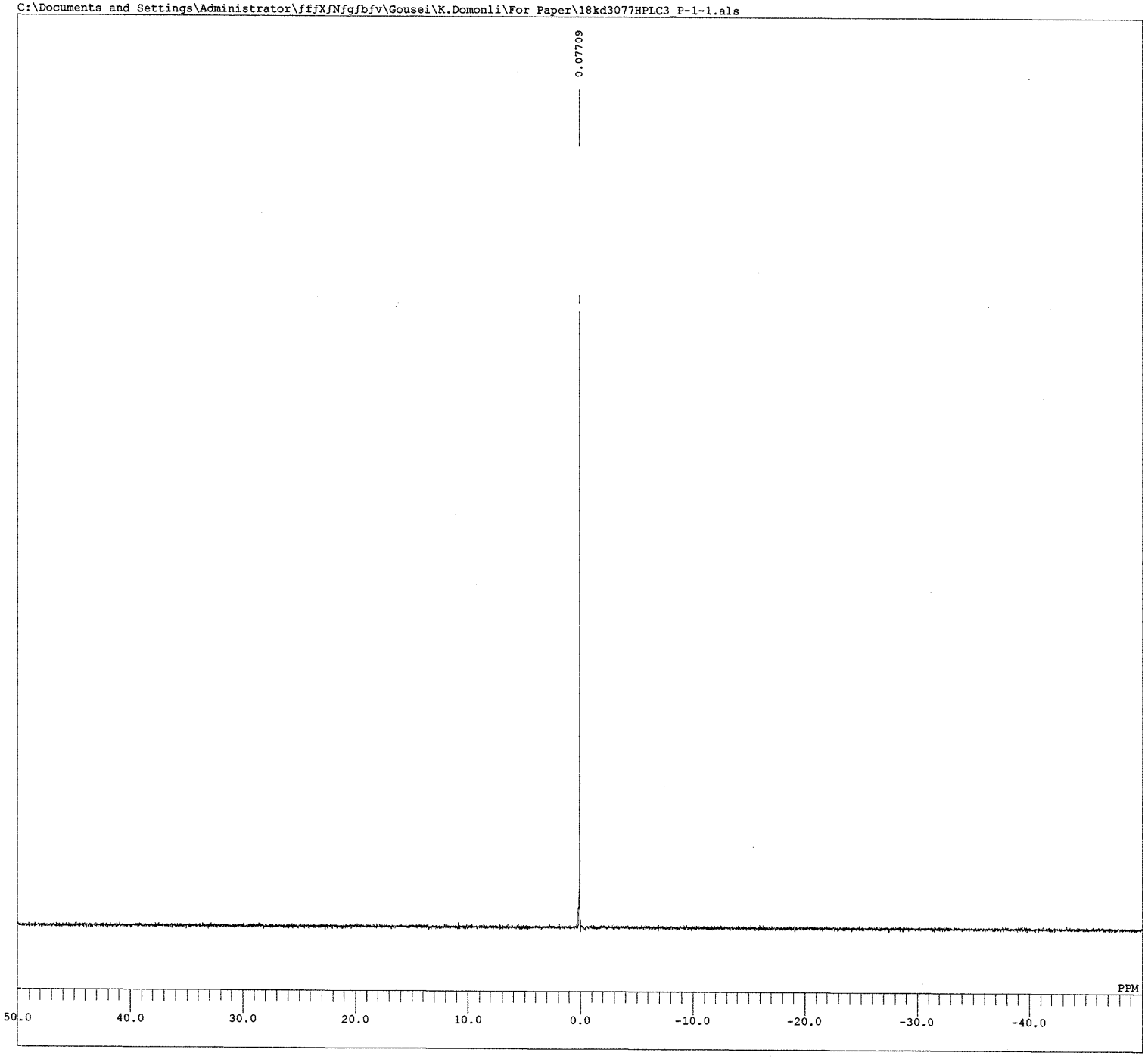


DFILE	18kd3077HPLC3_carbon-1-1.als
COMNT	
DATIM	2018-09-01 03:56:52
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	120
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	21.8 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

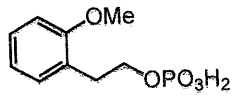


4

C:\Documents and Settings\Administrator\ffjXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3077HPLC3_P-1-1.als

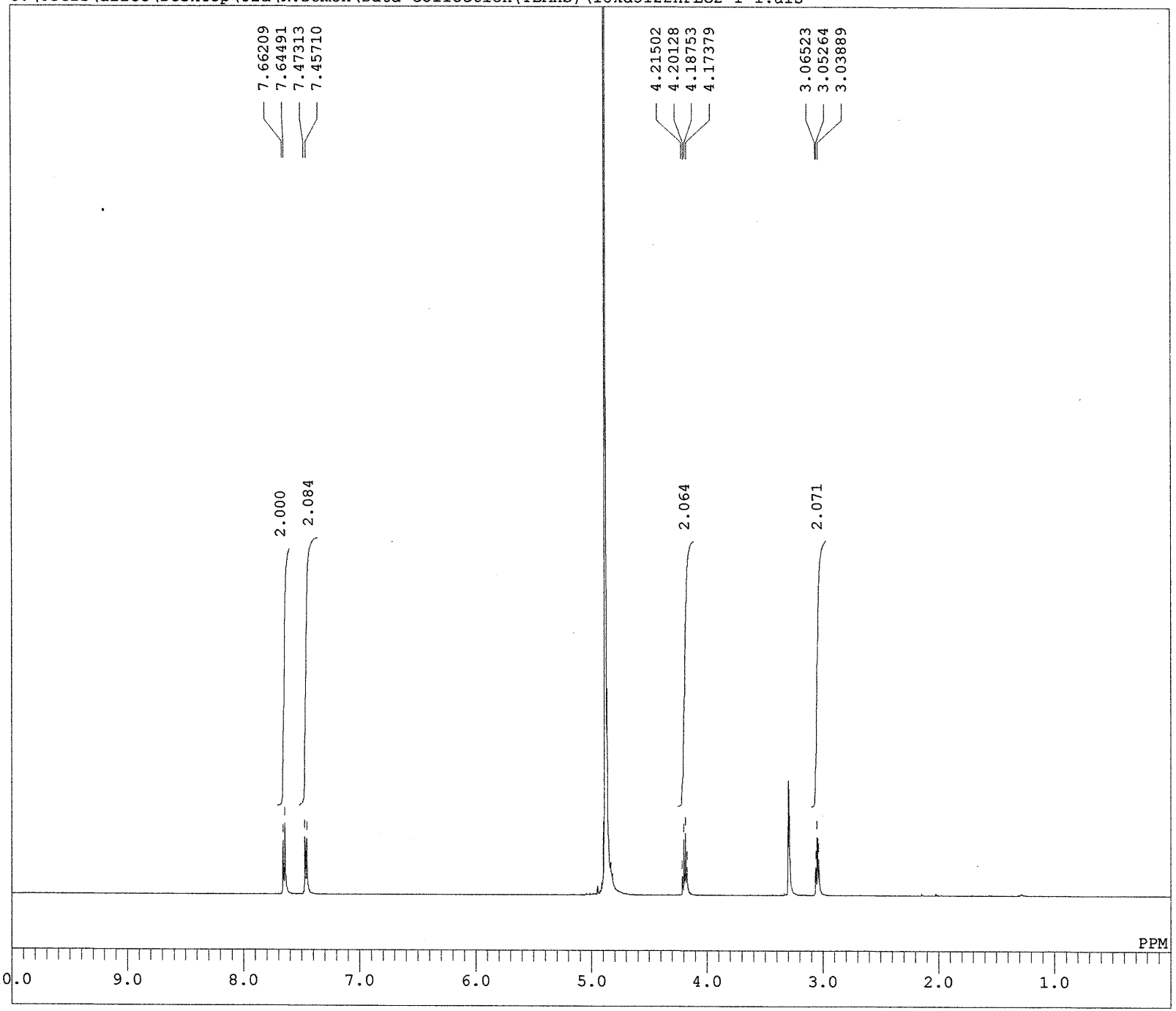



```
DFILE  18kd3077HPLC3_P-1-1.als
COMNT
DATIM  01-09-2018 05:44:45
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            41
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.6 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

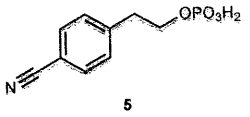


4

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3122HPLC2-1-1.als

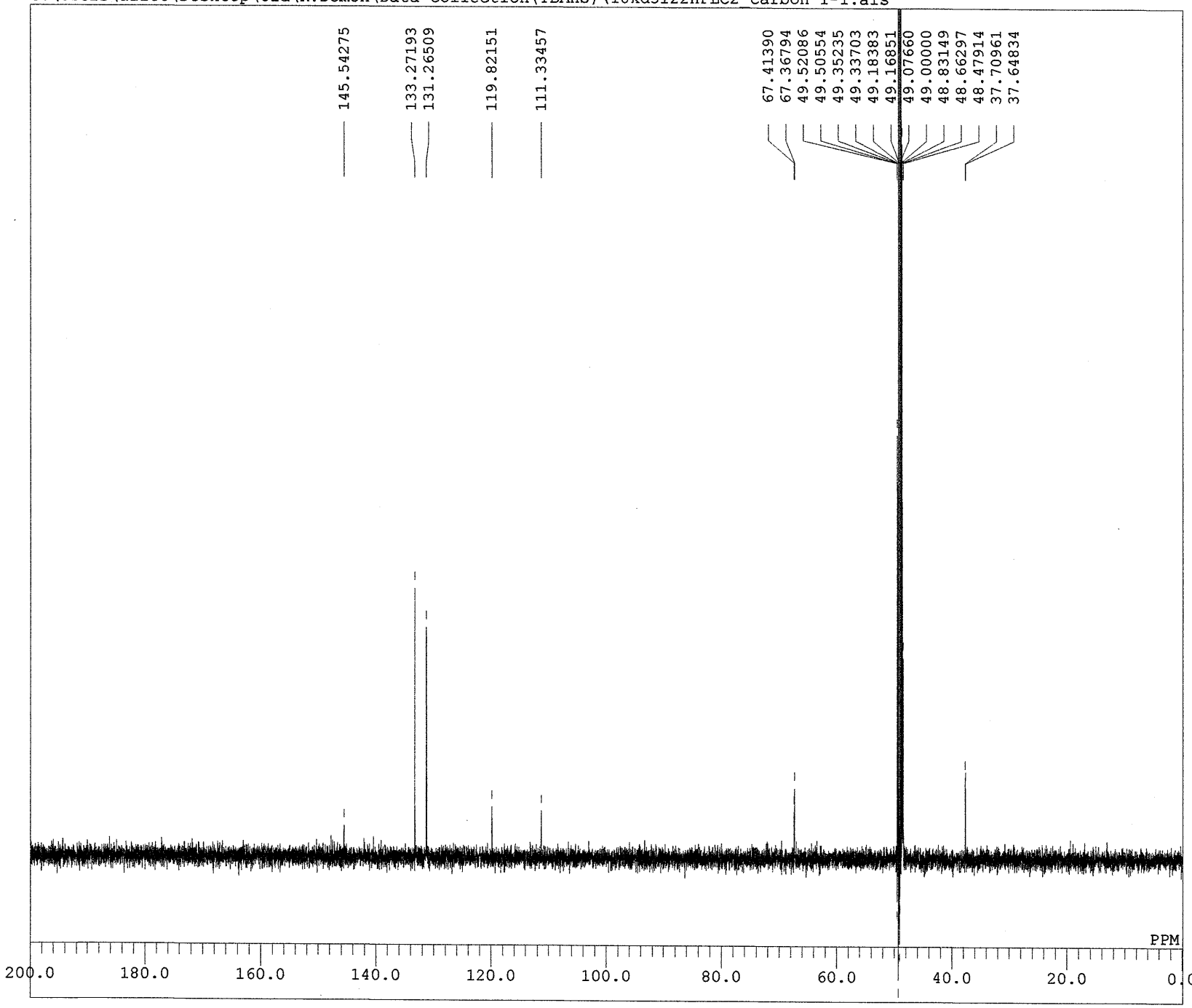



```
DFILE   18kd3122HPLC2-1-1.als
COMNT
DATIM   2018-09-20 07:43:10
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         500.16 MHz
OBSET           2.41 KHz
OBFIN           6.01 Hz
POINT          13107
FREQU        7507.51 Hz
SCANS                6
ACQTM          1.7459 sec
PD             5.0000 sec
PW1              5.55 usec
IRNUC   1H
CTEMP           22.0 c
SLVNT   CD3OD
EXREF            3.30 ppm
BF               0.12 Hz
RGAIN              30
```

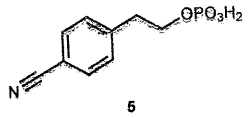


5

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3122HPLC2_carbon-1-1.als

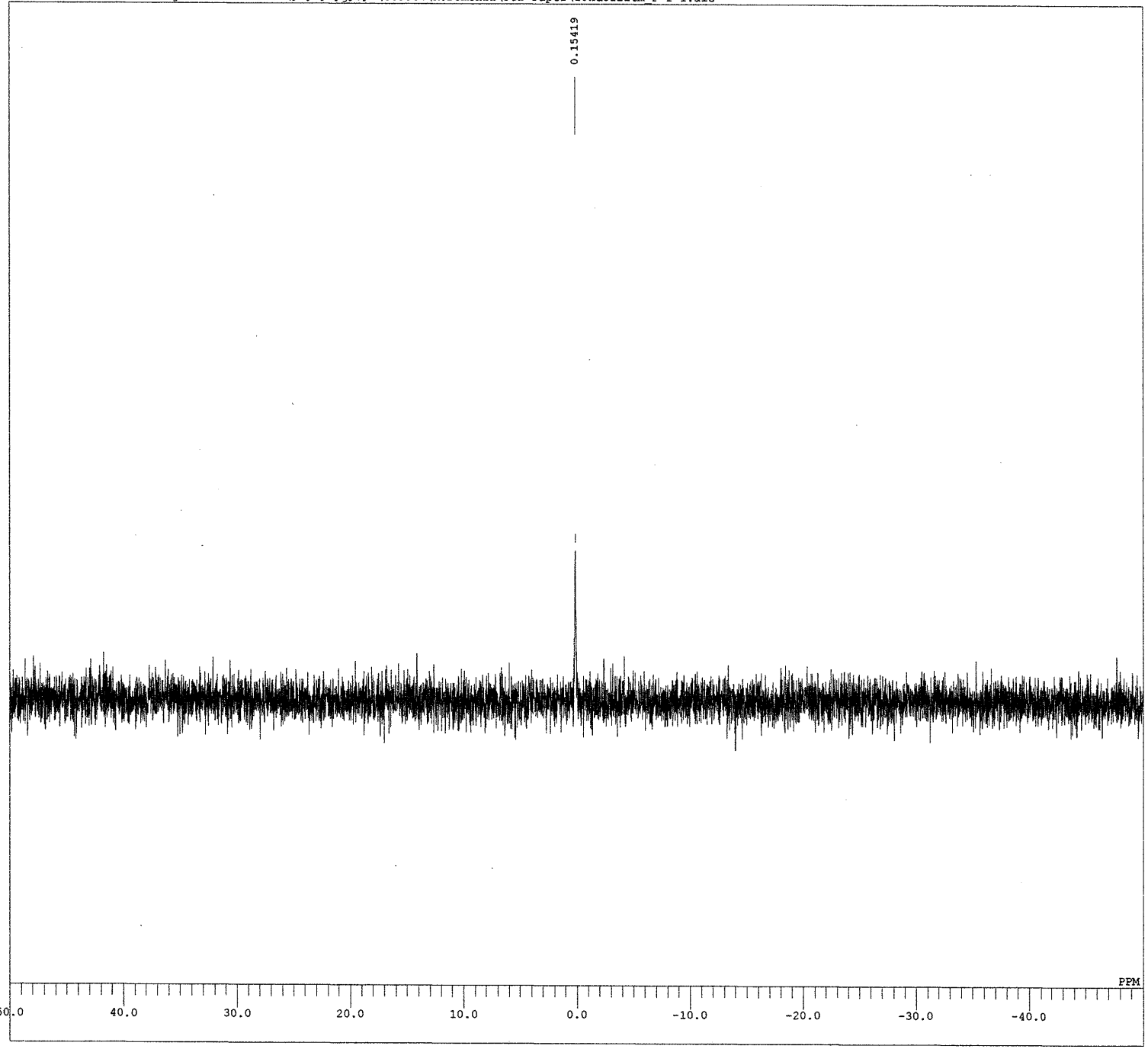



```
DFILE   18kd3122HPLC2_carbon-1-1.als
COMNT
DATIM   2018-09-20 07:44:28
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           1.58 KHz
OBFIN           5.95 Hz
POINT          26214
FREQU       50505.05 Hz
SCANS           1149
ACQTM         0.5190 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           22.2 c
SLVNT   CD3OD
EXREF          49.00 ppm
BF              0.12 Hz
RGAIN             60
```

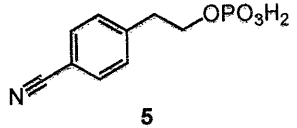


5

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3122tm_P-1-1.als

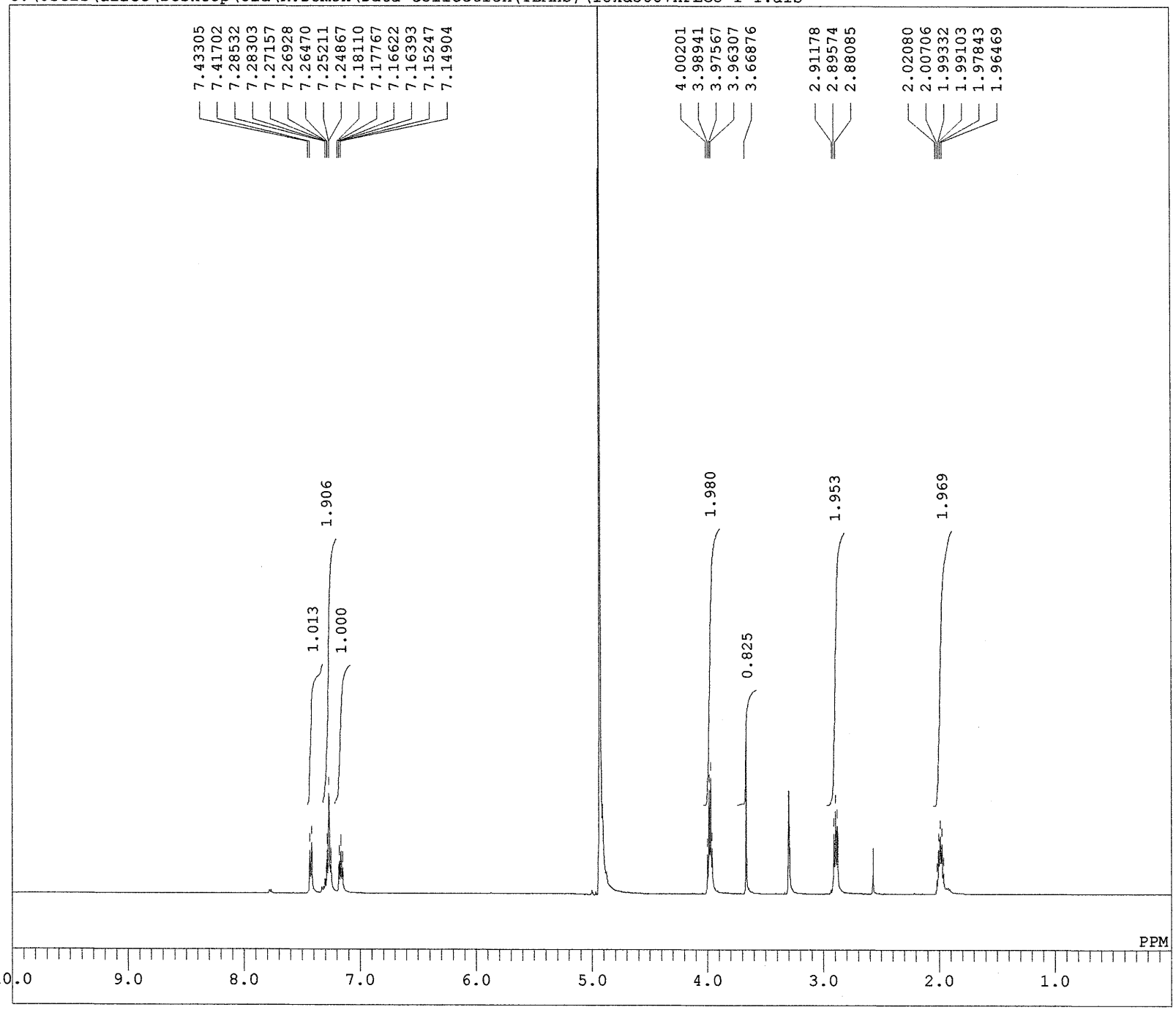


DFILE	18kd3122tm_P-1-1.als
COMNT	
DATIM	07-03-2019 05:13:36
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	16
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	20.1 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56



5

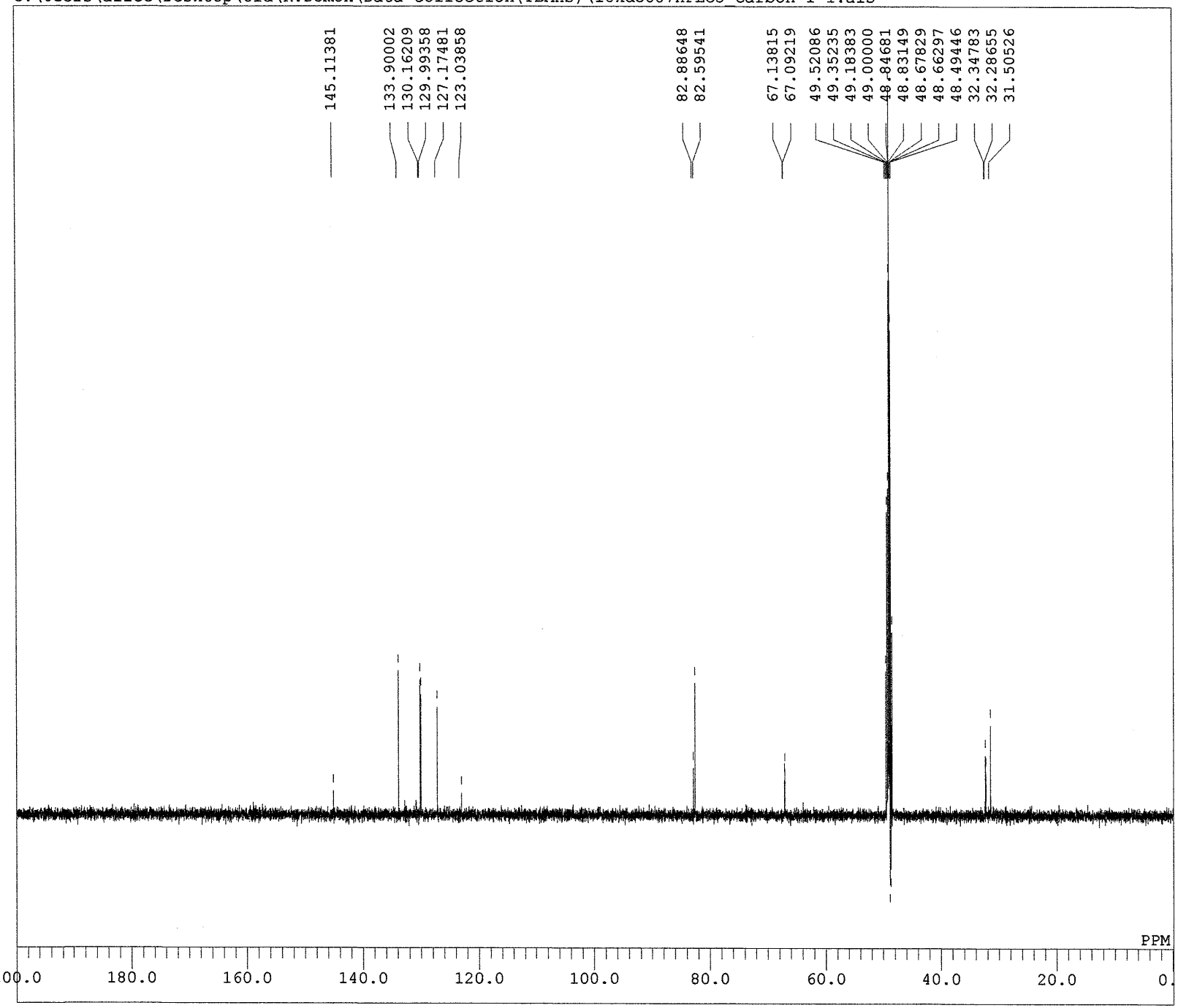
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3087HPLC3-1-1.als



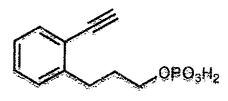
DFILE	18kd3087HPLC3-1-1.als
COMNT	
DATIM	2018-09-01 04:56:42
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

6

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3087HPLC3_carbon-1-1.als

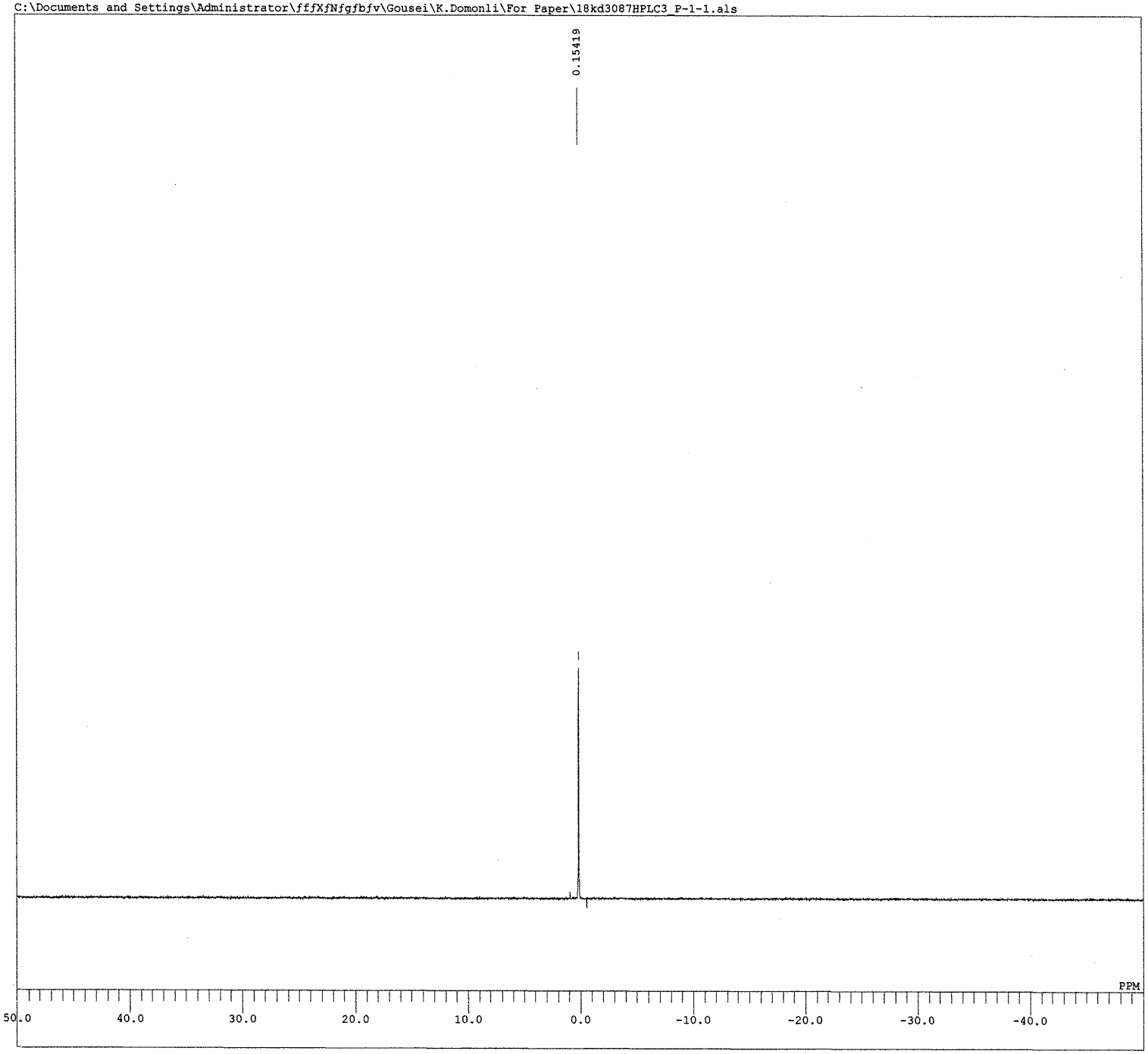



```
DFILE   18kd3087HPLC3_carbon-1-1.als
COMNT
DATIM   2018-09-01 05:06:20
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           1.58 KHz
OBFIN           5.95 Hz
POINT          26214
FREQU       50505.05 Hz
SCANS            301
ACQTM          0.5190 sec
PD             2.0000 sec
PW1              3.40 usec
IRNUC   1H
CTEMP           22.1 c
SLVNT   CD3OD
EXREF           49.00 ppm
BF               0.12 Hz
RGAIN              60
```

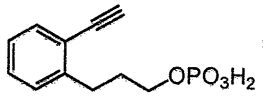


6

C:\Documents and Settings\Administrator\ffjXjNfgjbjv\Gousei\K.Domonli\For Paper\18kd3087HPLC3_P-1-1.als

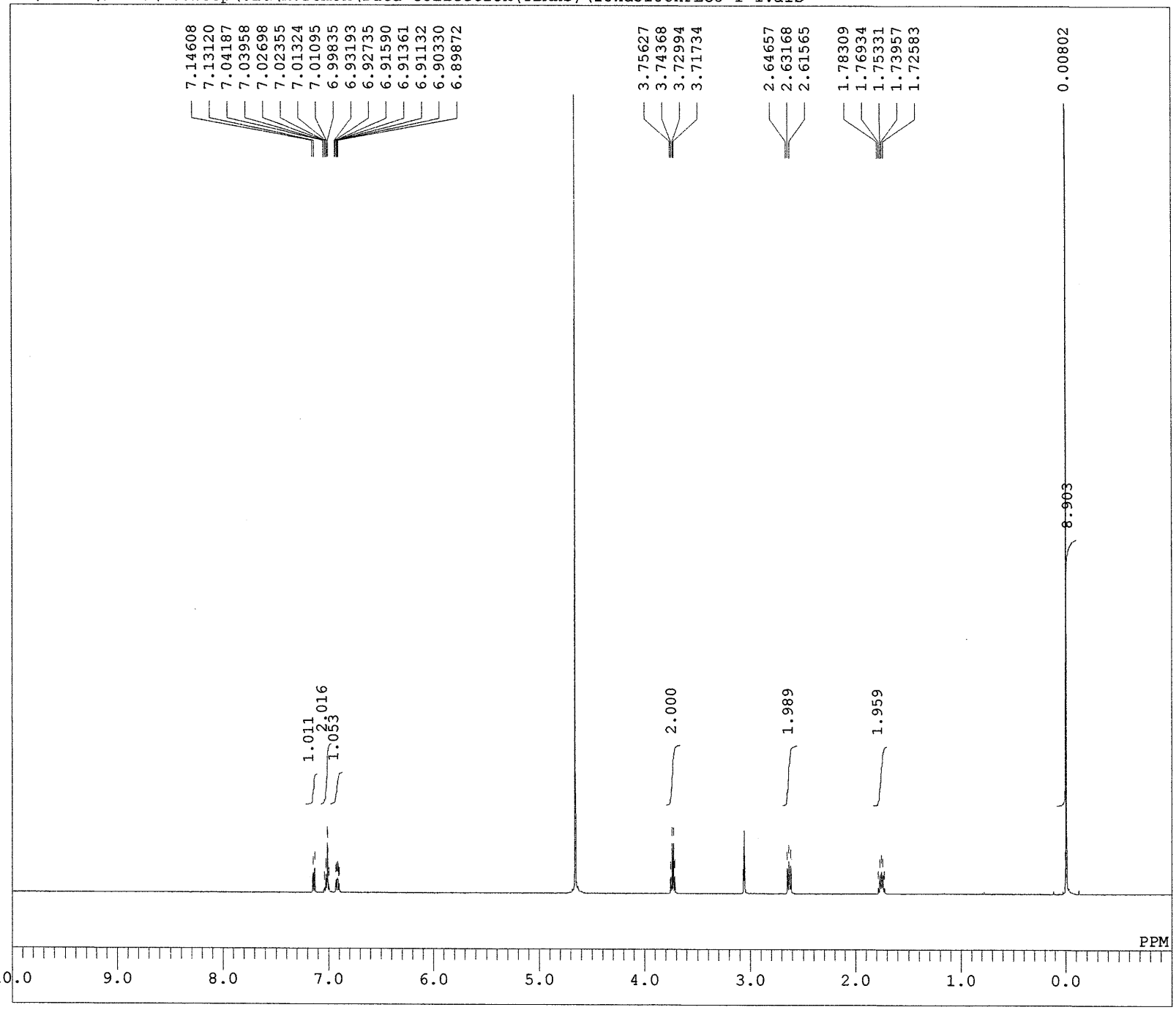



```
DFILE  18kd3087HPLC3_P-1-1.als
COMNT
DATIM  01-09-2018 23:06:27
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            29
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.2 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

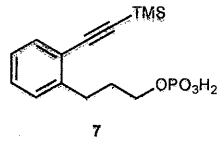


6

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3180HPLC8-1-1.als

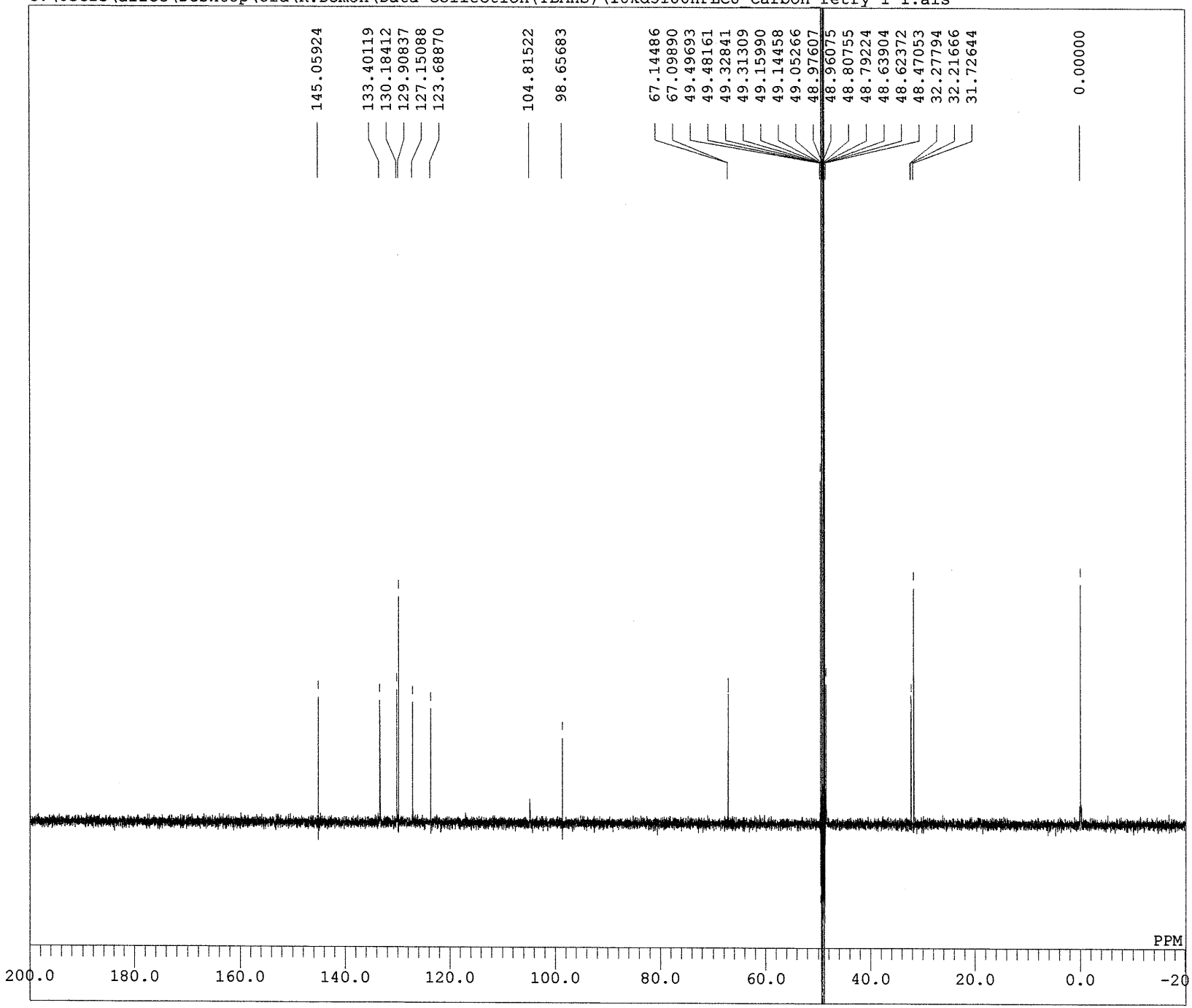


DFILE 18kd3180HPLC8-1-1.als
COMNT
DATIM 2018-10-03 08:25:20
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 8.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CD3OD
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 32

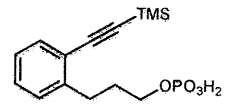


7

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3180HPLC8_carbon_retry-1-1.als

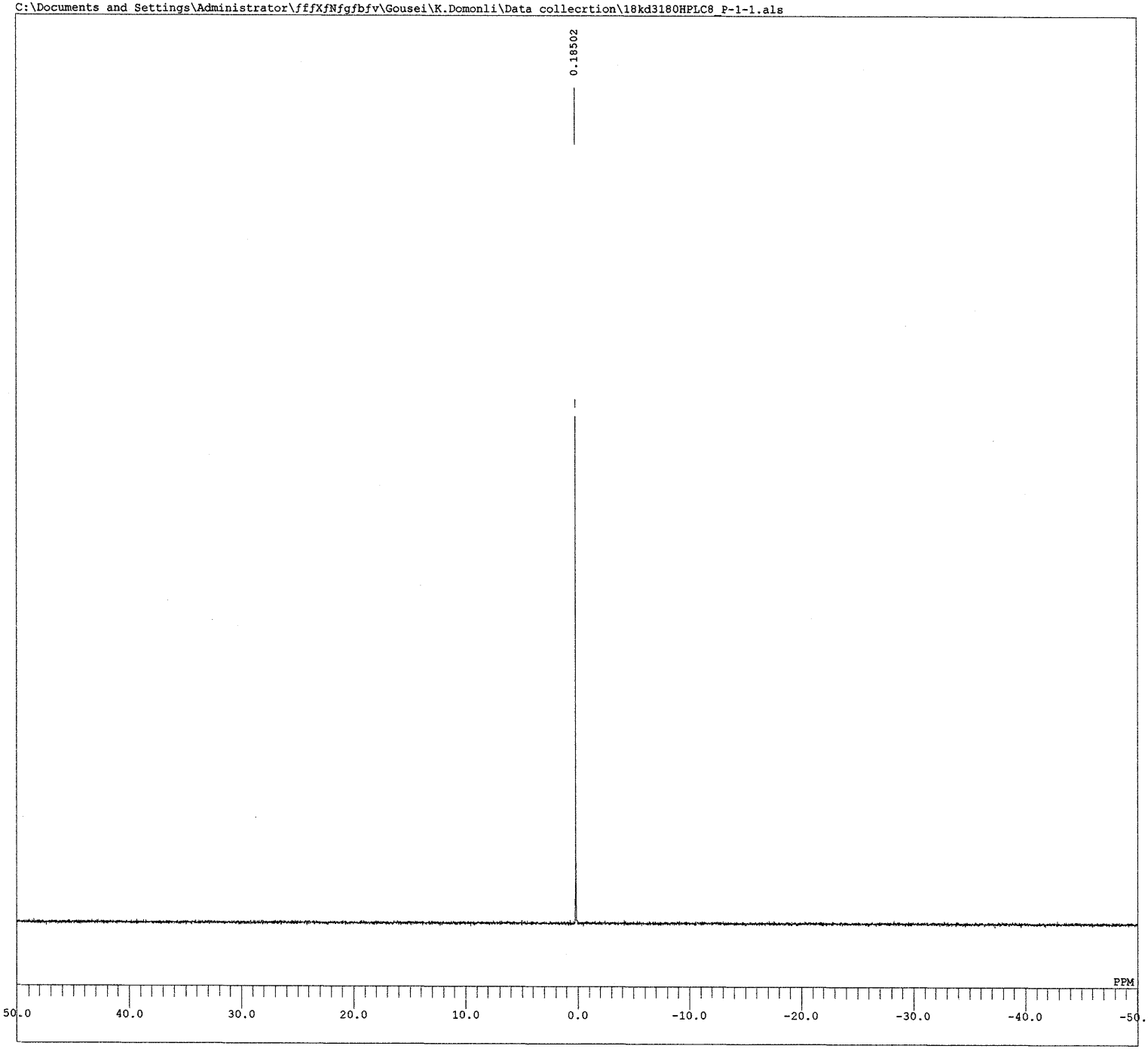



```
DFILE   18kd3180HPLC8_carbon_retry-1-1.
COMNT
DATIM   2018-10-03 08:37:09
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           1.58 KHz
OBFIN           5.95 Hz
POINT          26214
FREQU       50505.05 Hz
SCANS           1637
ACQTM         0.5190 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           22.2 c
SLVNT   CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             60
```

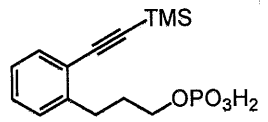


7

C:\Documents and Settings\Administrator\ffjXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd3180HPLC8_P-1-1.als

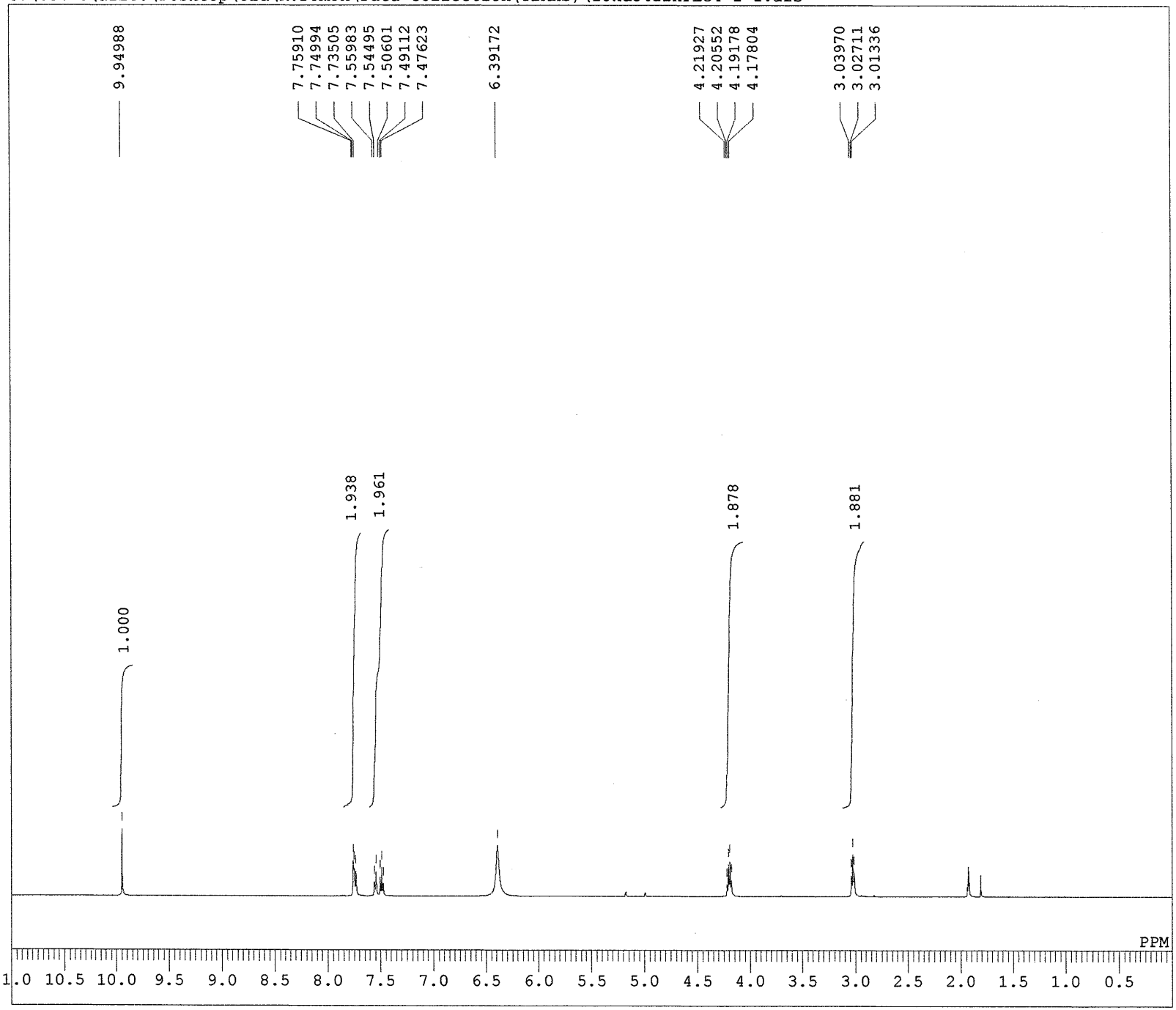



```
DFILE  18kd3180HPLC8_P-1-1.als
COMNT
DATIM  03-10-2018 22:05:51
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            72
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.3 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

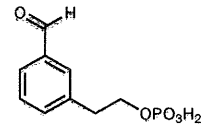


7

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3412HPLC4-1-1.als

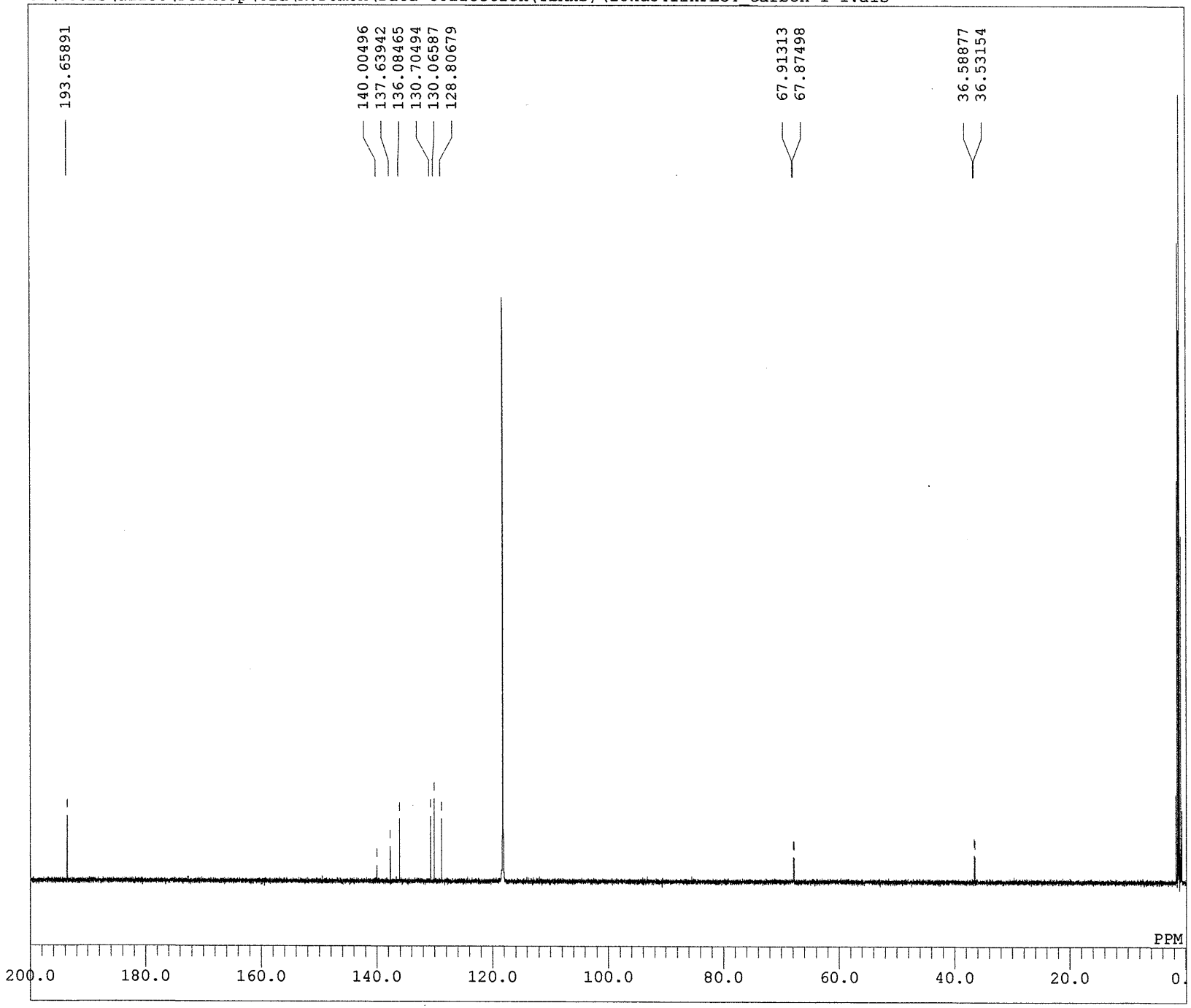


DFILE	18kd3412HPLC4-1-1.als
COMNT	
DATIM	2019-02-01 02:54:45
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	4
ACQTM	1.7459 sec
PD	6.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.6 c
SLVNT	CD3CN
EXREF	1.93 ppm
BF	0.12 Hz
RGAIN	36

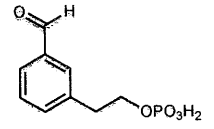


8

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3412HPLC4_carbon-1-1.als

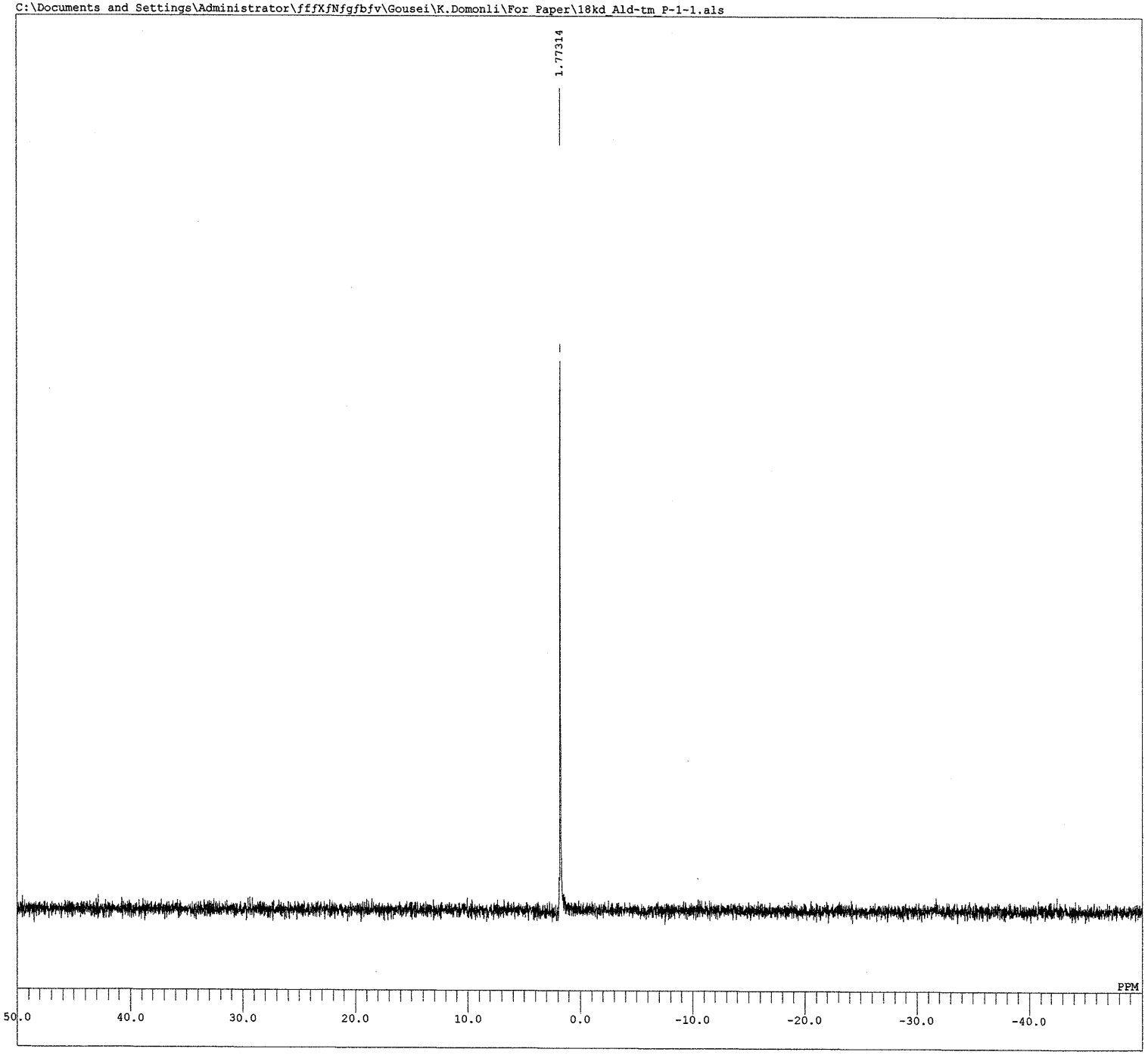


DFILE	18kd3412HPLC4_carbon-1-1.als
COMNT	
DATIM	2019-02-01 02:55:59
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	323
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.0 c
SLVNT	CD3CN
EXREF	118.20 ppm
BF	0.12 Hz
RGAIN	60

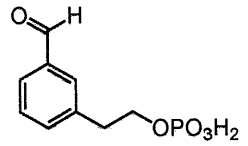


8

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd_Ald-tm_P-1-1.als

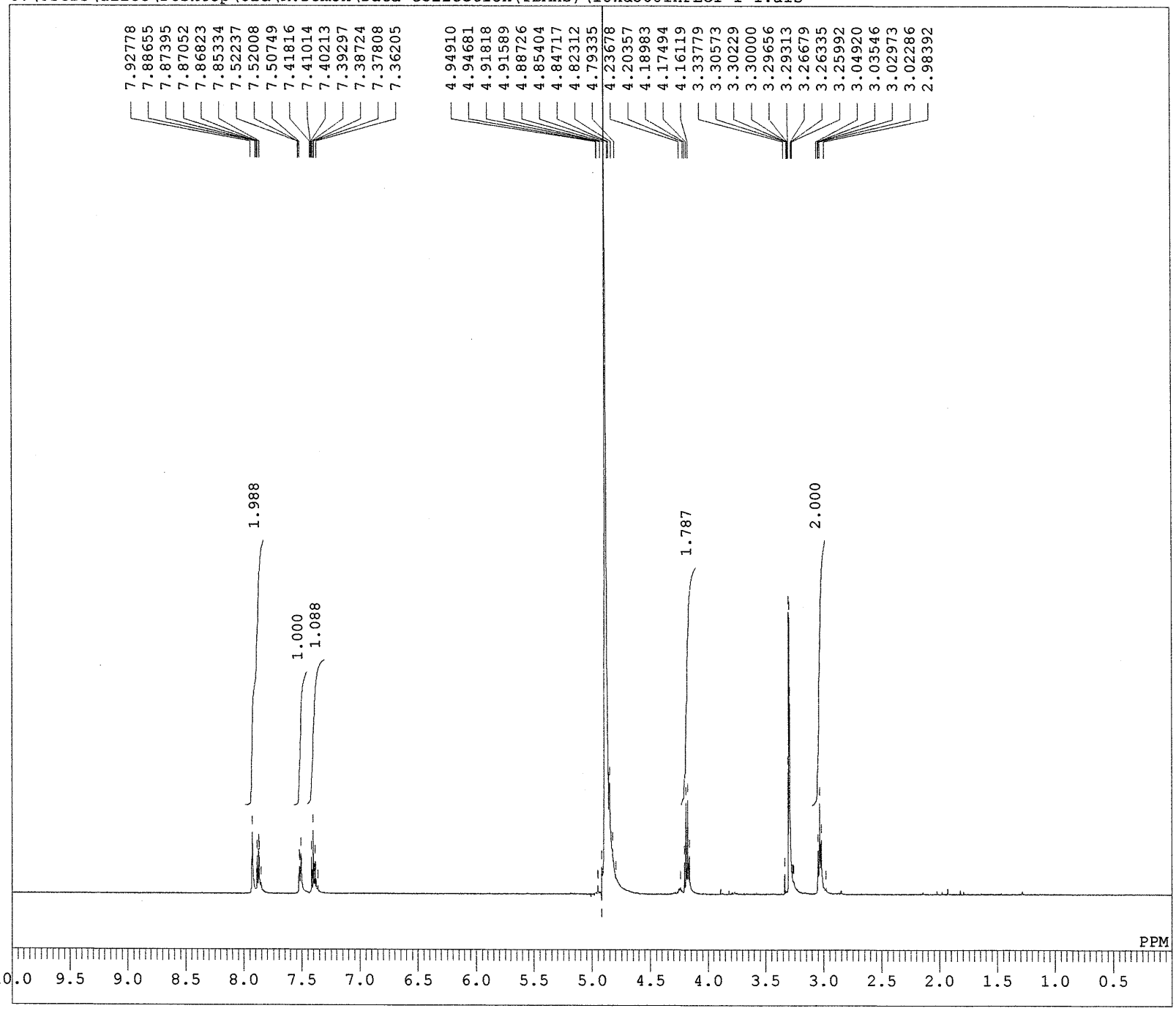


DFILE	18kd_Ald-tm_P-1-1.als
COMNT	
DATIM	07-03-2019 05:00:51
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	5
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

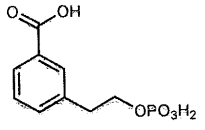


8

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3081HPLC1-1-1.als

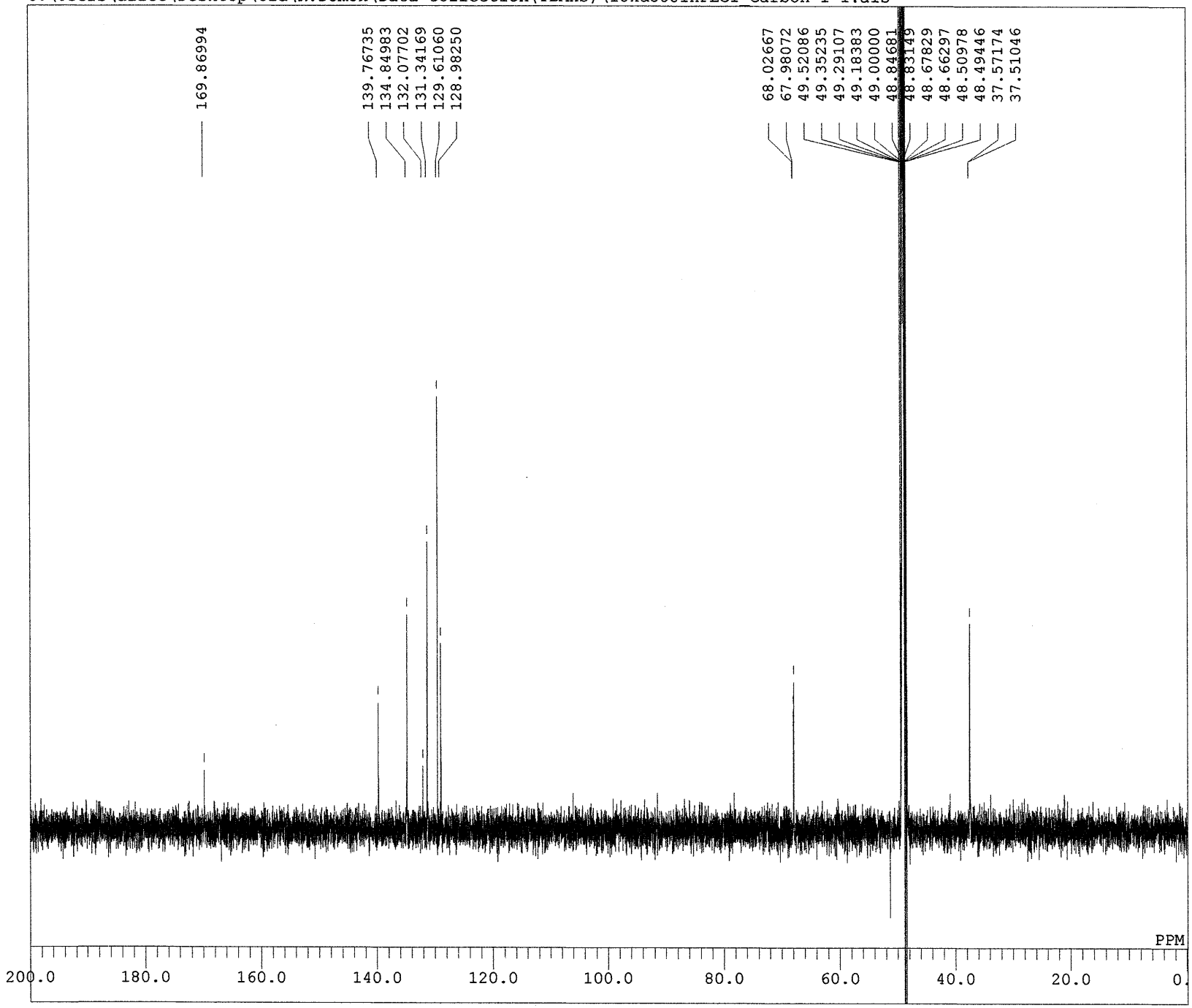


DFILE	18kd3081HPLC1-1-1.als
COMNT	
DATIM	2018-09-04 01:59:37
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	7
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.7 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

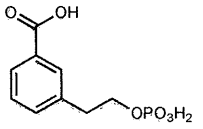


9

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3081HPLC1_carbon-1-1.als

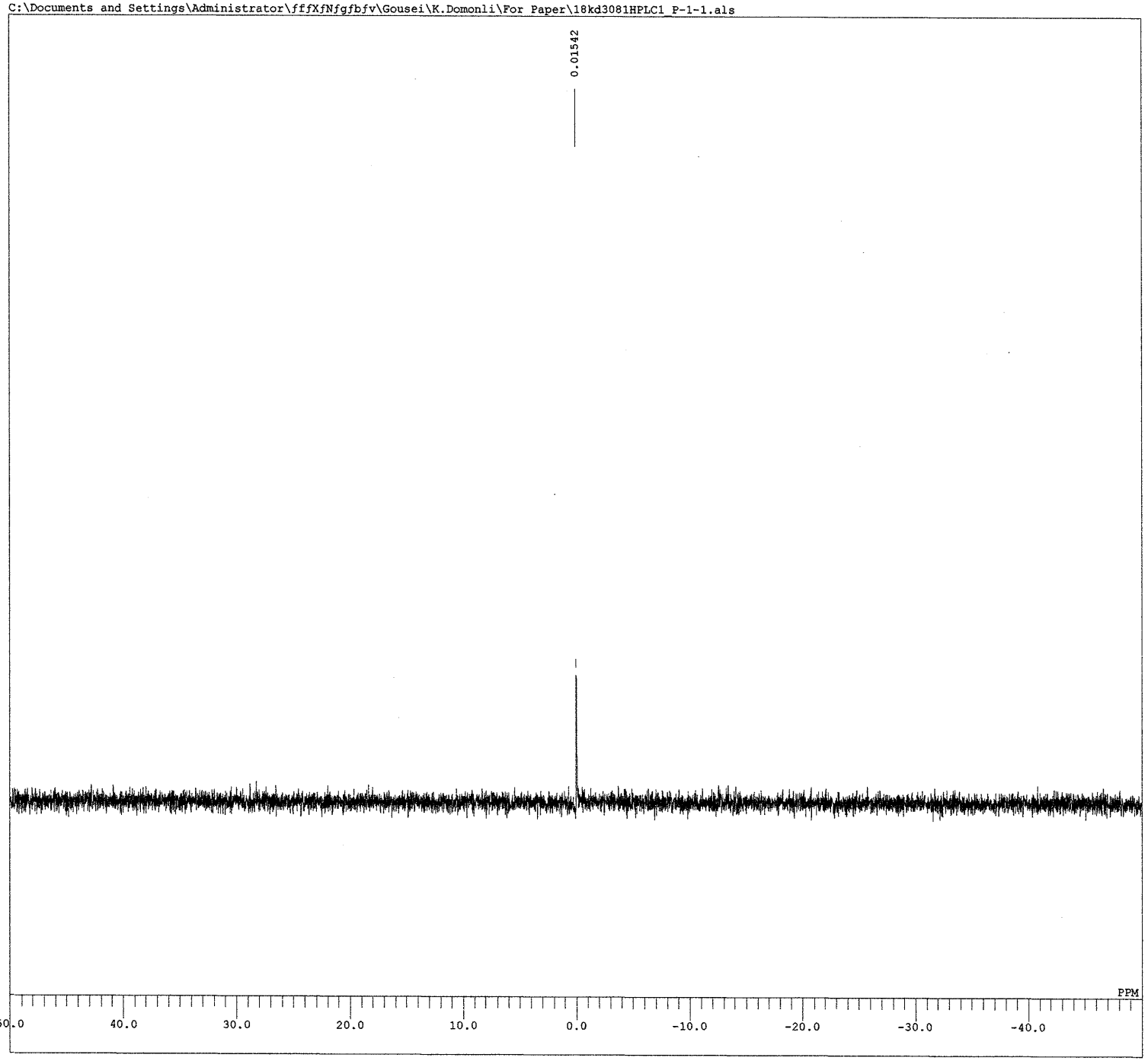



```
DFILE   18kd3081HPLC1_carbon-1-1.als
COMNT
DATIM   2018-09-04 02:06:54
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           1.58 KHz
OBFIN           5.95 Hz
POINT          26214
FREQU       50505.05 Hz
SCANS           6201
ACQTM         0.5190 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           22.4 c
SLVNT   CD3OD
EXREF          49.00 ppm
BF              0.12 Hz
RGAIN             60
```

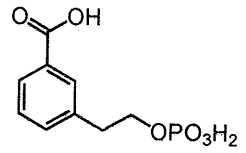


9

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3081HPLC1_P-1-1.als

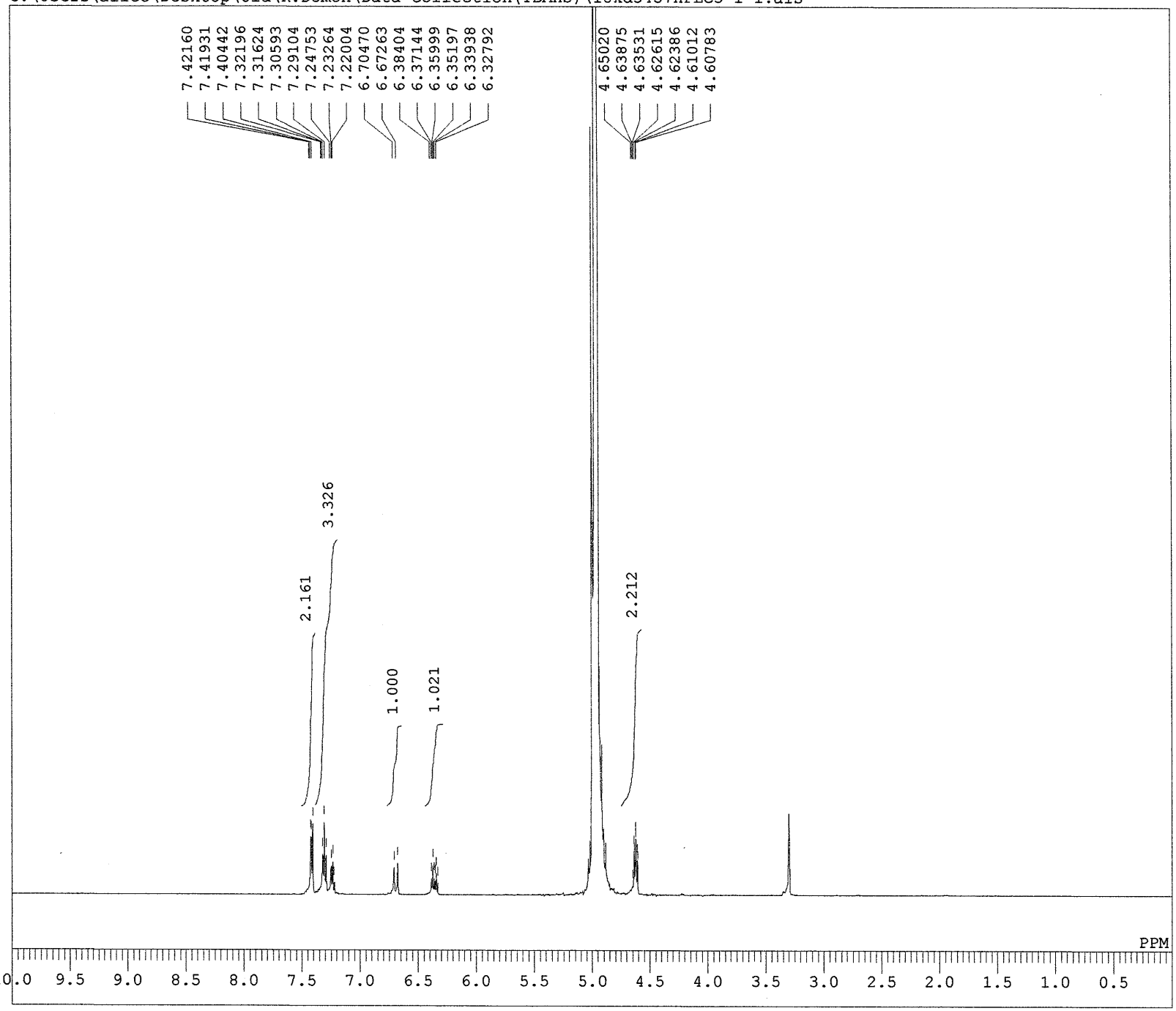



```
DFILE  18kd3081HPLC1_P-1-1.als
COMNT
DATIM  04-09-2018 07:09:38
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             5
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.1 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



9

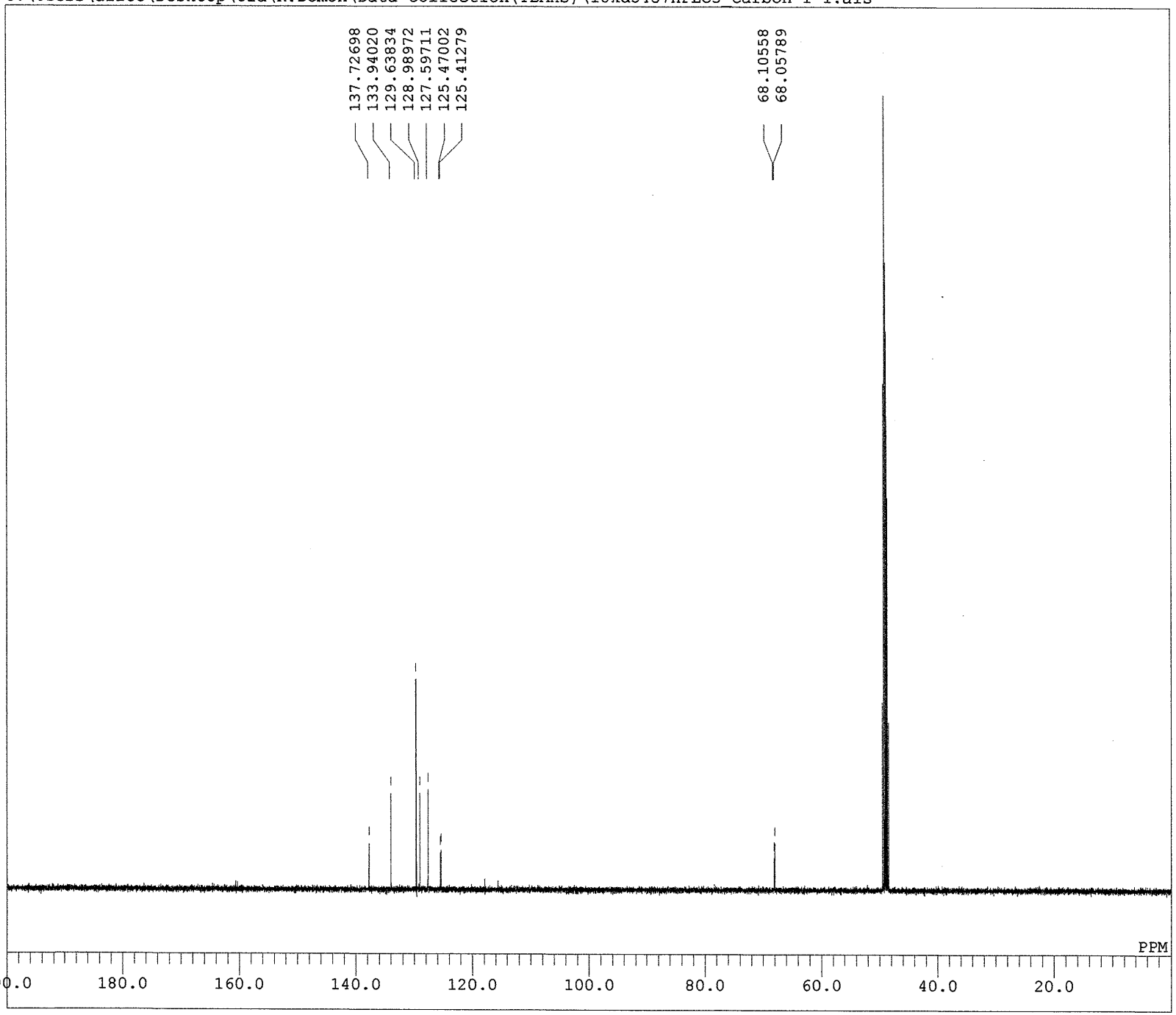
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3457HPLC3-1-1.als



DFILE	18kd3457HPLC3-1-1.als
COMNT	
DATIM	2019-03-13 00:06:17
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	4
ACQTM	1.7459 sec
PD	6.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	26

10

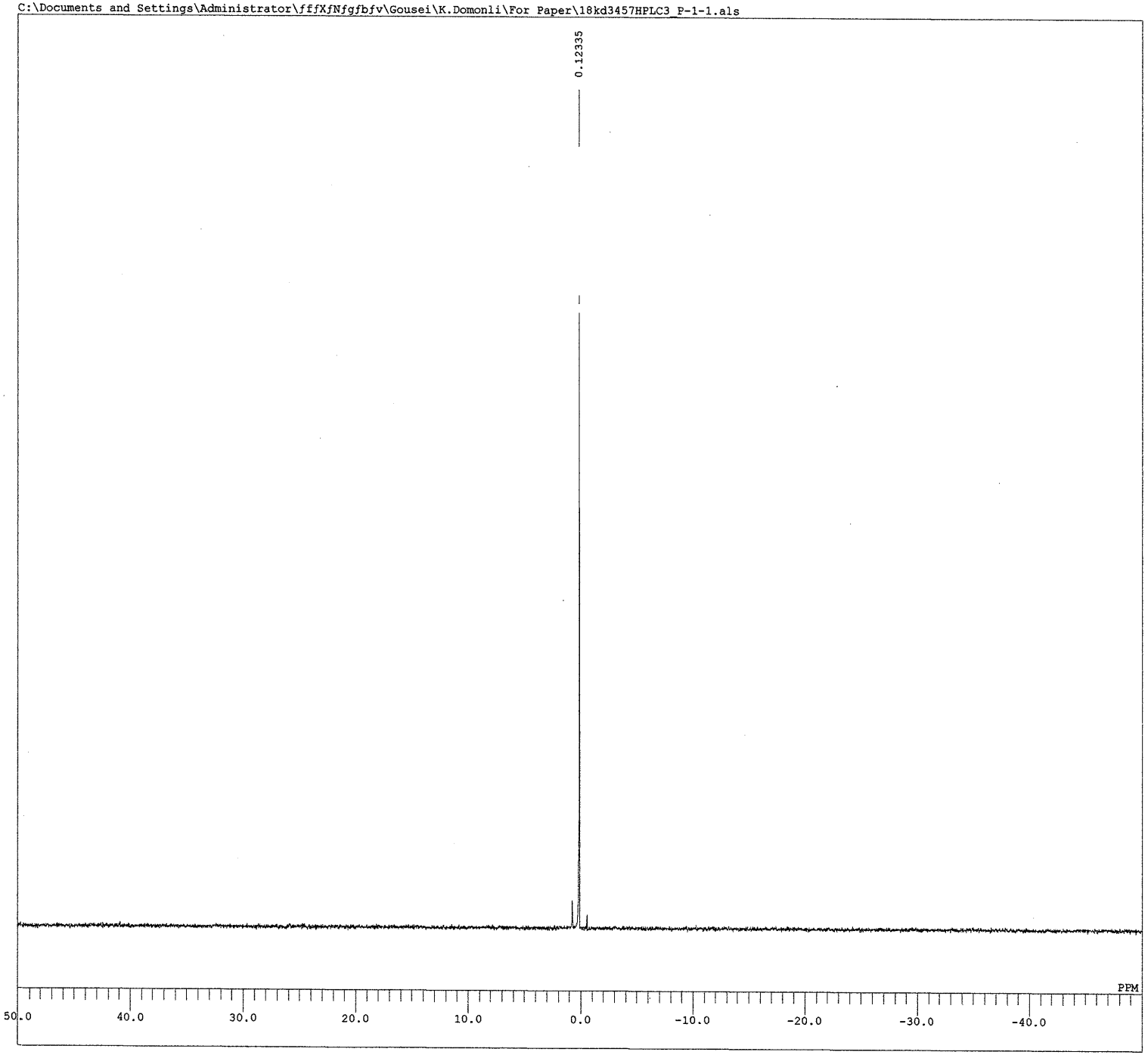
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3457HPLC3_carbon-1-1.als



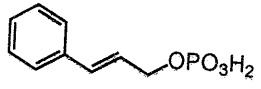

```
DFILE   18kd3457HPLC3_carbon-1-1.als
COMNT
DATIM   2019-03-13 00:16:29
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           7.87 KHz
OBFIN           4.21 Hz
POINT          26214
FREQU       31446.54 Hz
SCANS           1656
ACQTM         0.8336 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           21.9 c
SLVNT   CD3OD
EXREF           49.00 ppm
BF              0.12 Hz
RGAIN             60
```

10

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3457HPLC3_P-1-1.als

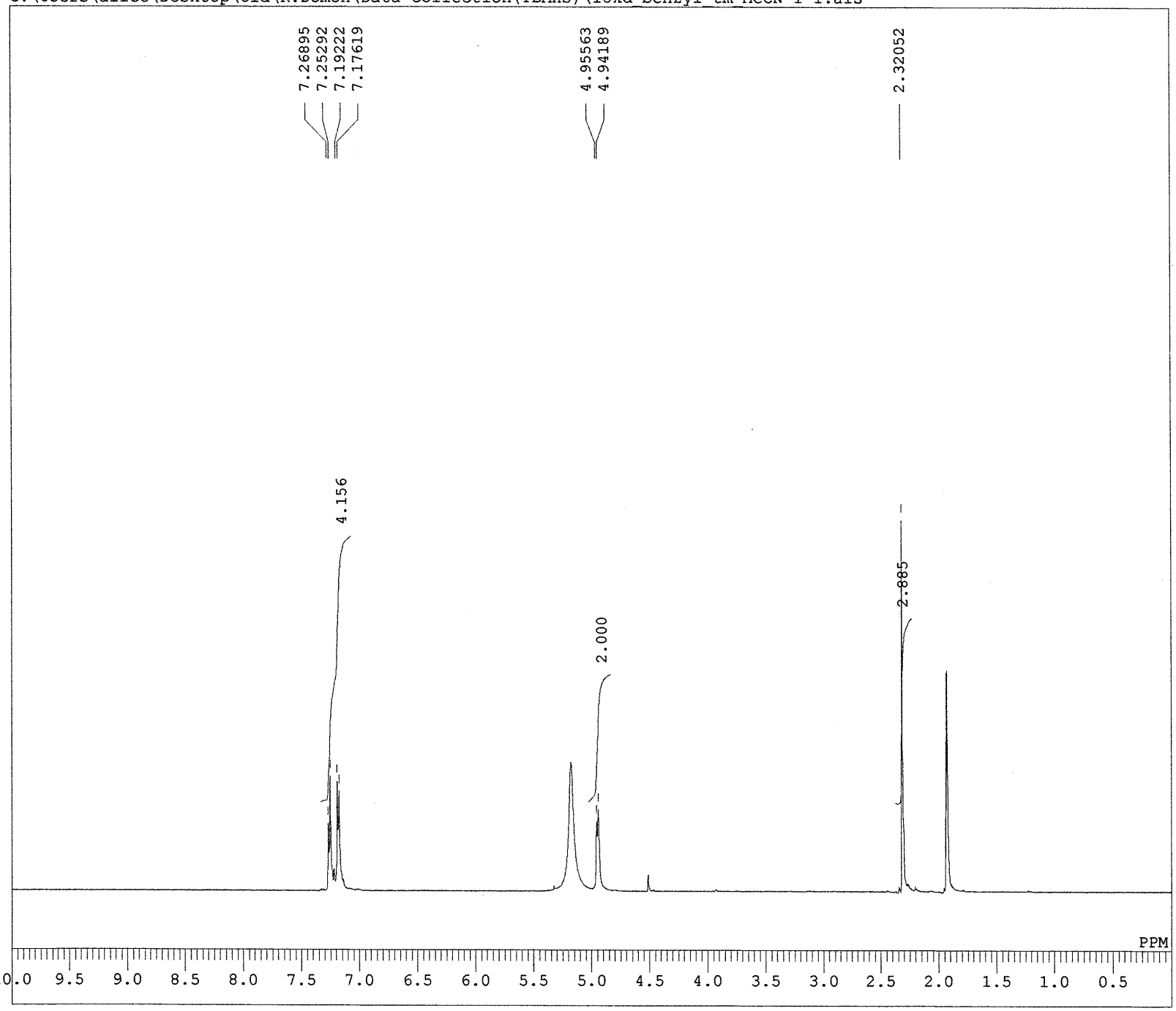


DFILE	18kd3457HPLC3_P-1-1.als
COMNT	
DATIM	13-03-2019 00:49:53
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	29
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	56

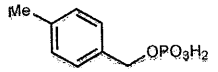


10

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd_benzyl_tm_MeCN-1-1.als

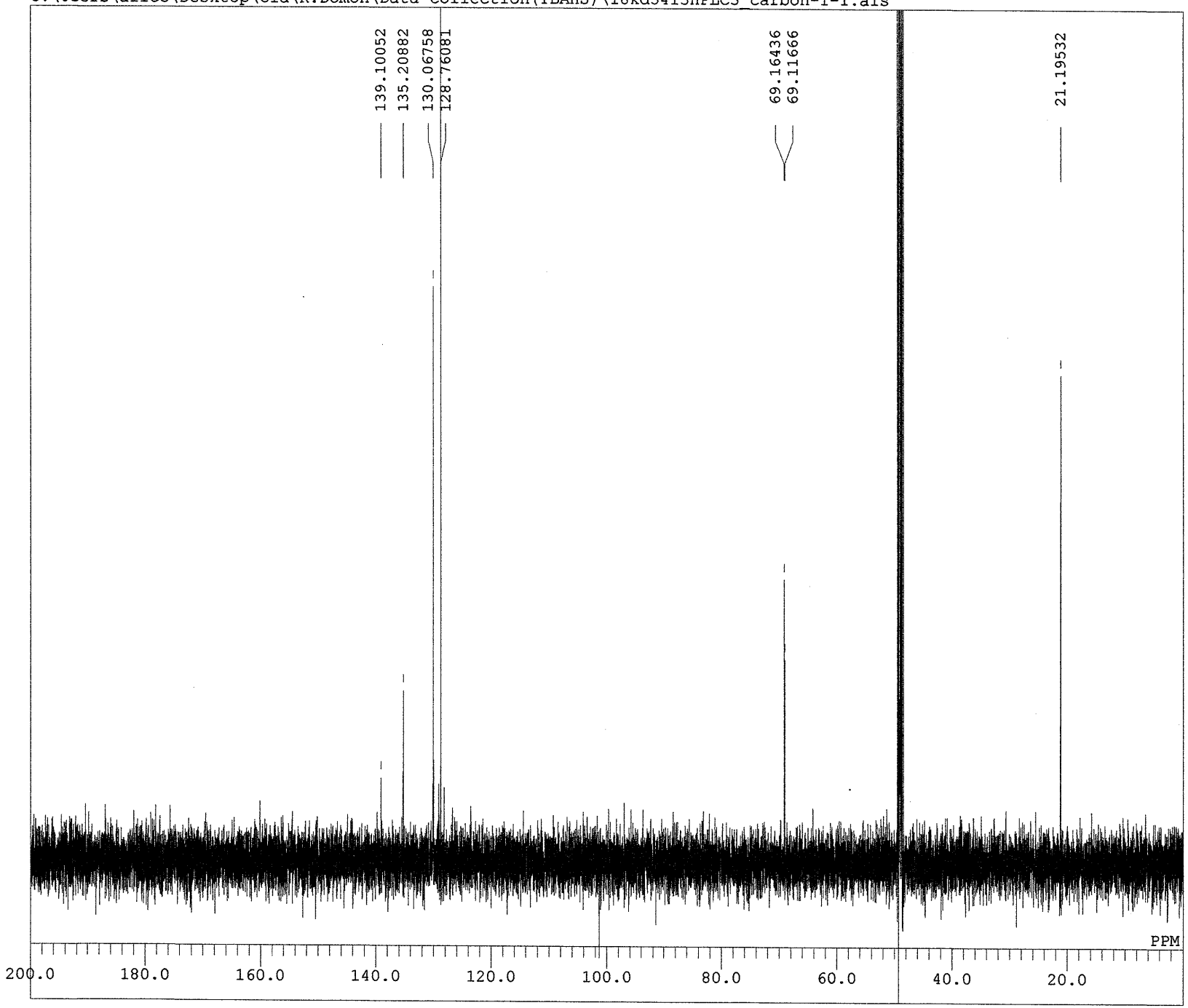


DFILE	18kd_benzyl_tm_MeCN-1-1.als
COMNT	
DATIM	2019-03-20 00:46:47
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	5
ACQTM	1.7459 sec
PD	6.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	CD3CN
EXREF	1.93 ppm
BF	0.12 Hz
RGAIN	40

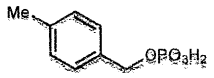


11

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3413HPLC3_carbon-1-1.als

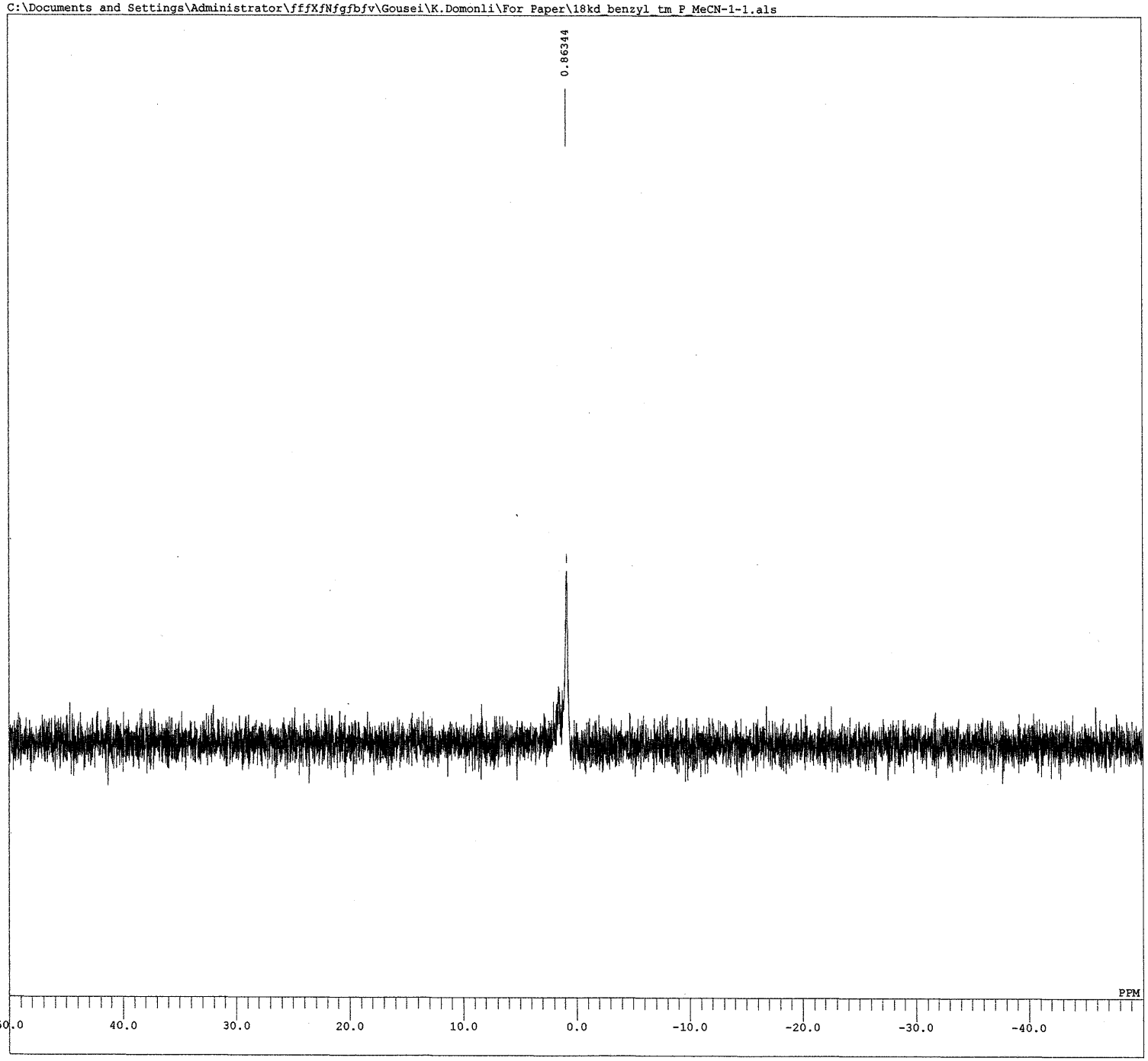


DFILE	18kd3413HPLC3_carbon-1-1.als
COMNT	
DATIM	2019-02-01 05:02:49
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	249
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

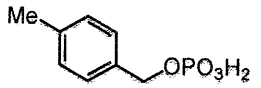


11

C:\Documents and Settings\Administrator\ffffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd_benzyl_tm_P_MeCN-1-1.als

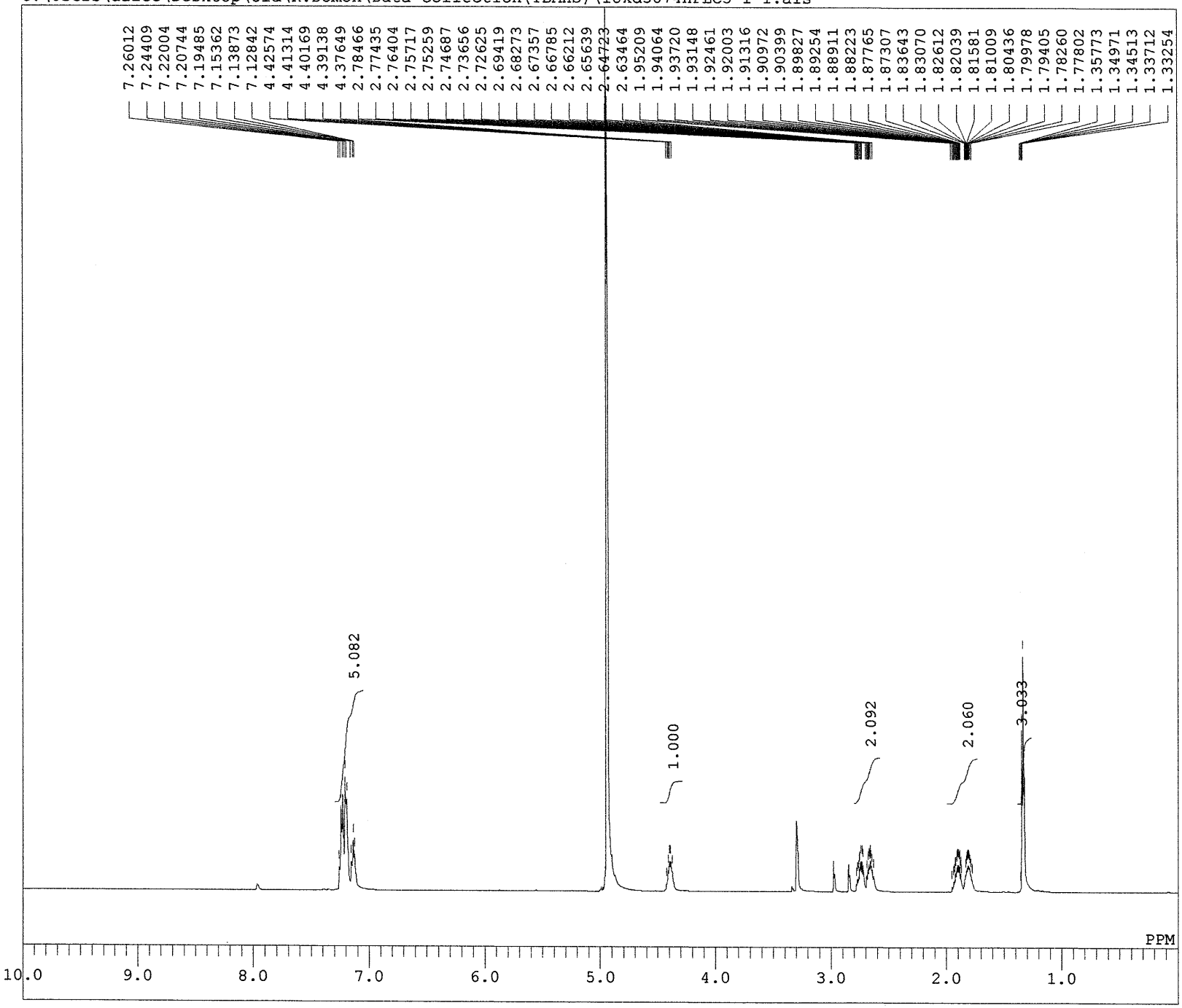


DFILE	18kd_benzyl_tm_P_MeCN-1-1.als
COMNT	
DATIM	20-03-2019 01:33:49
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	21
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	19.7 c
SLVNT	CD3CN
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

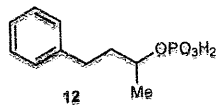


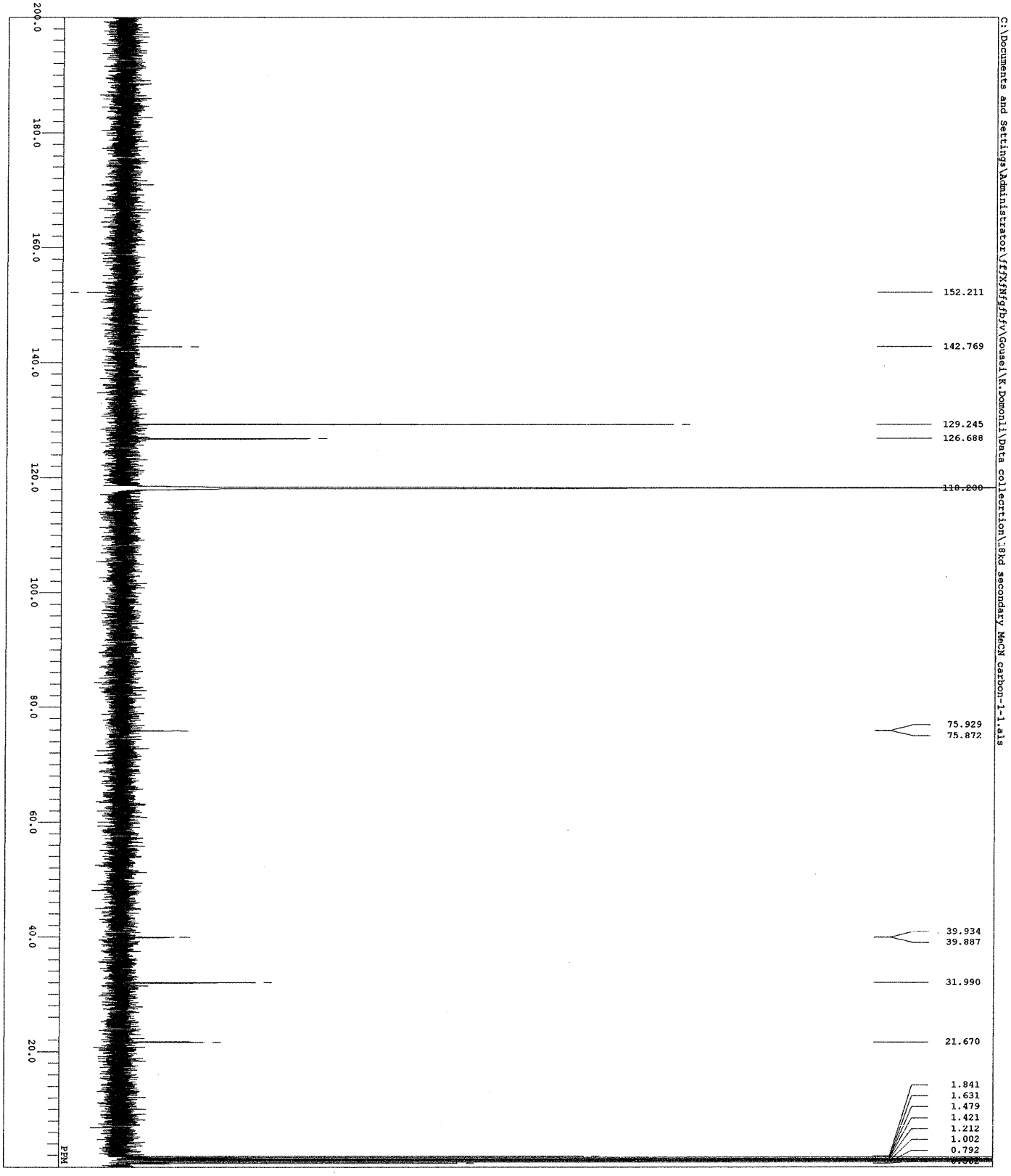
11

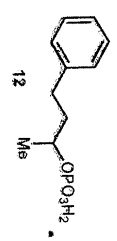
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3074HPLC3-1-1.als



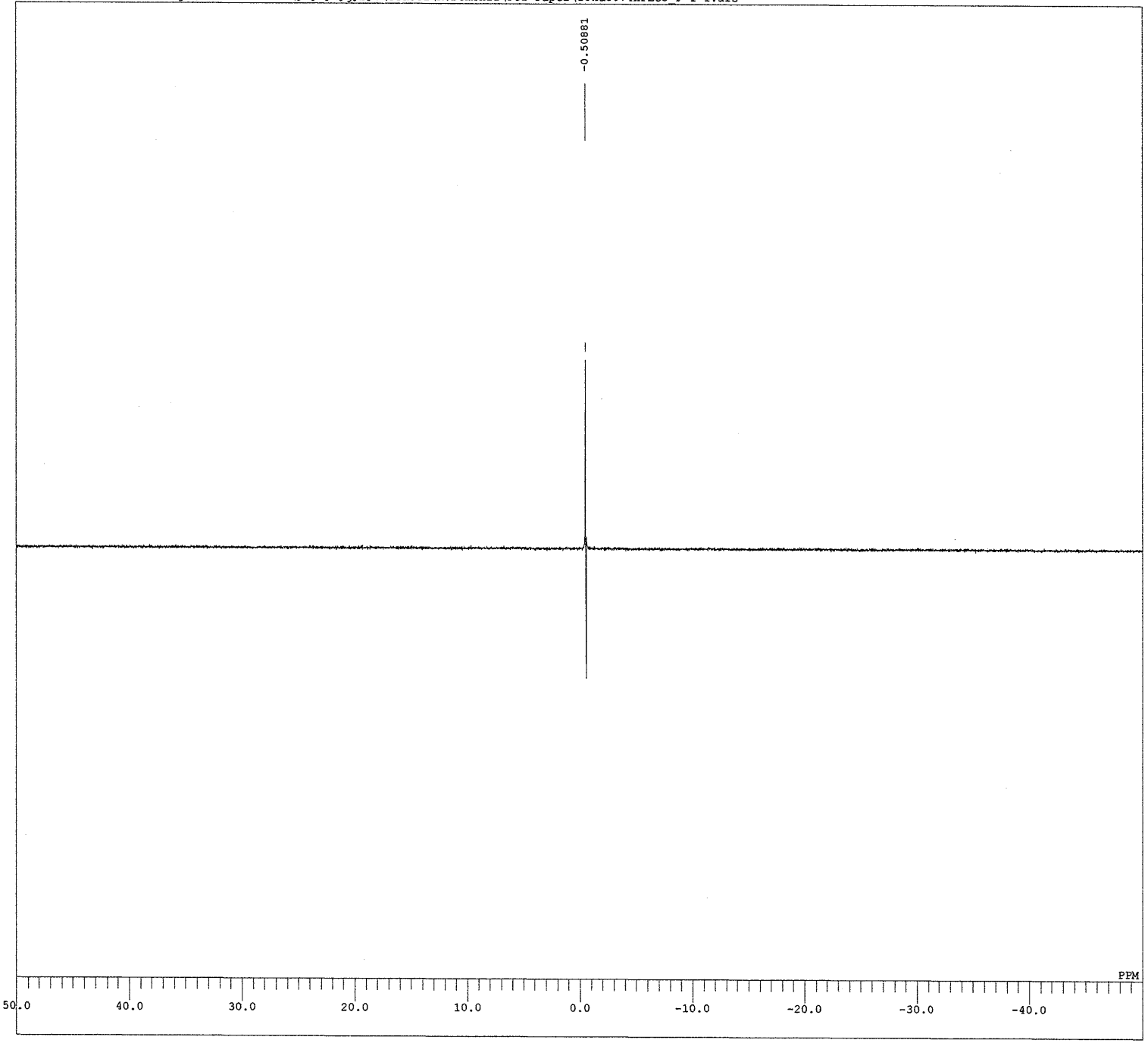

```
DFILE   18kd3074HPLC3-1-1.als
COMNT
DATIM   2018-09-01 03:02:12
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         500.16 MHz
OBSET           2.41 KHz
OBFIN           6.01 Hz
POINT          13107
FREQU        7507.51 Hz
SCANS             8
ACQTM         1.7459 sec
PD            5.0000 sec
PW1             5.55 usec
IRNUC   1H
CTEMP           21.2 c
SLVNT   CD3OD
EXREF           3.30 ppm
BF              0.12 Hz
RGAIN             30
```



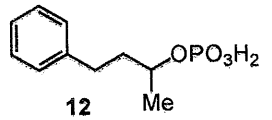

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd secondary MeCN carbon-1-1.als
152.211
142.769
129.245
126.688
118.200
75.929
75.872
39.934
39.887
31.990
21.670
1.841
1.631
1.479
1.421
1.212
1.002
0.792
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
PPM
DFILE 18kd_secondary_MeCN_carbon-1-1.als
COMNT
DATIM 21-03-2019 00:26:41
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 98.52 MHz
OBSET 4.64 KHz
OBFIN 8.74 Hz
POINT 26214
FREQU 24630.54 Hz
SCANS 545
ACQTM 1.0643 sec
PD 2.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 19.9 c
SLVNT CD3CN
EXREF 118.20 ppm
BF 0.12 Hz
RGAIN 58


12
Me
OPO3H2

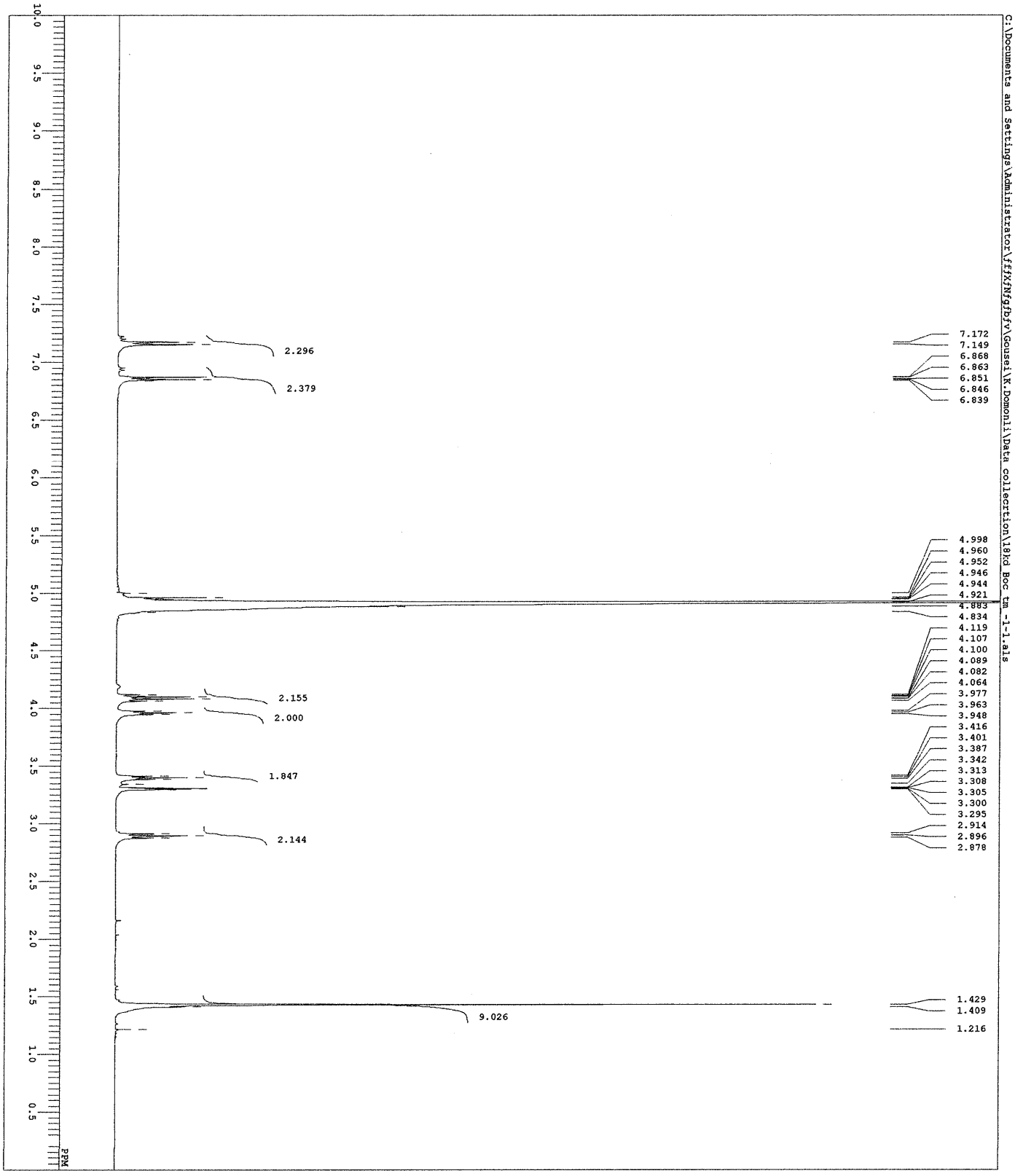
C:\Documents and Settings\Administrator\ƒfƒXƒNƒgƒbƒv\Gousei\K.Domonli\For Paper\18kd3074HPLC3_P-1-1.als



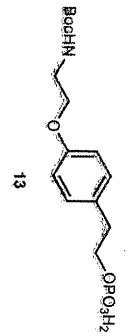

```
DFILE   18kd3074HPLC3_P-1-1.als
COMNT
DATIM   01-09-2018 23:03:20
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS              5
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC   1H
CTEMP          20.1 c
SLVNT   CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



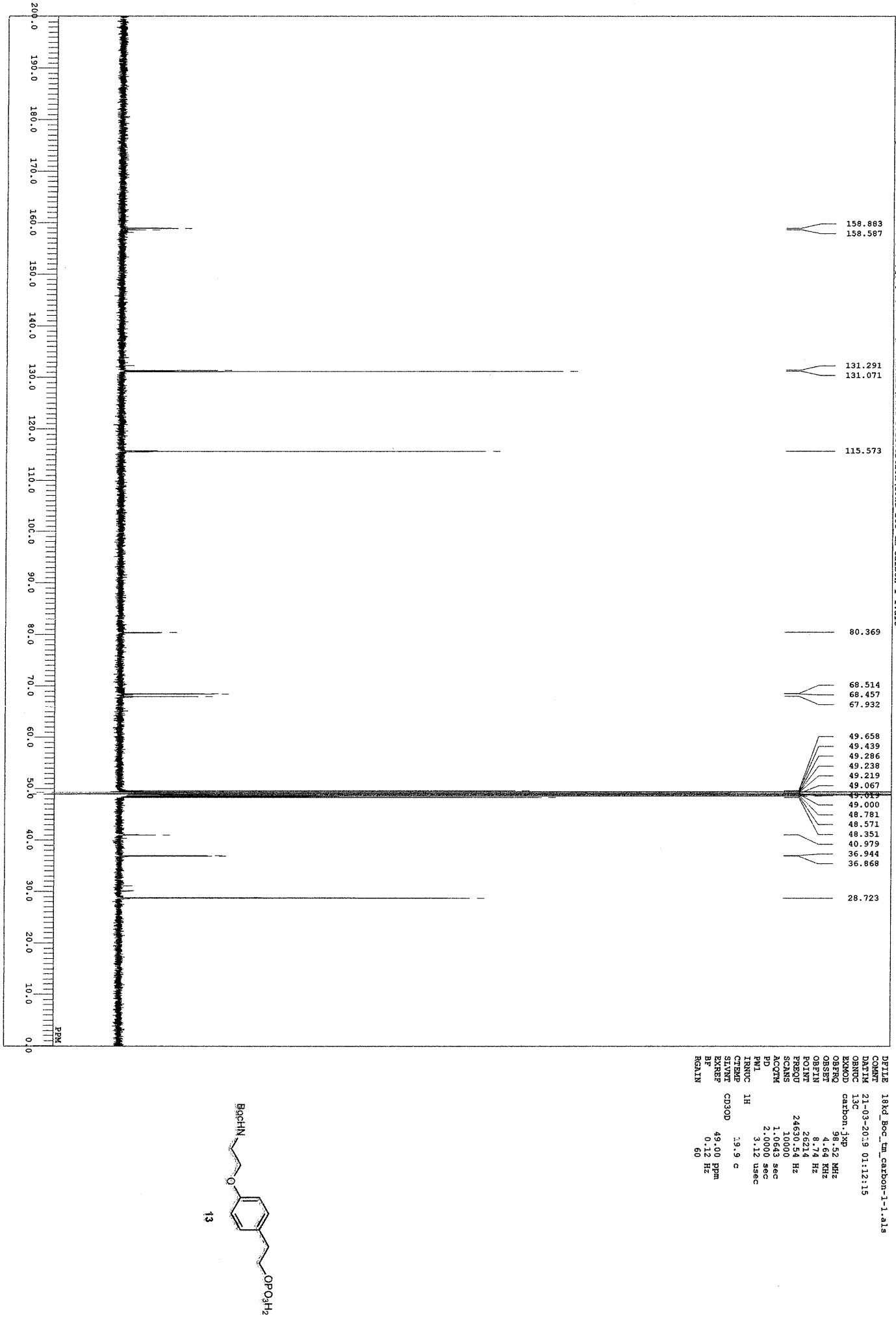
12



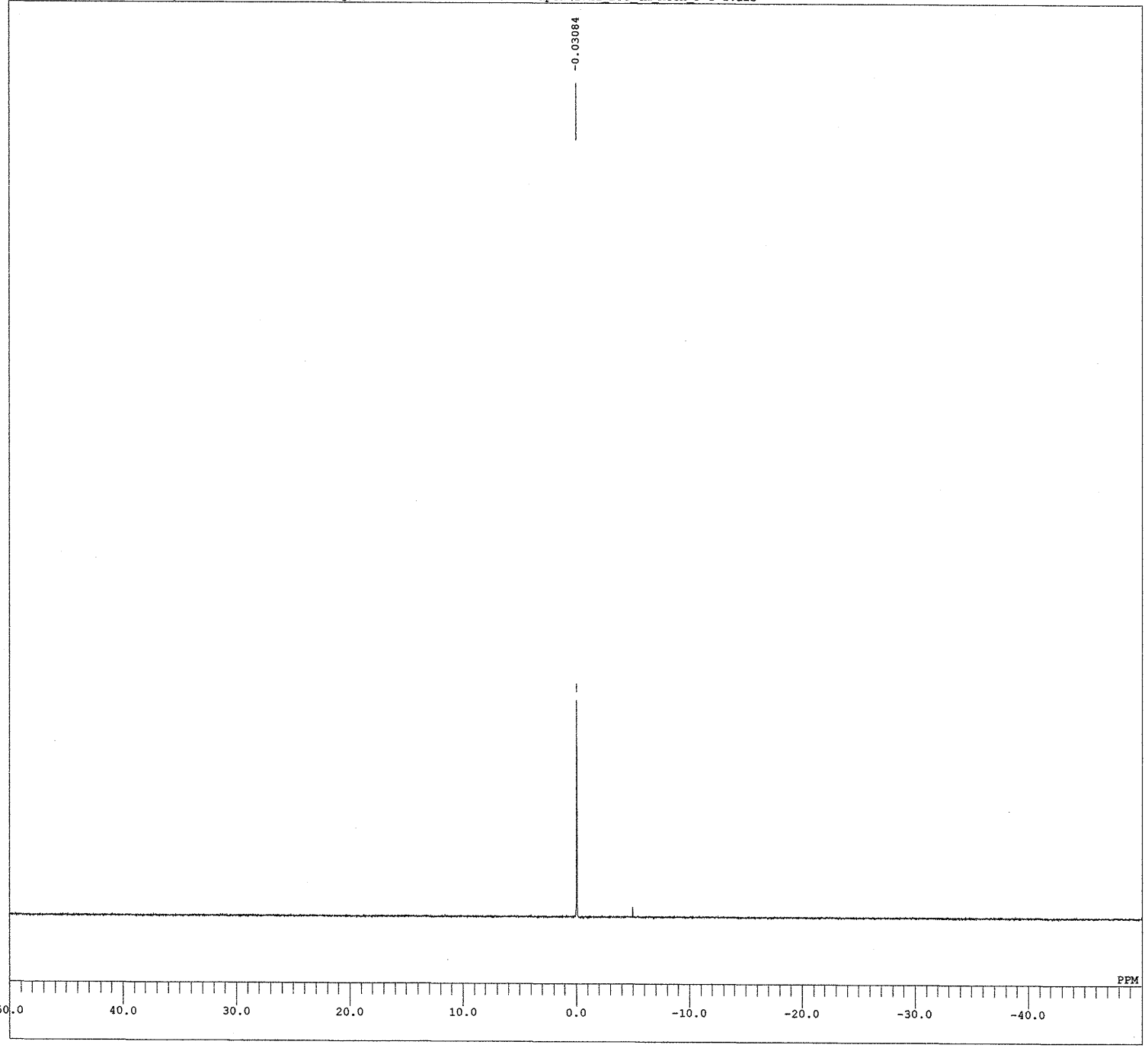
DFILE 18kd_Boc_tm_-1-1.als
COMNT
DATIM 21-03-2019 09:59:43
OBNUC 1H
EXMOD proton.jxp
OBFRQ 391.78 MHz
OBSET 8.51 KHz
OBFIN 3.34 Hz
POINT 13107
FREQU 5878.90 Hz
SCANS 8
ACQTM 2.2295 sec
PD 5.0000 sec
PW1 5.22 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 24



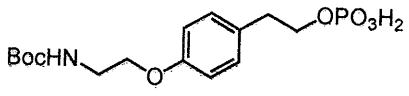
13


C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\Data collection\18kd_Boc_tm_carbon-1-1.als
158.883
158.587
131.291
131.071
115.573
80.369
68.514
68.457
67.932
49.658
49.439
49.286
49.238
49.219
49.067
49.000
48.781
48.571
48.351
40.979
36.944
36.868
28.723
PPM
DFILE 18kd_Boc_tm_carbon-1-1.als
COMNT
DATIM 21-03-20:9 01:12:15
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 96.52 MHz
OBSET 4.64 KHz
OBFIN 8.74 Hz
POINT 26214
FREQU 24630.54 Hz
SCANS 10000
ACQTM 1.0643 sec
PD 2.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP :9.9 c
SLVNT CD3OD
EXREF 49.00 ppm
BF 0.12 Hz
RGAIN 60
BocHN
O
OPO3H2
13

C:\Documents and Settings\Administrator\ffjXjNfgfbjv\Gousei\K.Domonli\For Paper\18kd_Boc_tm_MeOH_P-1-1.als

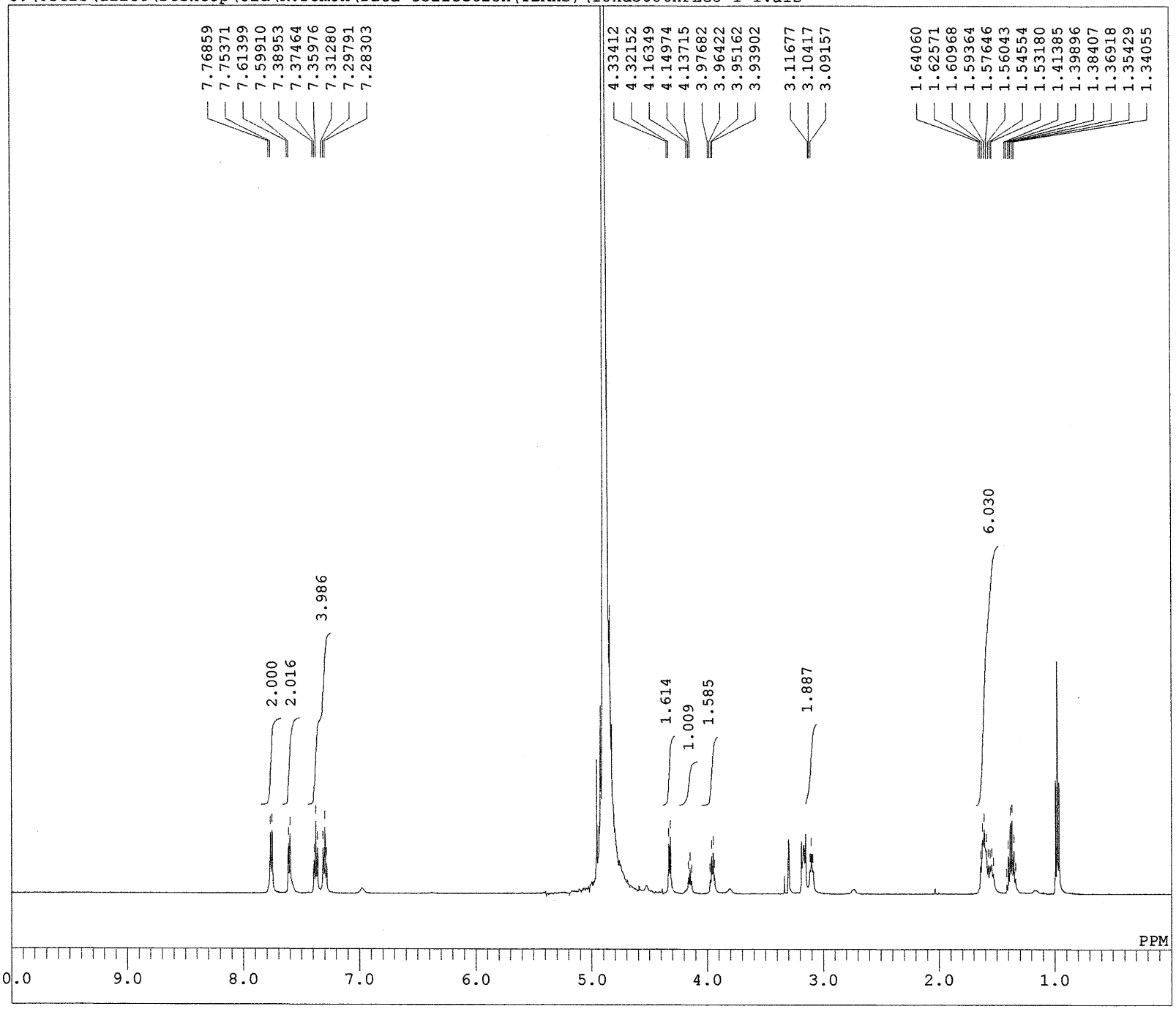



```
DFILE  18kd_Boc_tm_MeOH_P-1-1.als
COMNT
DATIM  21-03-2019 10:04:21
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            22
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP           19.8 c
SLVNT  CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



13

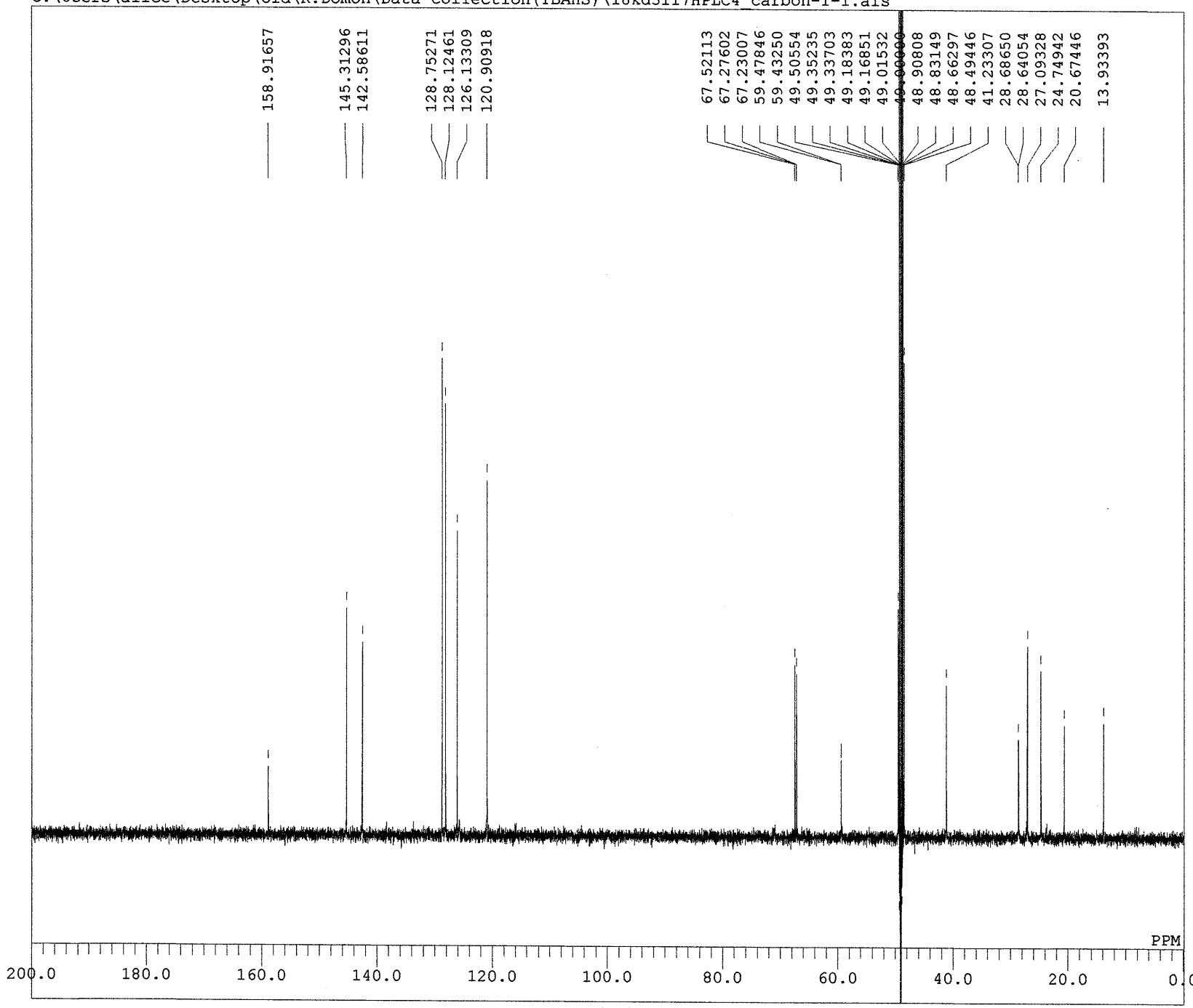
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3086HPLC8-1-1.als



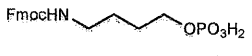
DFILE	18kd3086HPLC8-1-1.als
COMNT	
DATIM	2018-09-01 04:53:19
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.7 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	18

14

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3117HPLC4_carbon-1-1.als



DFILE	18kd3117HPLC4_carbon-1-1.als
COMNT	
DATIM	2018-09-20 04:16:60
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	1895
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.2 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60



14

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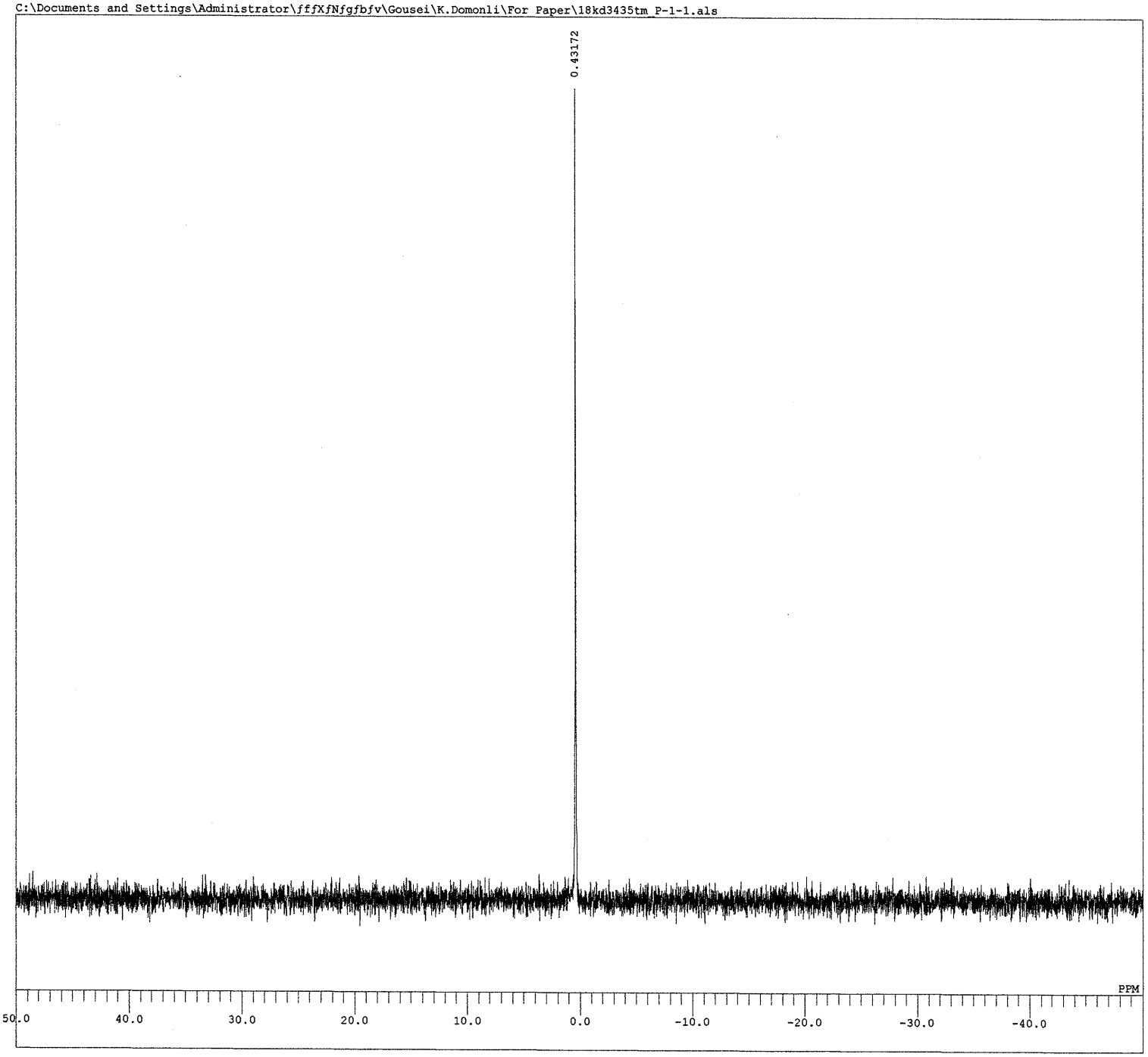
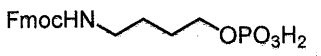
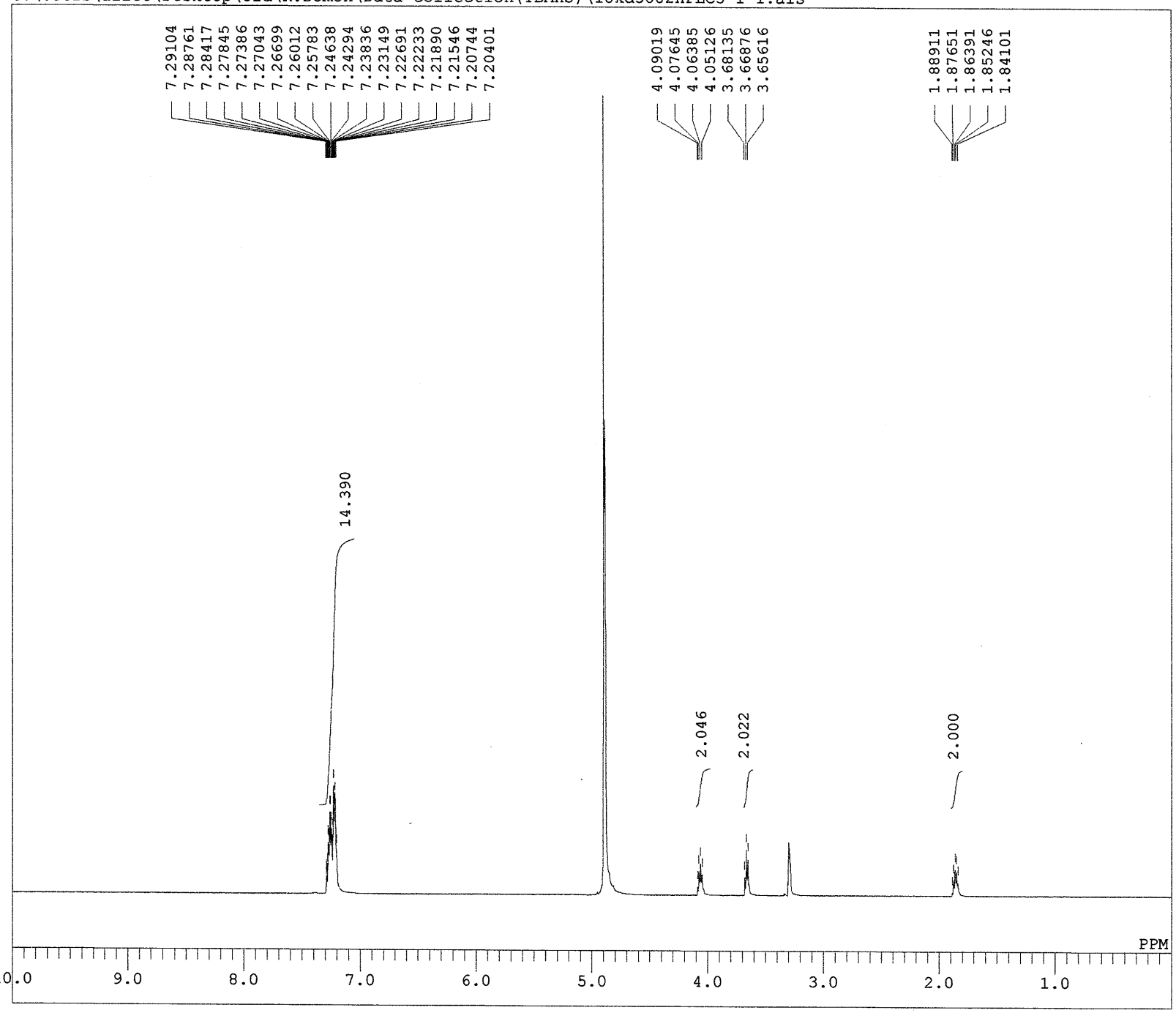


DFILE	18kd3435tm_P-1-1.als
COMNT	
DATIM	07-03-2019 05:16:05
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	8
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	19.9 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

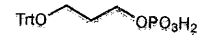


14

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3082HPLC3-1-1.als

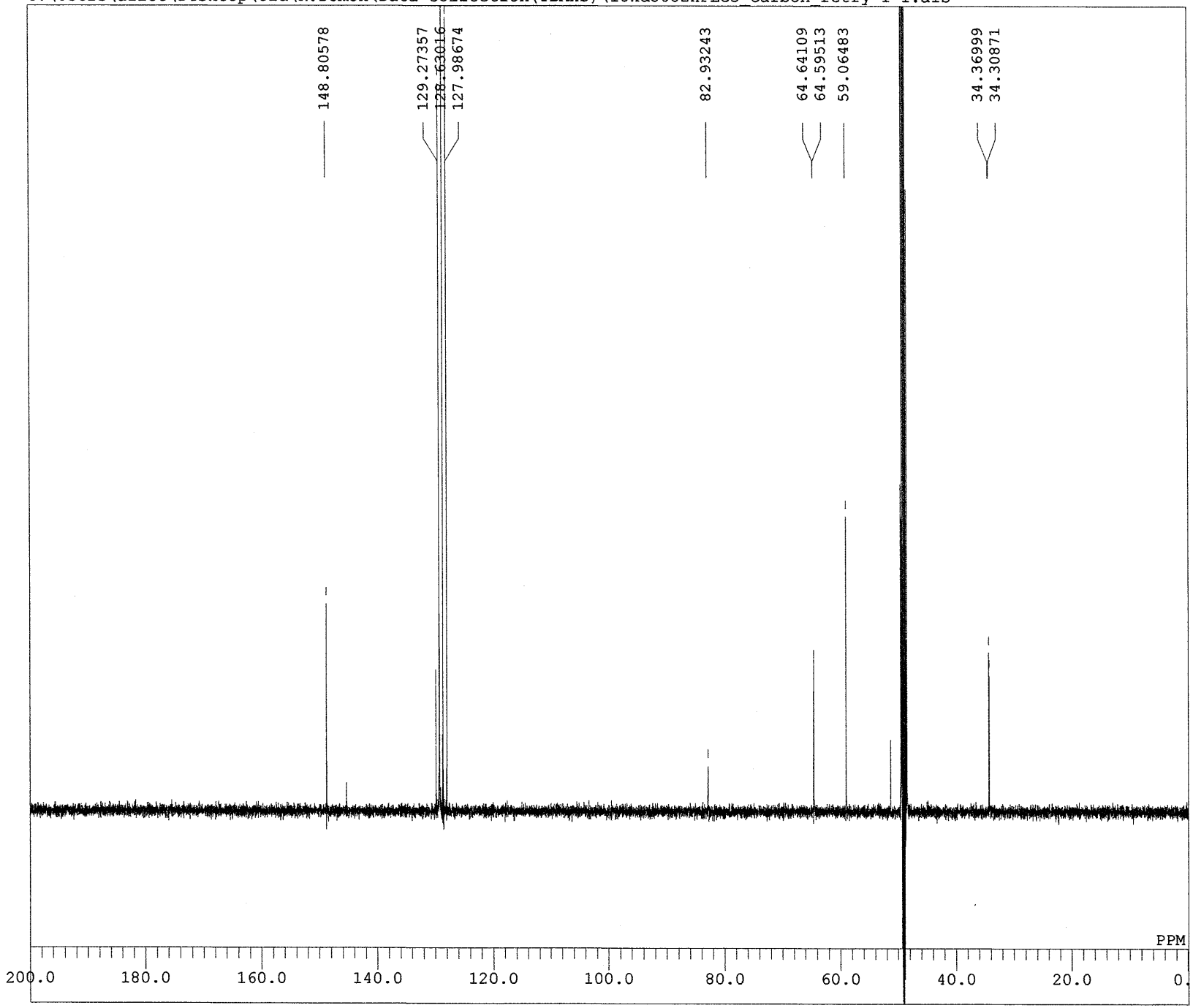


DFILE	18kd3082HPLC3-1-1.als
COMNT	
DATIM	2018-09-01 04:24:23
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	4
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

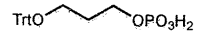


15

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3082HPLC3_carbon_retry-1-1.als



DFILE	18kd3082HPLC3_carbon_retry-1-1.
COMNT	
DATIM	2018-09-01 05:34:16
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	6623
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60



15

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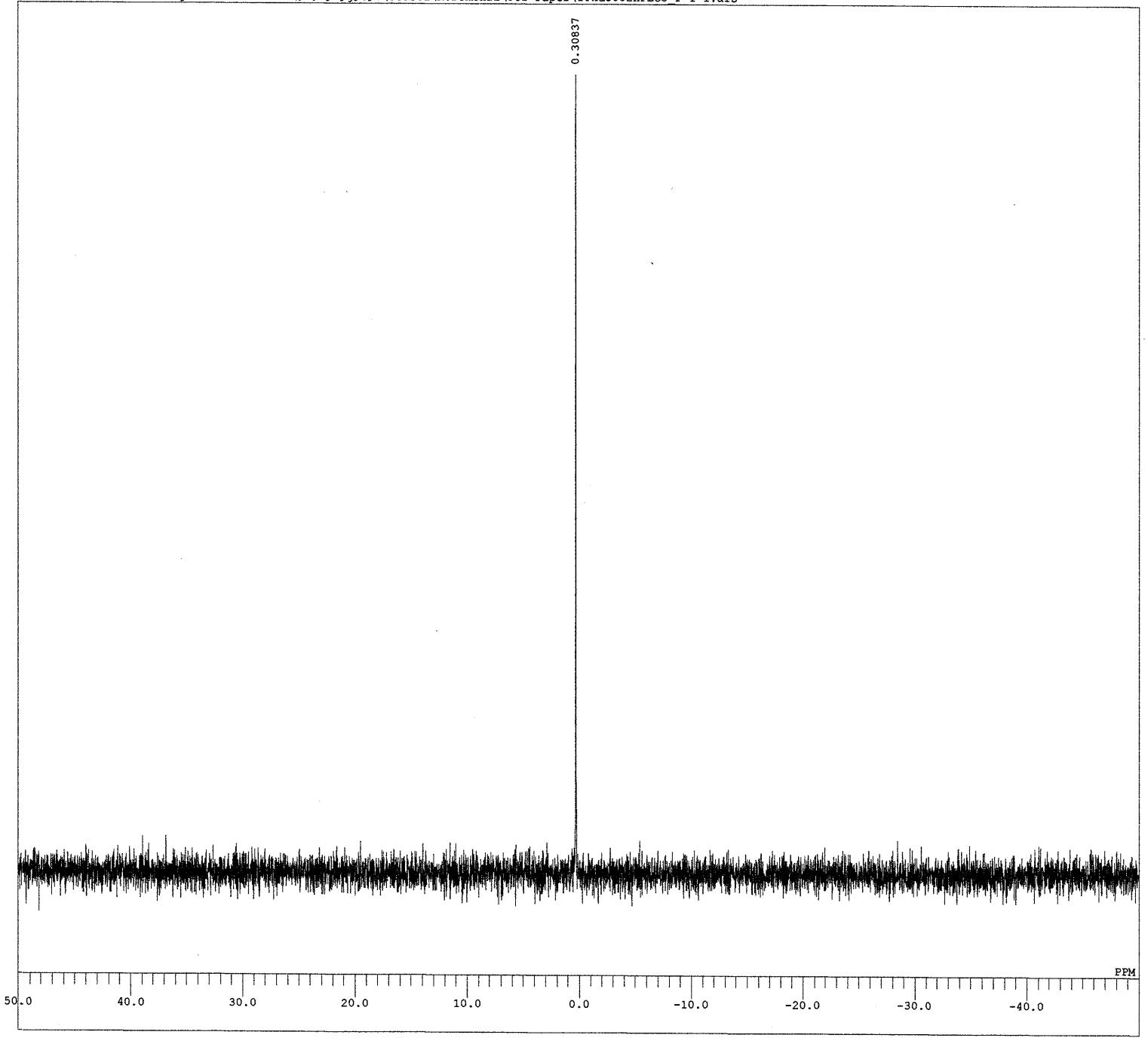
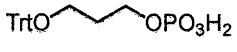



```
DFILE  18kd3082HPLC3_P-1-1.als
COMNT
DATIM  01-09-2018 06:02:21
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             8
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP         20.4 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



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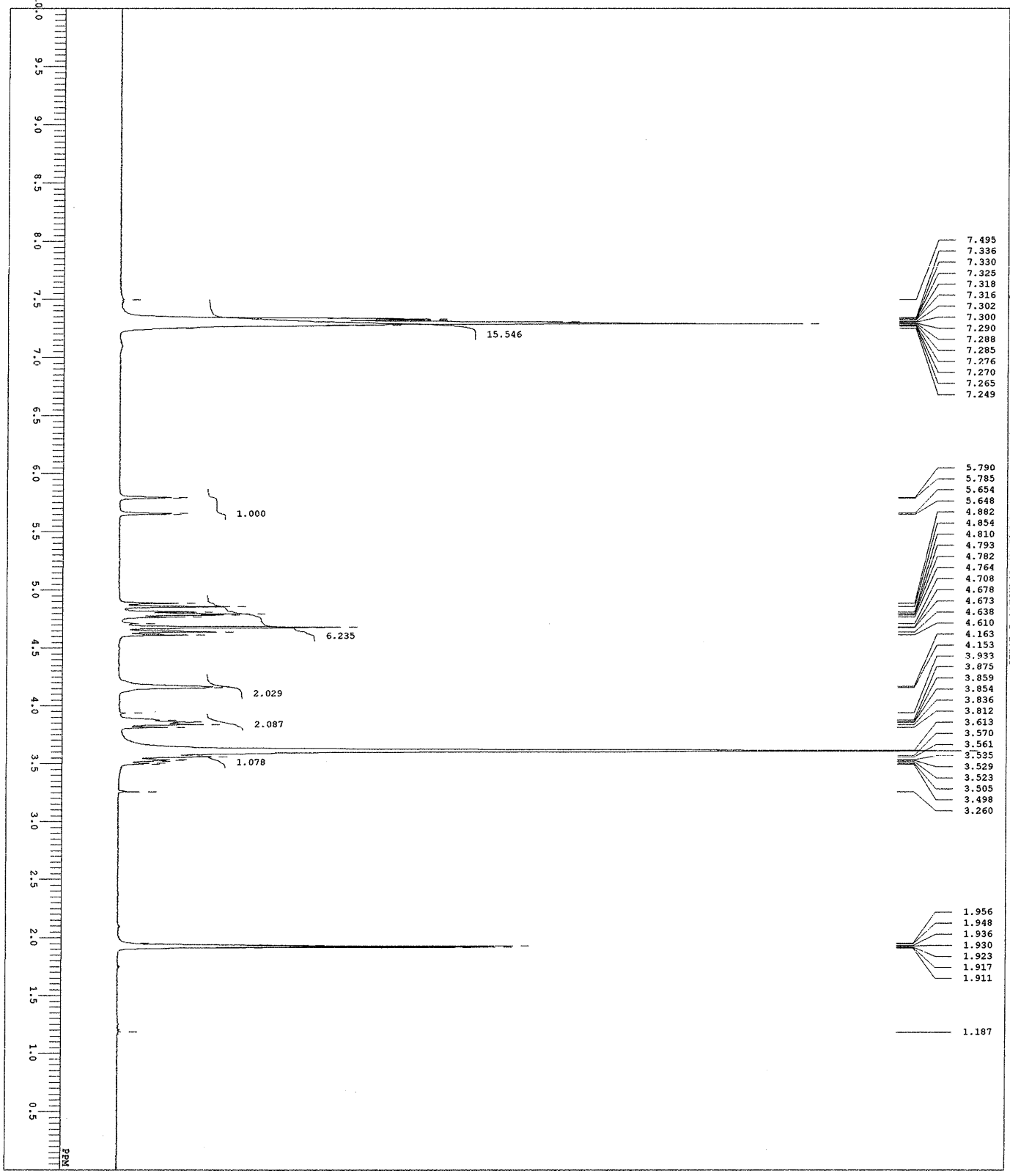
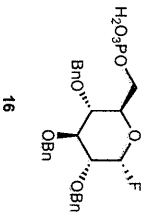
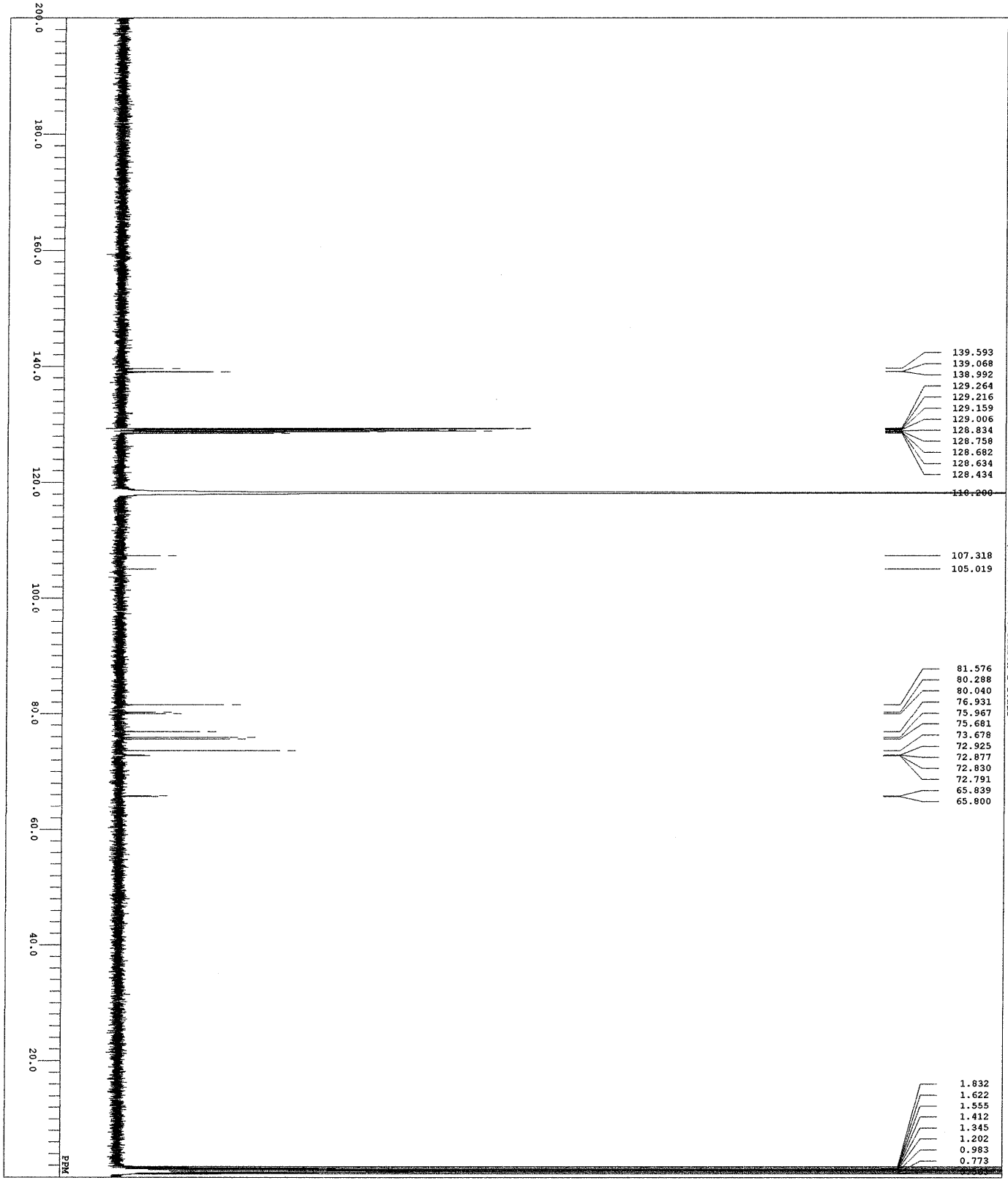


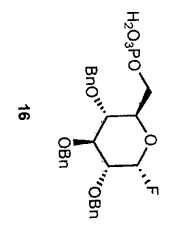
DFILE 18kd3454HPLC6-1-1.als
COMNT
DATIM 13-03-2019 05:24:30
OBNUC 1H
EXMOD proton.jxp
OBFRQ 391.78 MHz
OBSET 8.51 KHz
OBFIN 3.34 Hz
POINT 13107
FREQU 5882.35 Hz
SCANS 8
ACQTM 2.2282 sec
PD 5.0000 sec
PW1 5.22 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CD3CN
EXREF 1.93 ppm
BF 0.12 Hz
RGAIN 38



16



DFILE 18kd3454HPLC6_carbon-1-1.als
COMNT
DATIM 14-03-2019 02:29:20
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 98.52 MHz
OBSET 4.64 KHz
OBFIN 8.74 Hz
POINT 26214
FREQU 24630.54 Hz
SCANS 9522
ACQTM 1.0643 sec
PD 2.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CD3CN
EXREF 118.20 ppm
BF 0.12 Hz
RGAIN 60



16

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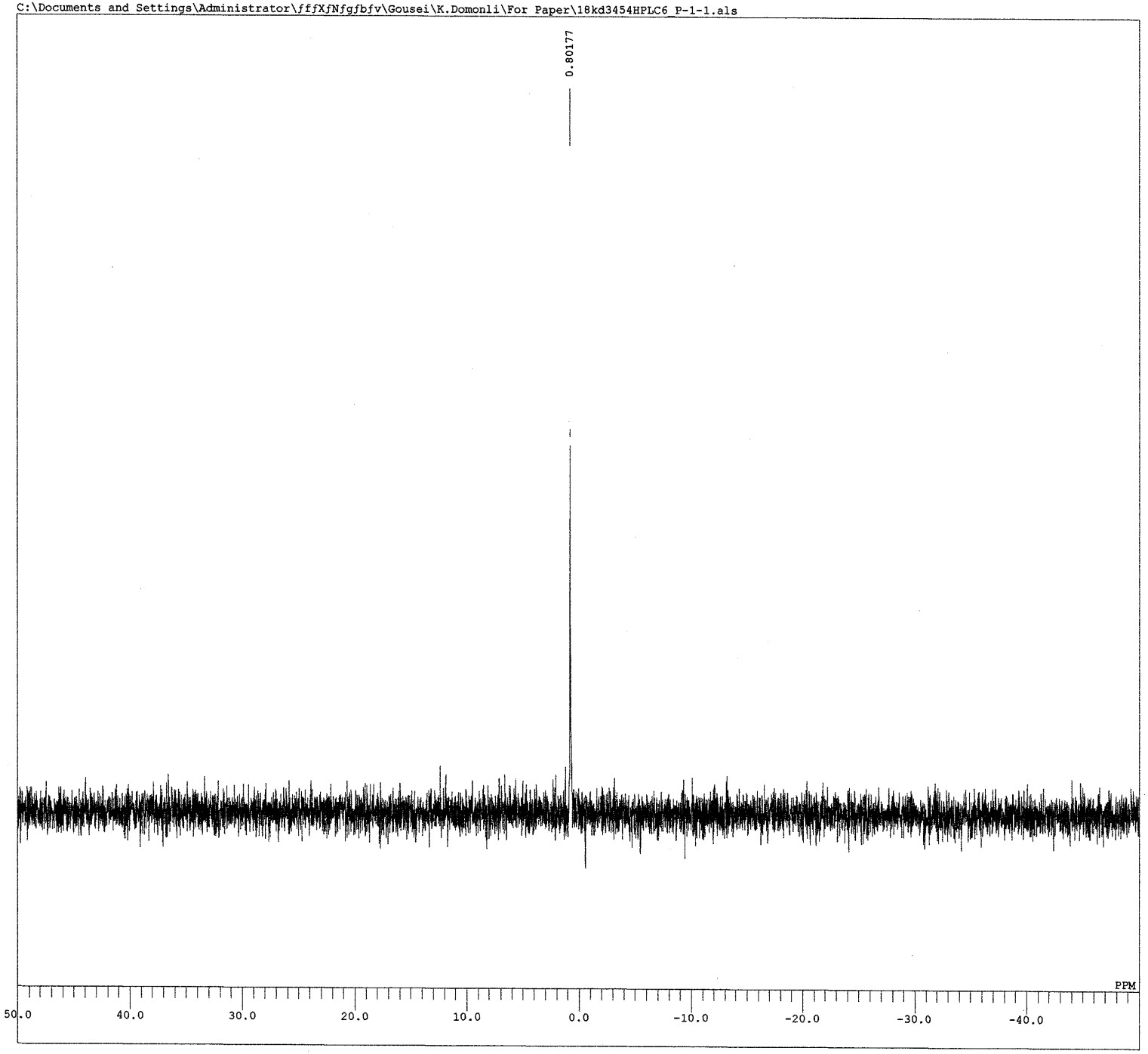
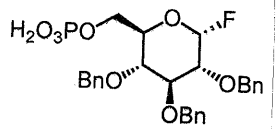
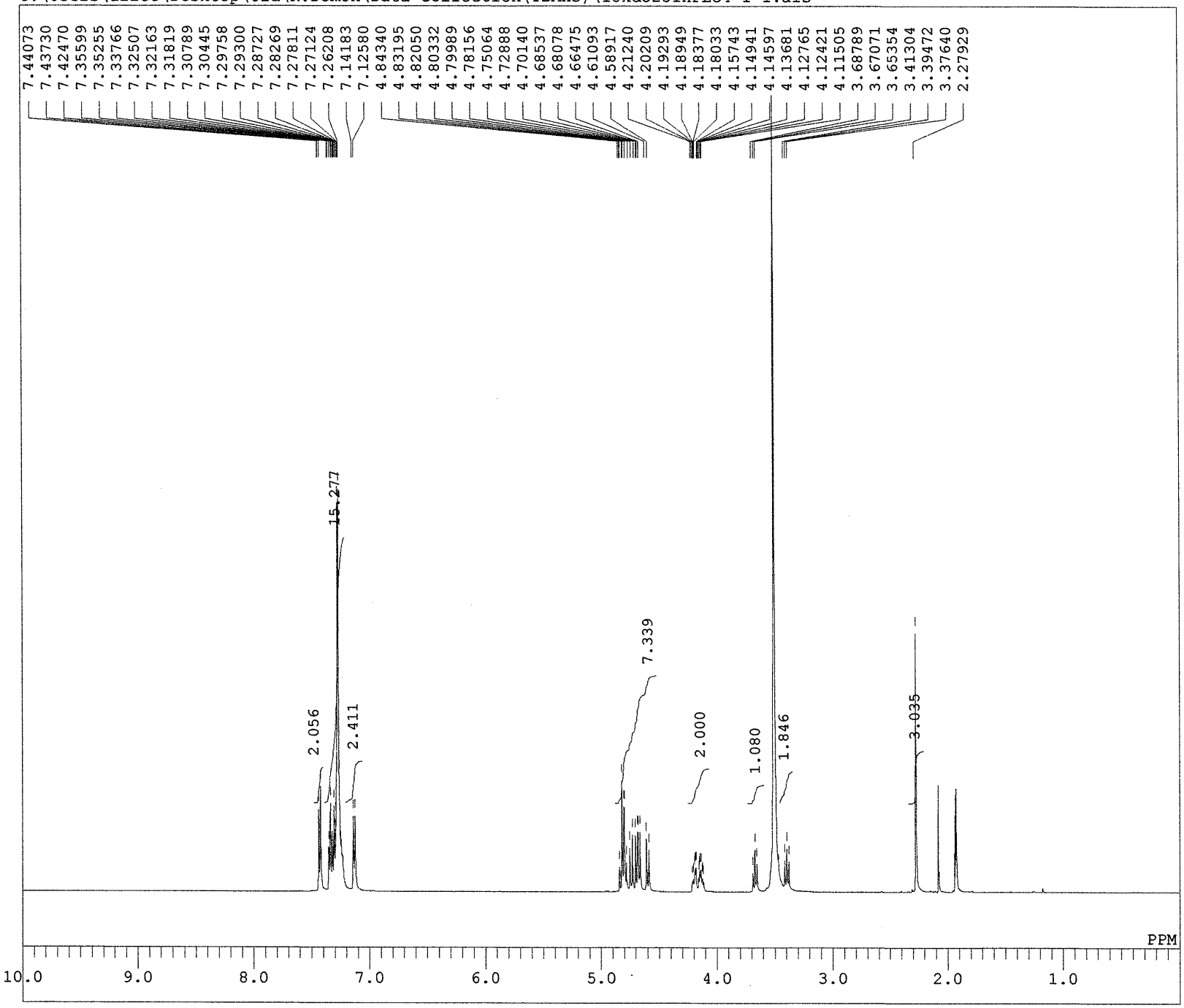



```
DFILE  18kd3454HPLC6_P-1-1.als
COMNT
DATIM  13-03-2019 05:33:12
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            10
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          19.6 c
SLVNT  CD3CN
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

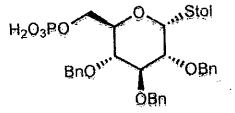


16

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3251HPLC4-1-1.als

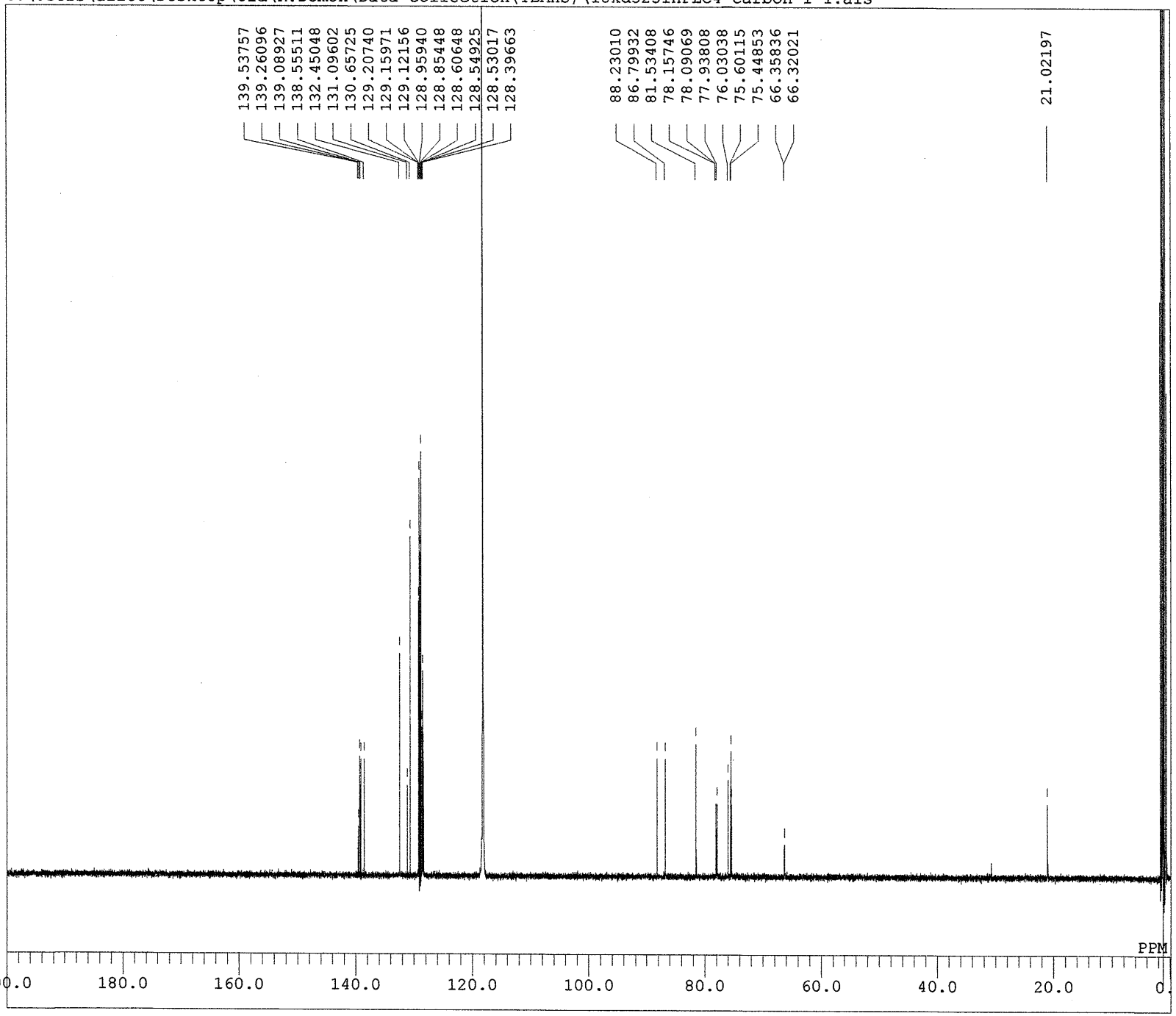


DFILE	18kd3251HPLC4-1-1.als
COMNT	
DATIM	2018-10-25 00:16:04
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CD3CN
EXREF	1.93 ppm
BF	0.12 Hz
RGAIN	30

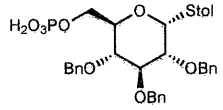


17

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3251HPLC4_carbon-1-1.als




```
DFILE   18kd3251HPLC4_carbon-1-1.als
COMNT
DATIM   2018-10-25 02:28:19
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           7.87 KHz
OBFIN           4.21 Hz
POINT          26214
FREQU       31446.54 Hz
SCANS           2926
ACQTM         0.8336 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           22.2 c
SLVNT   CD3CN
EXREF         118.20 ppm
BF              0.12 Hz
RGAIN             60
```



17

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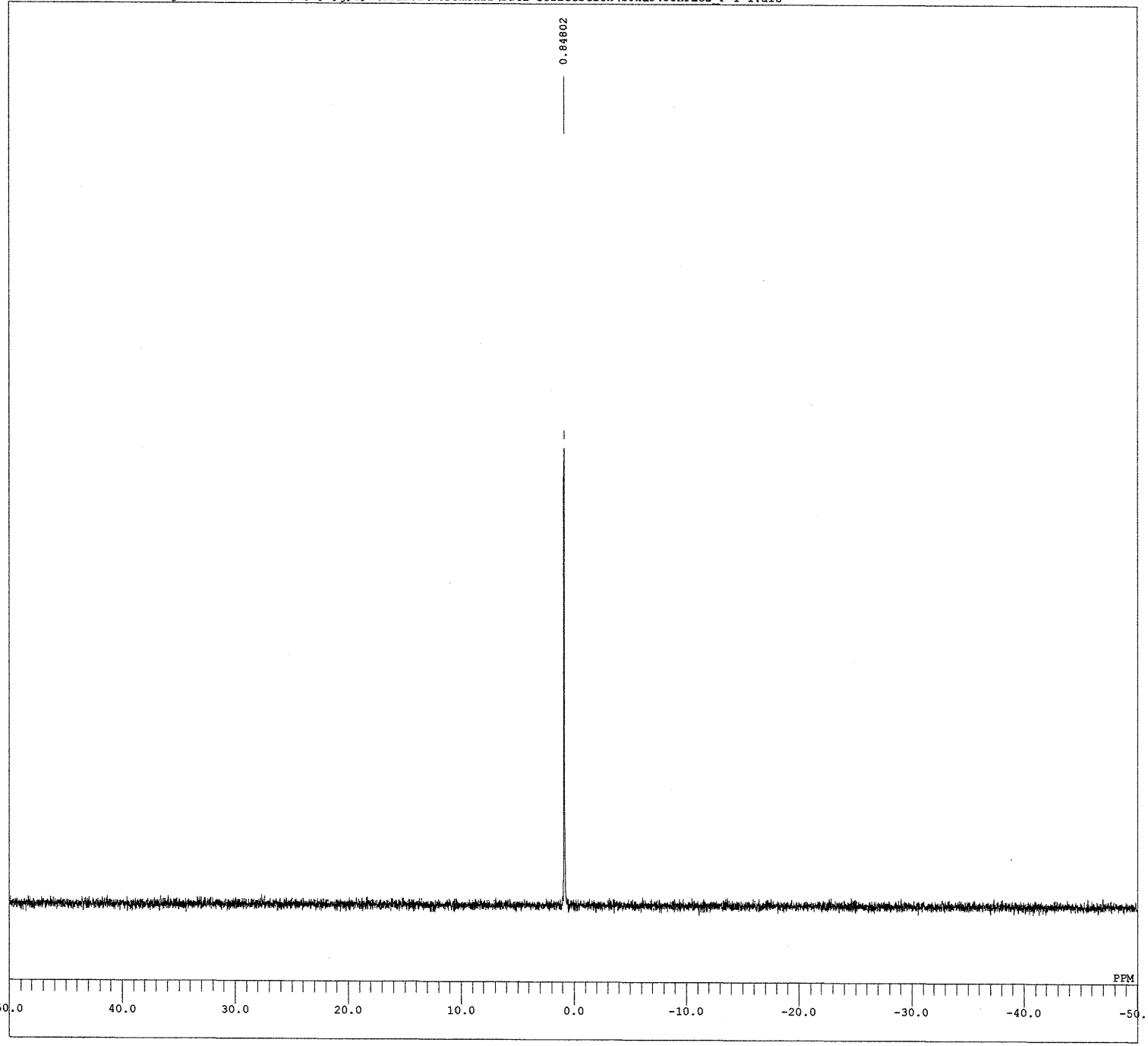
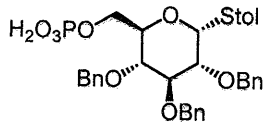
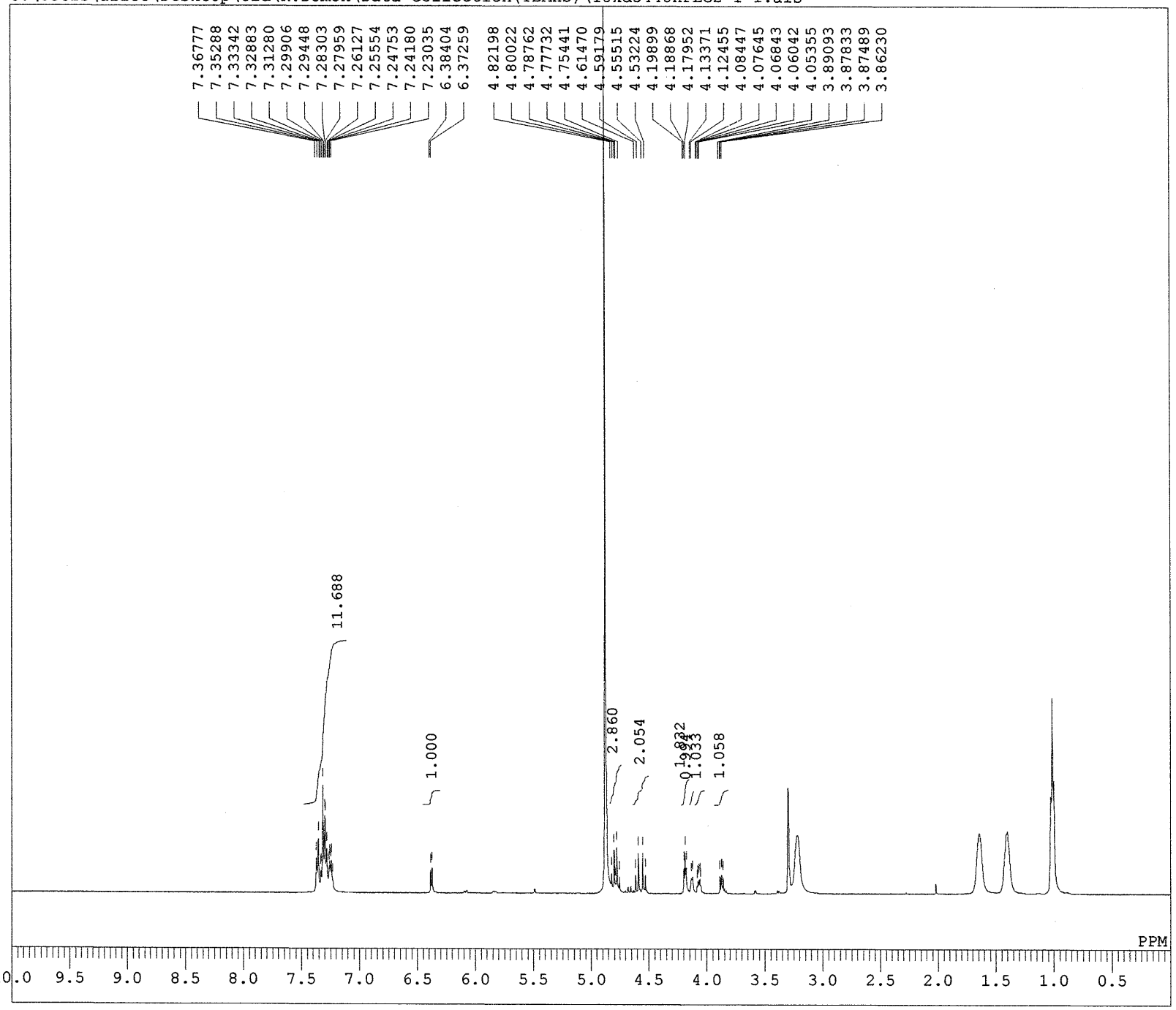



```
DFILE  18kd3455HPLC2_P-1-1.als
COMNT
DATIM  13-03-2019 05:35:34
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            11
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          19.7 c
SLVNT  CD3CN
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

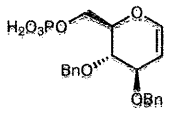


17

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3448HPLC2-1-1.als

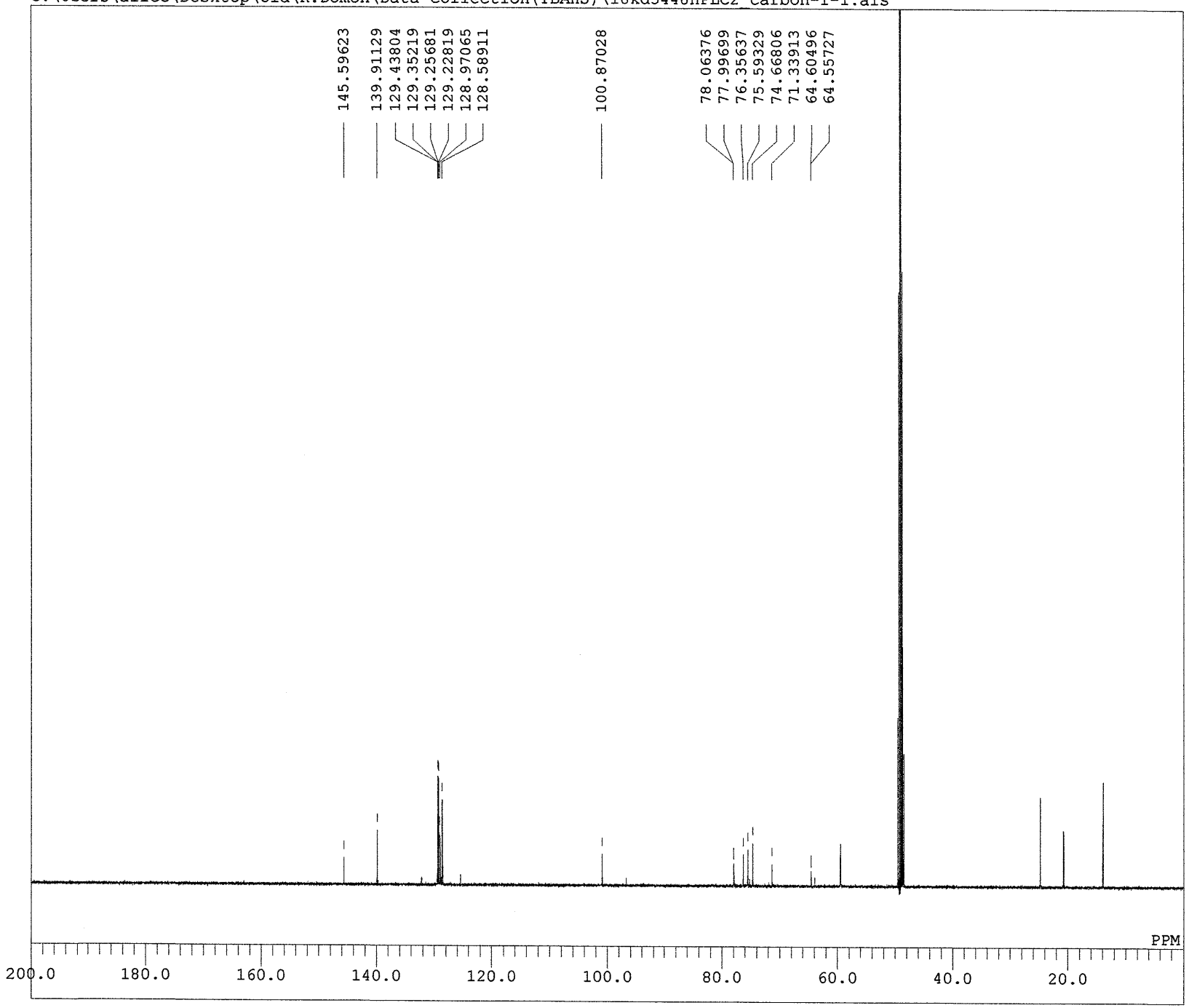


DFILE	18kd3448HPLC2-1-1.als
COMNT	
DATIM	2019-03-04 08:57:50
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	6.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	36

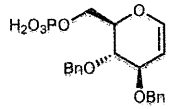


18

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3448HPLC2_carbon-1-1.als

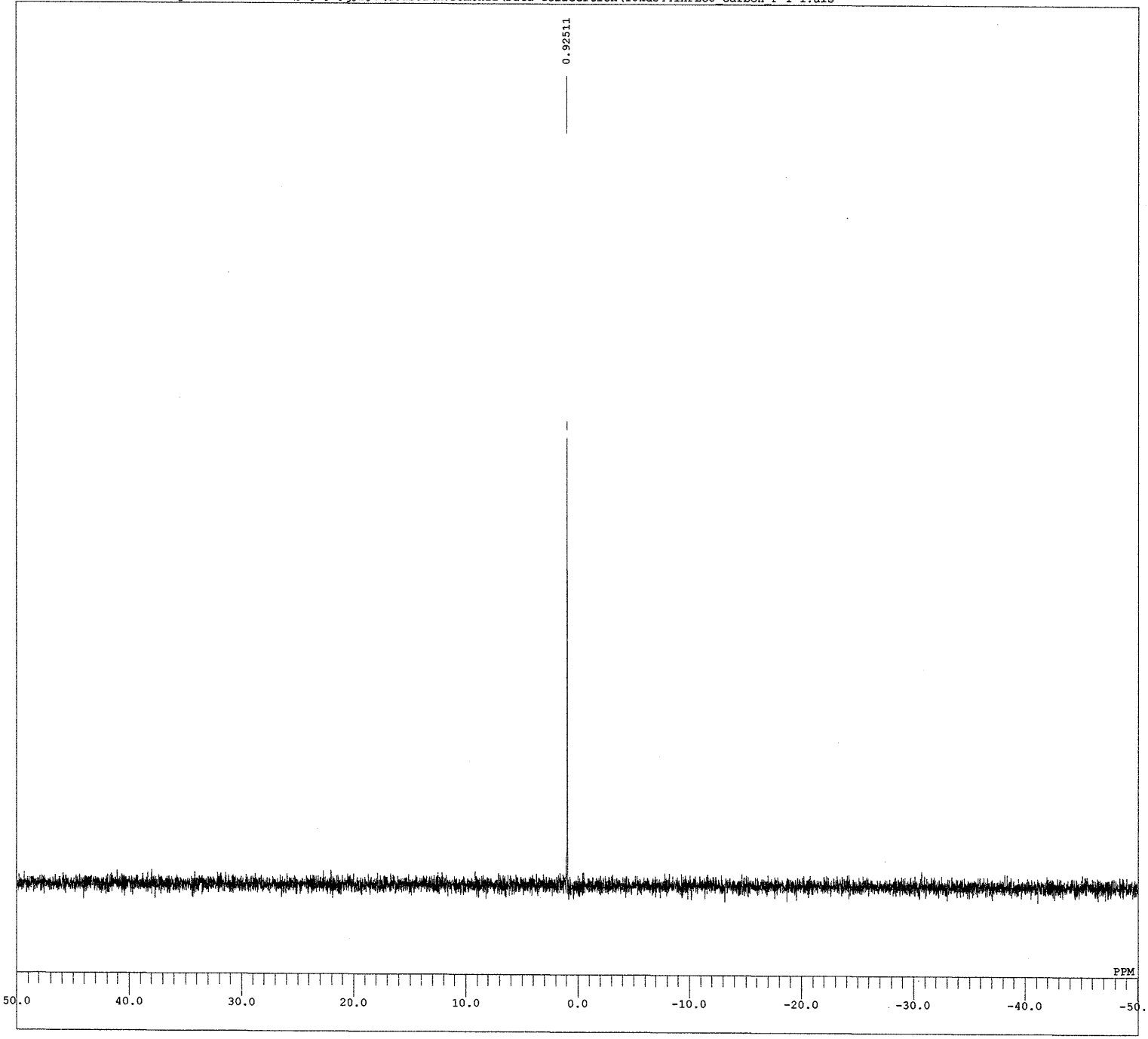



```
DFILE   18kd3448HPLC2_carbon-1-1.als
COMNT
DATIM   2019-03-05 23:17:21
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ         125.77 MHz
OBSET           7.87 KHz
OBFIN           4.21 Hz
POINT          26214
FREQU       31446.54 Hz
SCANS           4843
ACQTM         0.8336 sec
PD            2.0000 sec
PW1             3.40 usec
IRNUC   1H
CTEMP           22.1 c
SLVNT   CD3OD
EXREF           49.00 ppm
BF              0.12 Hz
RGAIN             60
```

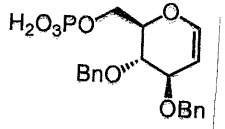


18

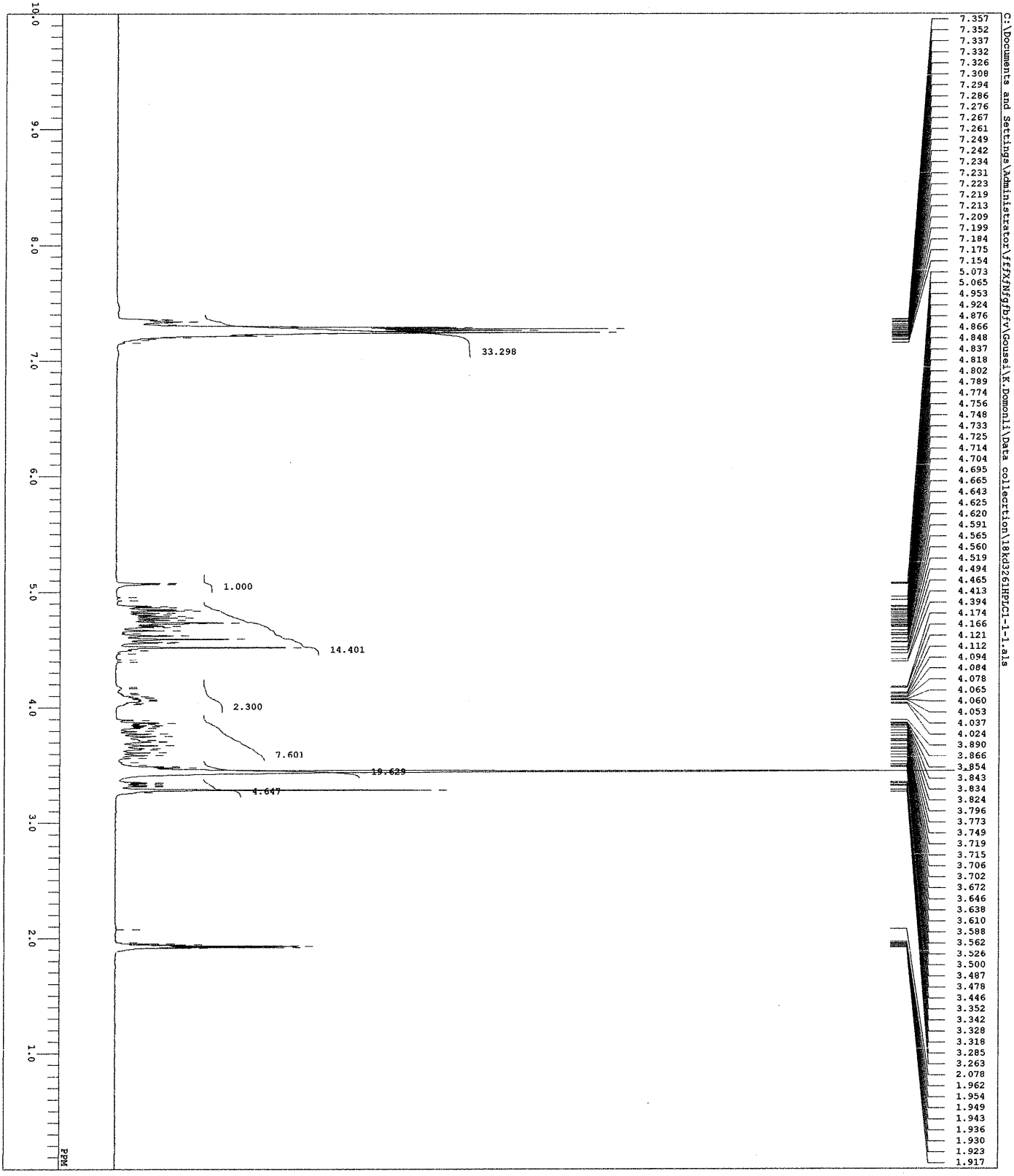
C:\Documents and Settings\Administrator\ffjXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd3441HPLC5_carbon_P-1-1.als




```
DFILE  18kd3441HPLC5_carbon_P-1-1.als
COMNT
DATIM  28-02-2019 16:03:57
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             6
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP         19.9 c
SLVNT  CD3OD
EXREF         0.00 ppm
BF            0.12 Hz
RGAIN           56
```



18


C:\Documents and Settings\Administrator\ffNfNfgfbfv\Gousei\K.Domonli\Data collection\18kd326lHPLC1-1-1.als
7.357
7.352
7.337
7.332
7.326
7.308
7.294
7.286
7.276
7.267
7.261
7.249
7.242
7.234
7.231
7.223
7.219
7.213
7.209
7.199
7.184
7.175
7.154
5.073
5.065
4.953
4.924
4.876
4.866
4.848
4.837
4.818
4.802
4.789
4.774
4.756
4.748
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4.725
4.714
4.704
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4.519
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4.166
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4.112
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4.084
4.078
4.065
4.060
4.053
4.037
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1.923
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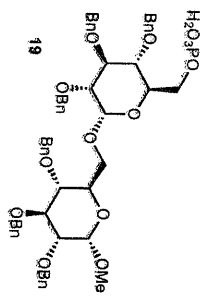
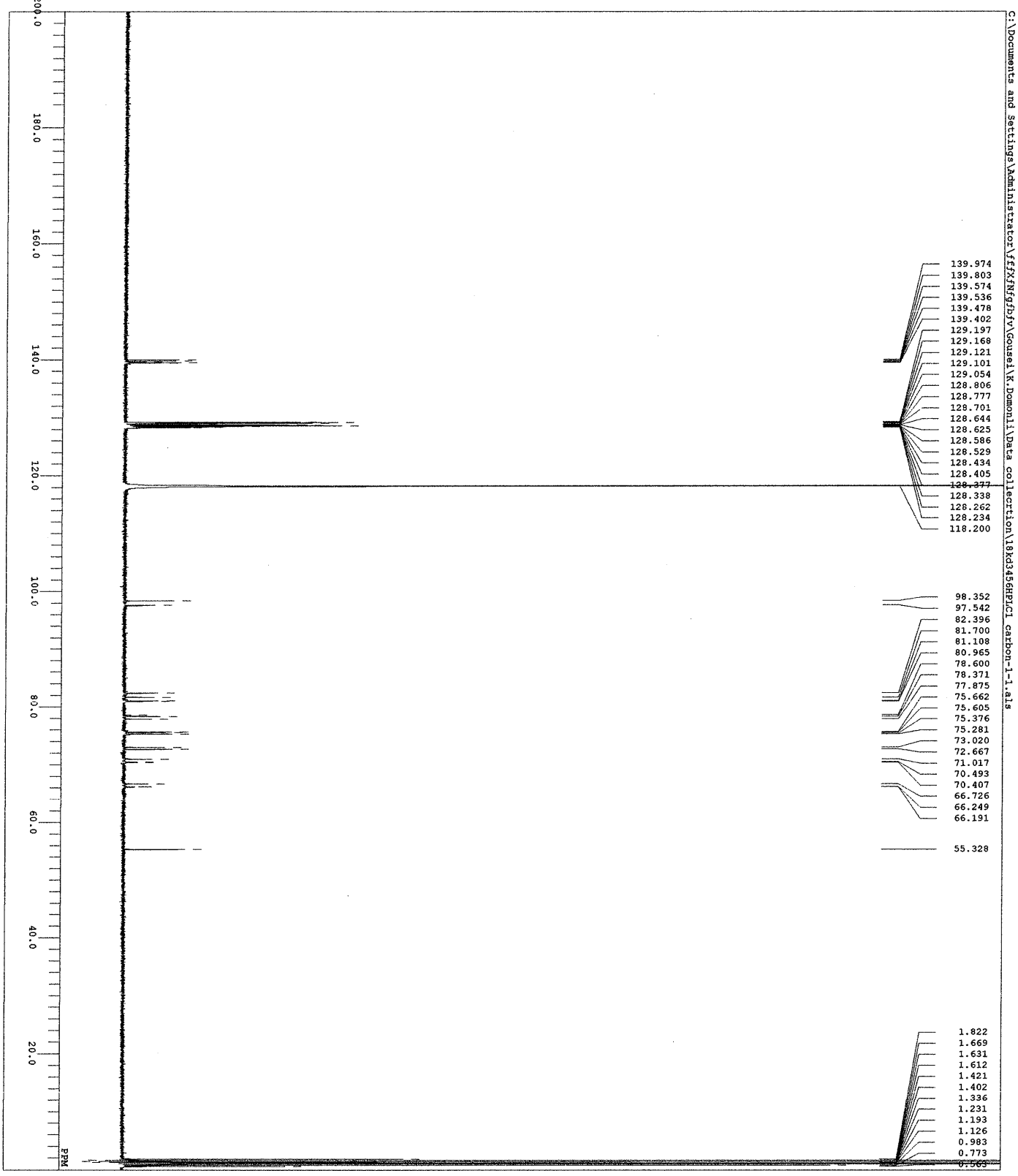
1.000
14.401
2.300
7.601
19.629
4.647
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
PPM
DFILE 18kd326lHPLC1-1-1.als
COMNT
DATIM 26-Jo-2018 06:41:41
OBNUC 1H
EXMOD proton.jxp
OBFRQ 391.78 MHz
OBSET 8.51 KHz
OBFIN 3.34 Hz
POINT 13107
FREQU 5882.35 Hz
SCANS 6
ACQTM 2.2282 sec
PD 5.0000 sec
PW1 5.22 usec
IRNUC 1H
CTEMP 19.8 c
SLVNT CD3CN
EXREF 1.93 ppm
BF 0.12 Hz
RGAIN 32


19
BnO
BnO
H2O3PO
OBn
BnO
OBn
OBn
OMe


C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd3456HPJC1_carbon-1-1.als
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129.168
129.121
129.101
129.054
128.806
128.777
128.701
128.644
128.625
128.586
128.529
128.434
128.405
128.377
128.338
128.262
128.234
118.200
98.352
97.542
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81.700
81.108
80.965
78.600
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77.875
75.662
75.605
75.376
75.281
73.020
72.667
71.017
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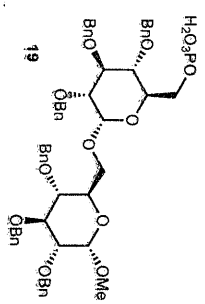
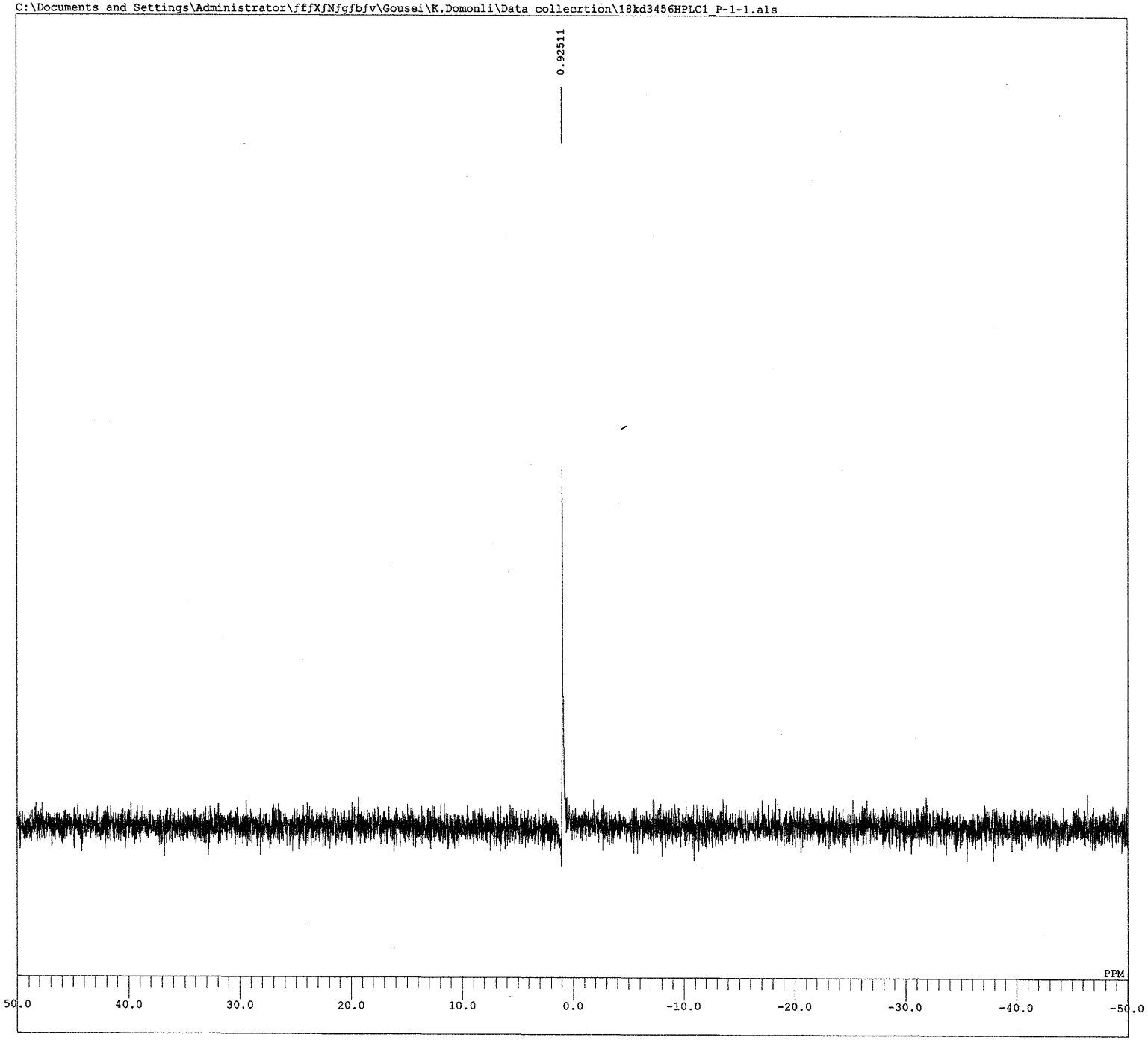
70.407
66.726
66.249
66.191
55.328
1.822
1.669
1.631
1.612
1.421
1.402
1.336
1.231
1.193
1.126
0.983
0.773
0.563
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
PPM
DFILE 18kd3456HPJC1_carbon-1-1.als
COMNT
DATIM 13-03-2019 06:23:57
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 98.52 MHz
OBSET 4.64 KHz
OBFIN 8.74 Hz
POINT 26214
FREQU 24630.54 Hz
SCANS 4575
ACQTM 1.0643 sec
PD 2.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CD3CN
EXREF 118.20 ppm
BF 0.12 Hz
RGAIN 60

19


BnO
BnO
H2O3PO
OBn
O
BnO
O
OBn
OBn
OMe

C:\Documents and Settings\Administrator\ffƒXƒNƒgƒbƒv\Gousei\K.Domonli\Data collecrtion\18kd3456HPLC1_P-1-1.als

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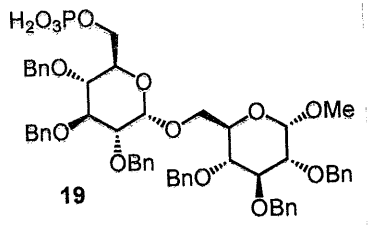
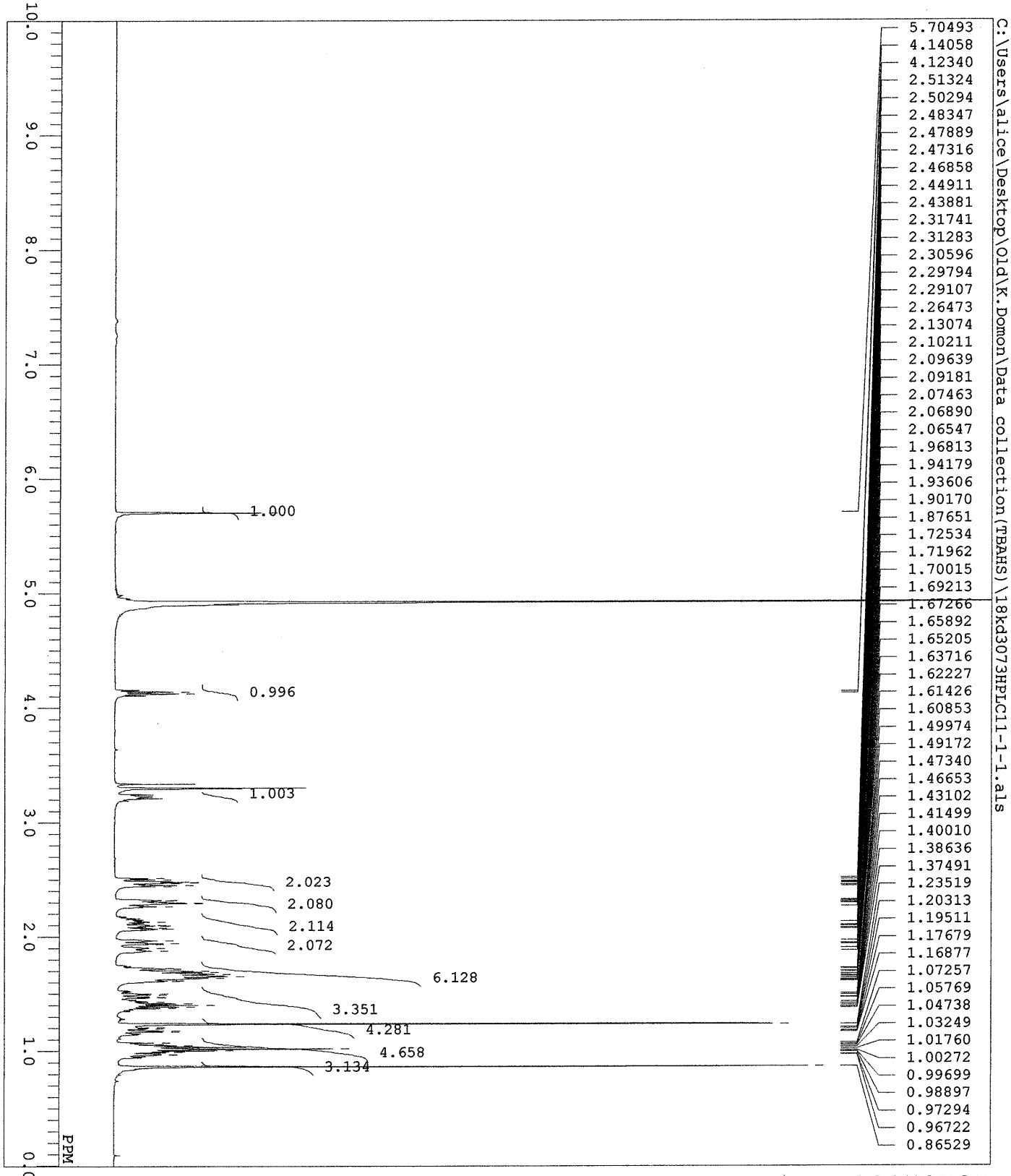
DFILE  18kd3456HPLC1_P-1-1.als
COMNT
DATIM  13-03-2019 05:38:02
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             7
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          19.8 c
SLVNT  CD3CN
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



19


C:\Users\alice\Desktop\old\K.Domon\Data collection(TBAHS)\18kd3073HPLC11-1-1.als
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2.46858
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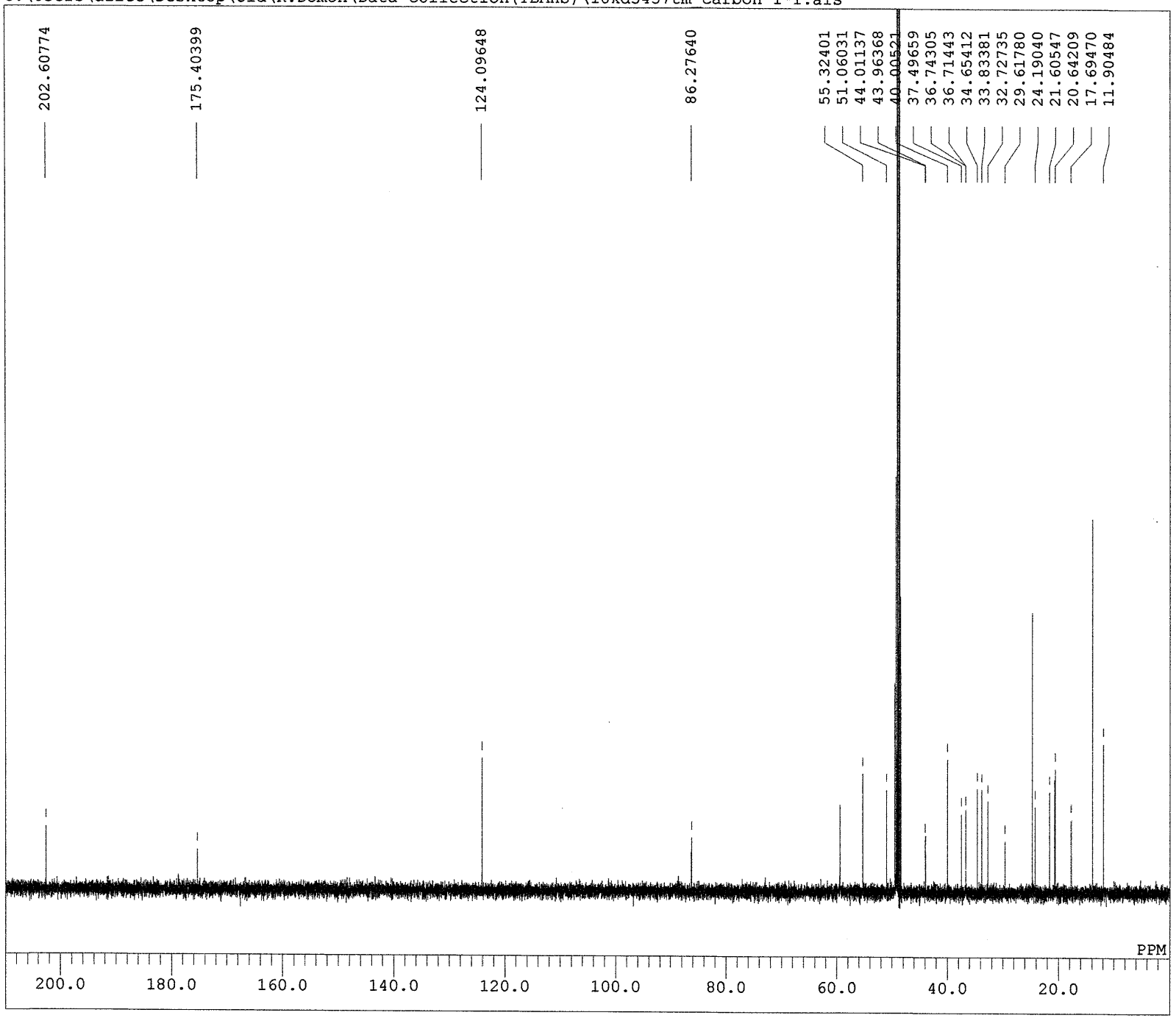
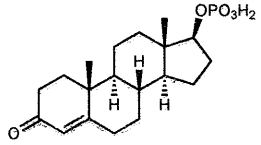
2.43881
2.31741
2.31283
2.30596
2.29794
2.29107
2.26473
2.13074
2.10211
2.09639
2.09181
2.07463
2.06890
2.06547
1.96813
1.94179
1.93606
1.90170
1.87651
1.72534
1.71962
1.70015
1.69213
1.67266
1.65892
1.65205
1.63716
1.62227
1.61426
1.60853
1.49974
1.49172
1.47340
1.46653
1.43102
1.41499
1.40010
1.38636
1.37491
1.23519
1.20313
1.19511
1.17679
1.16877
1.07257
1.05769
1.04738
1.03249
1.01760
1.00272
0.99699
0.98897
0.97294
0.96722
0.86529
1.000
0.996
1.003
2.023
2.080
2.114
2.072
6.128
3.351
4.281
4.658
3.134
PPM
DFILE 18kd3073HPLC11-1-1.als
COMNT
DATIM 2018-09-01 02:34:14
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 28
20
OPO3H2

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3437tm_carbon-1-1.als

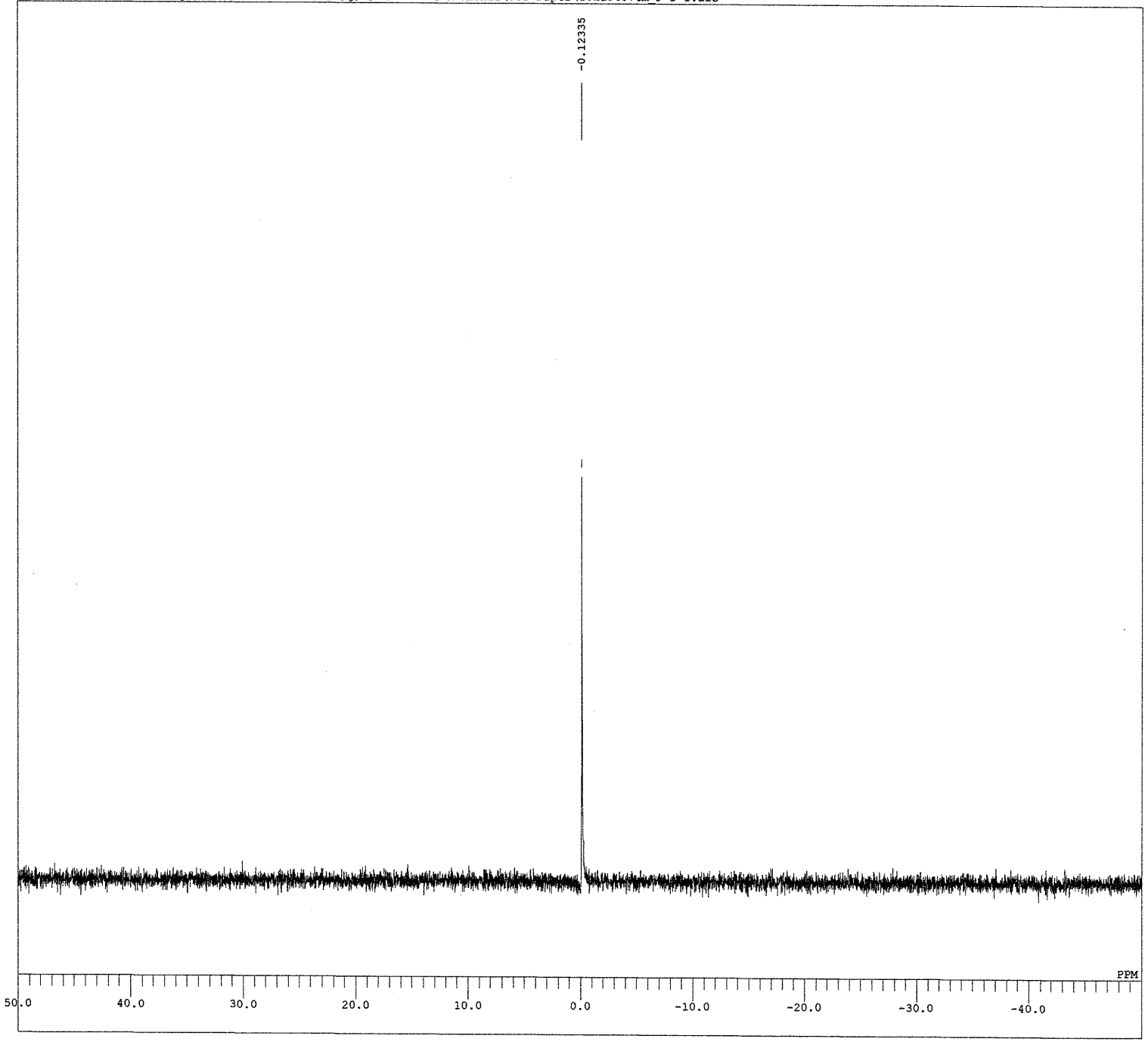


DFILE	18kd3437tm_carbon-1-1.als
COMNT	
DATIM	2019-03-20 00:49:18
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	355
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	21.9 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

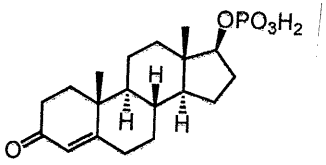


20

C:\Documents and Settings\Administrator\ffffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3437tm_P-1-1.als

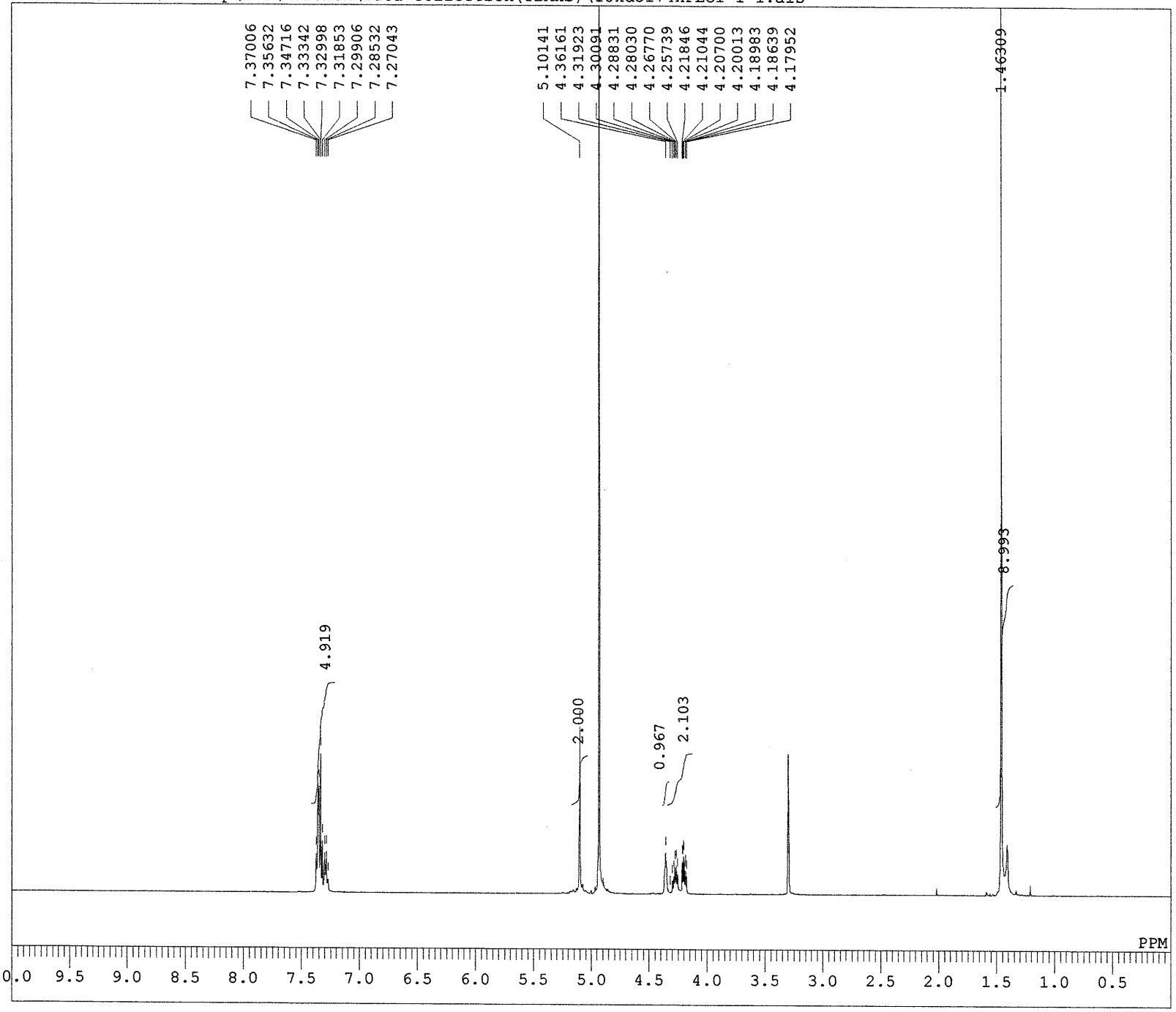



```
DFILE   18kd3437tm_P-1-1.als
COMNT
DATIM   07-03-2019 05:18:19
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS              5
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC   1H
CTEMP          19.9 c
SLVNT   CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



20

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3174HPLC1-1-1.als

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DFILE   18kd3174HPLC1-1-1.als
COMNT
DATIM   2018-10-01 02:22:51
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         500.16 MHz
OBSET           2.41 KHz
OBFIN           6.01 Hz
POINT          13107
FREQU        7507.51 Hz
SCANS                4
ACQTM          1.7459 sec
PD             5.0000 sec
PW1              5.55 usec
IRNUC   1H
CTEMP           21.8 c
SLVNT   CD3OD
EXREF           3.30 ppm
BF              0.12 Hz
RGAIN             30
```
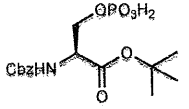
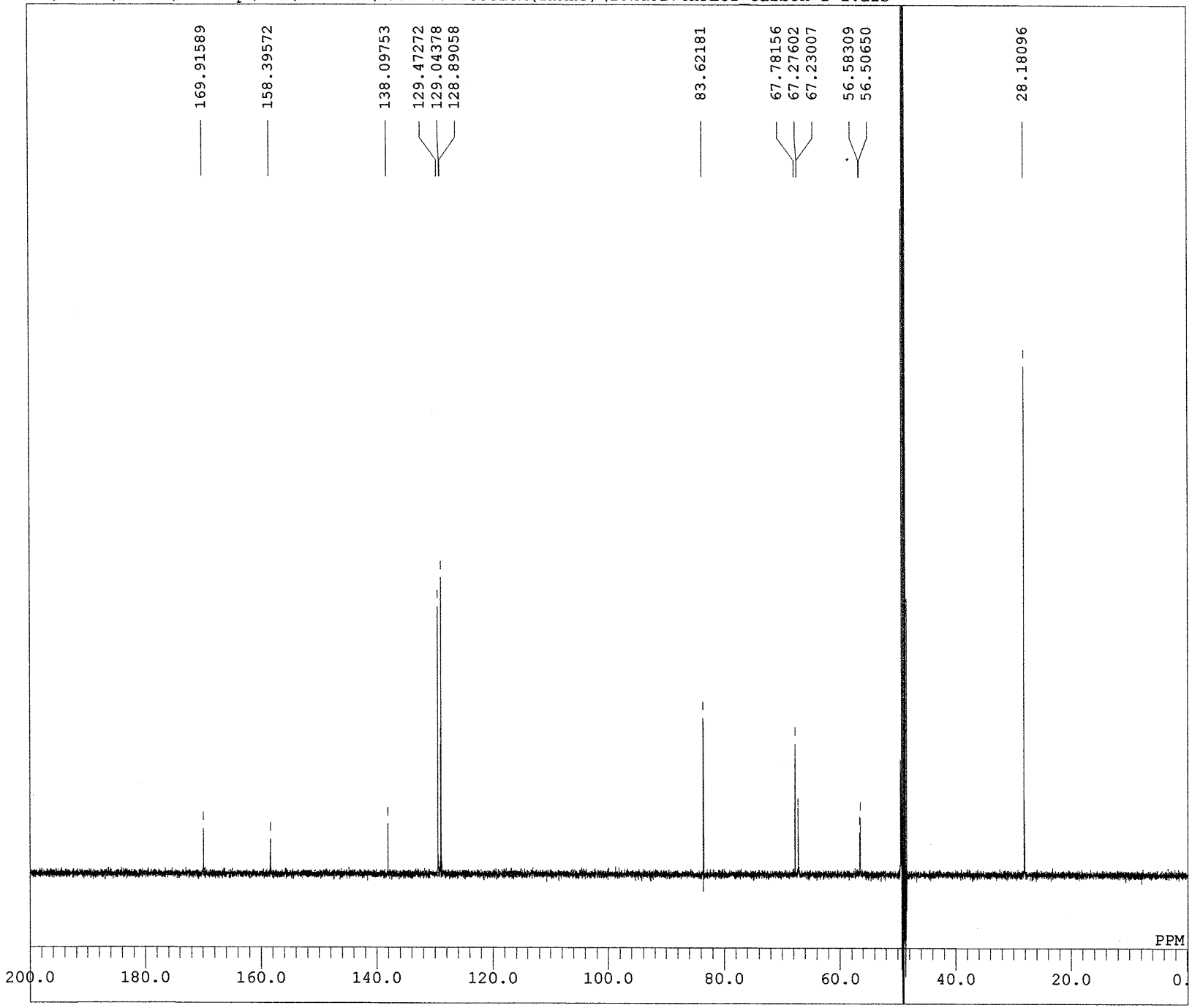
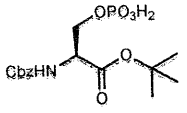



21

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3174HPLC1_carbon-1-1.als

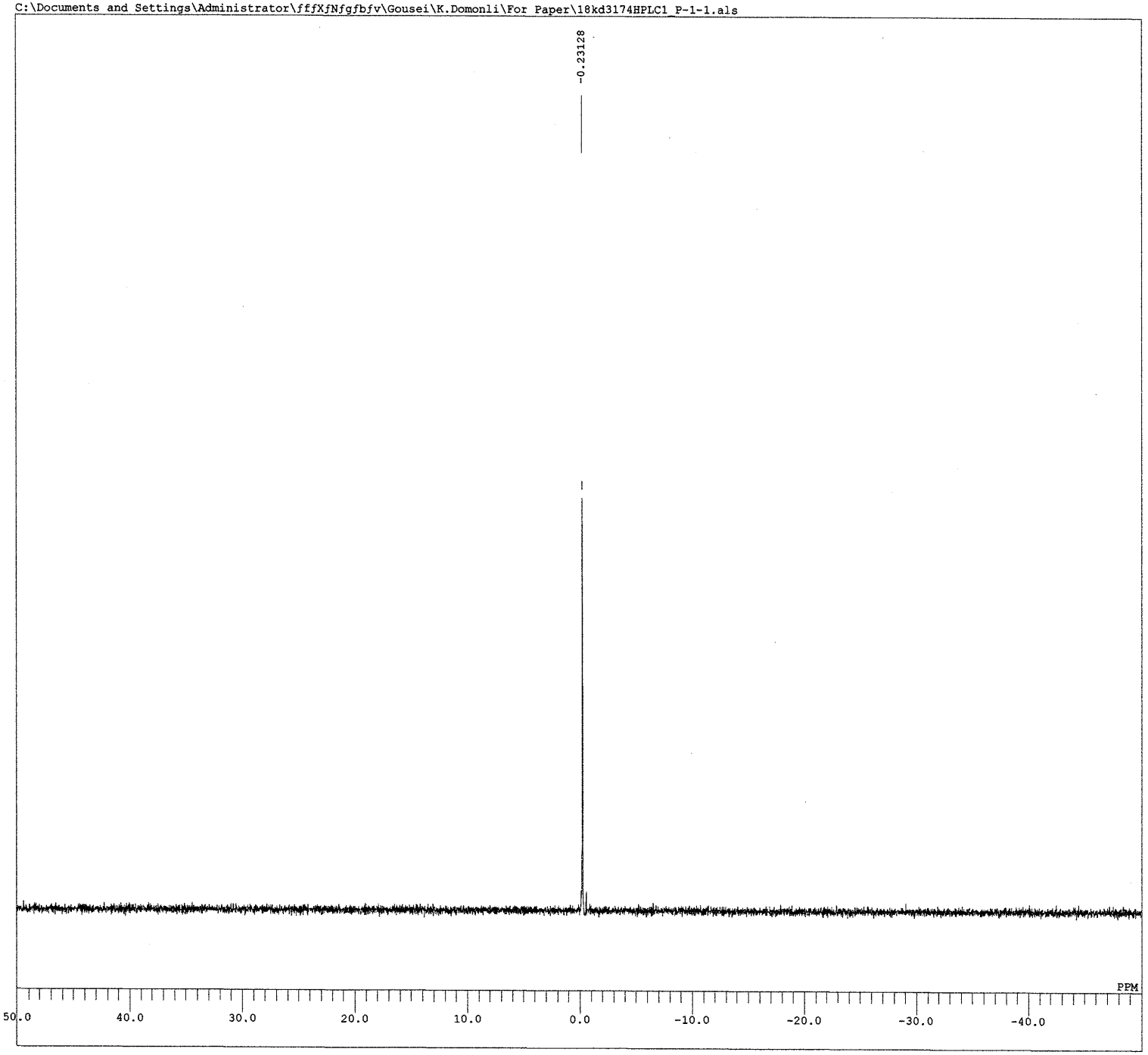


DFILE	18kd3174HPLC1_carbon-1-1.als
COMNT	
DATIM	2018-10-01 02:23:59
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	2248
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.3 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

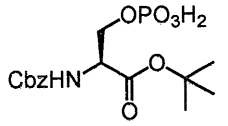


21

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3174HPLC1_P-1-1.als

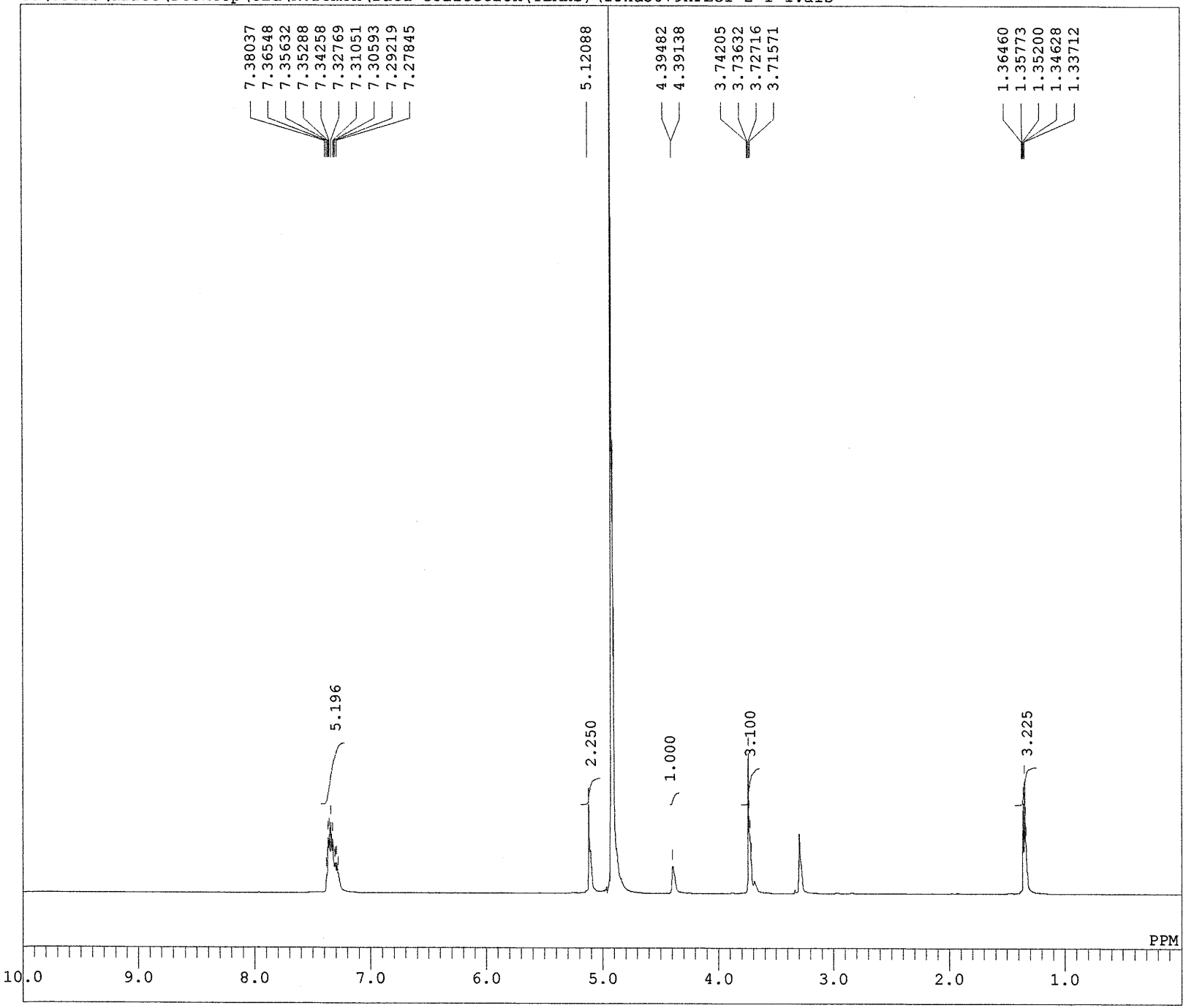


DFILE	18kd3174HPLC1_P-1-1.als
COMNT	
DATIM	01-10-2018 04:38:41
OBNUC	31P
EXMOD	carbon.jxp
OBFRQ	158.59 MHz
OBSET	7.99 KHz
OBFIN	9.23 Hz
POINT	26214
FREQU	64102.56 Hz
SCANS	10
ACQTM	0.4089 sec
PD	2.0000 sec
PW1	4.80 usec
IRNUC	1H
CTEMP	20.2 c
SLVNT	CD3OD
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	56

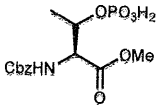


21

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3079HPLC1-2-1-1.als

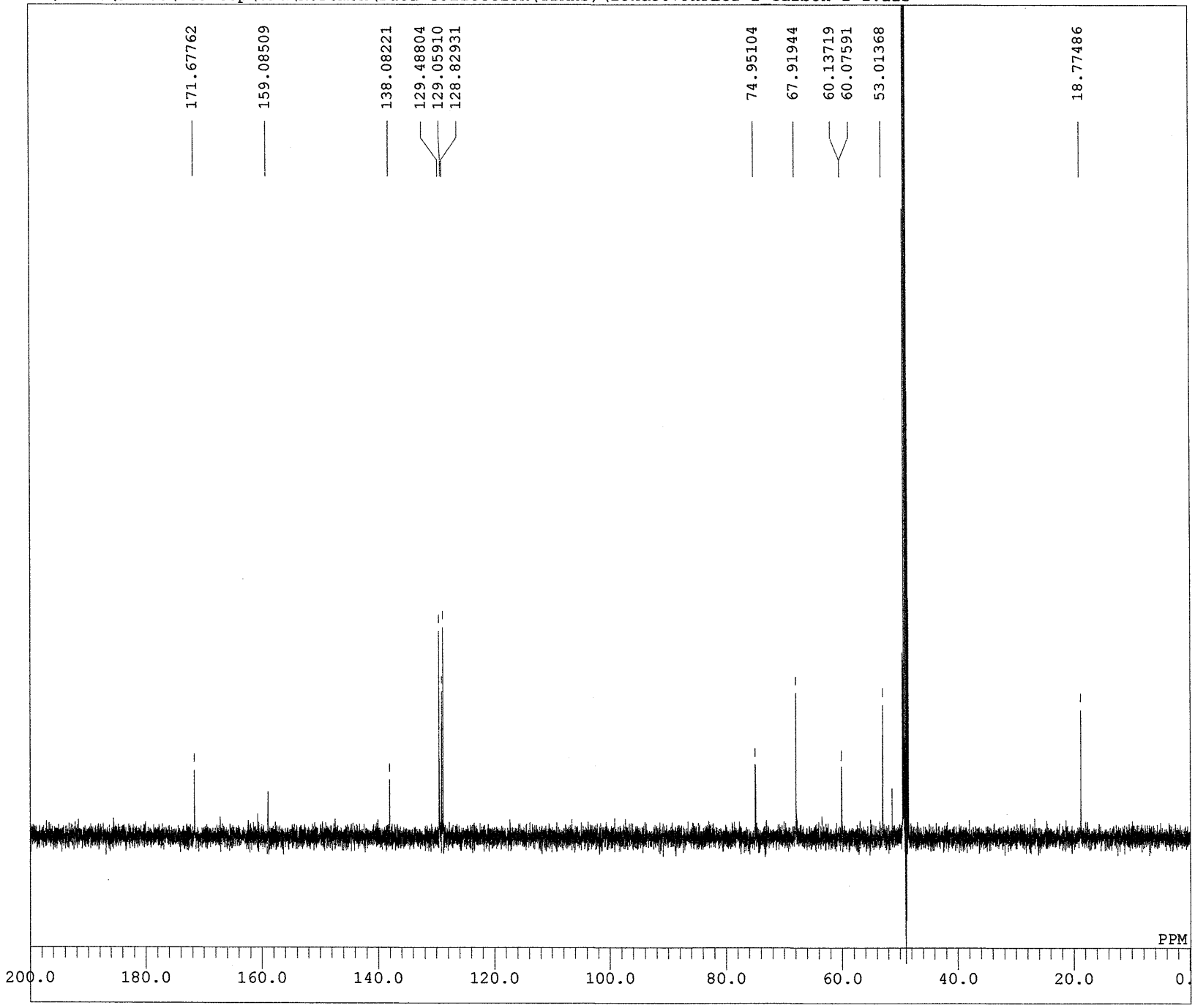


DFILE	18kd3079HPLC1-2-1-1.als
COMNT	
DATIM	2018-09-01 03:17:05
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.4 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

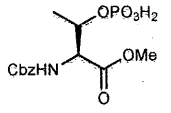


22

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3079HPLC1-2_carbon-1-1.als

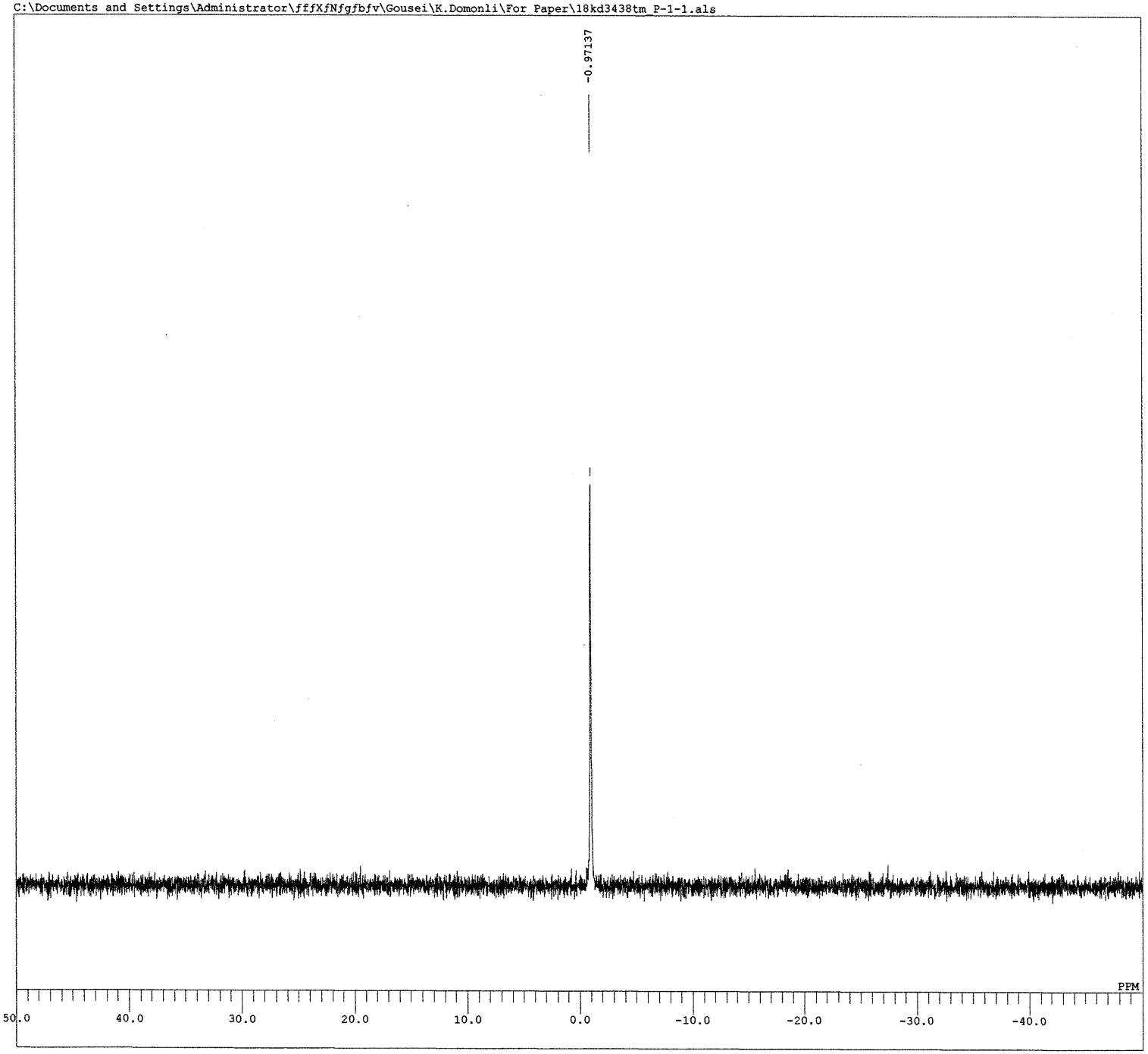


DFILE	18kd3079HPLC1-2_carbon-1-1.als
COMNT	
DATIM	2018-09-01 03:22:33
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	761
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	21.9 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

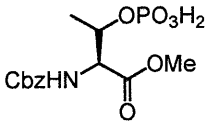


22

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3438tm_P-1-1.als

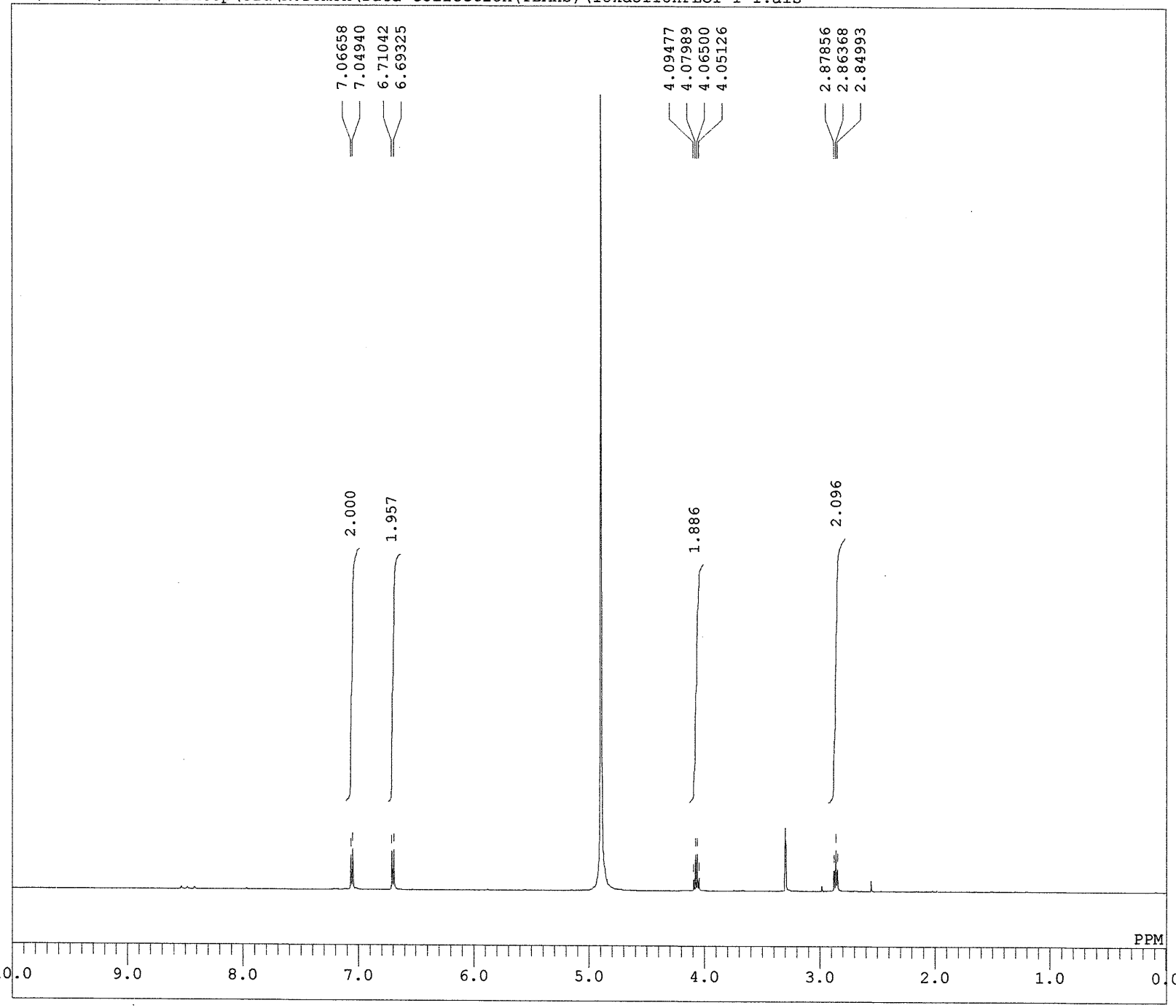



```
DFILE  18kd3438tm_P-1-1.als
COMNT
DATIM  07-03-2019 05:20:26
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            13
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP         19.9 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

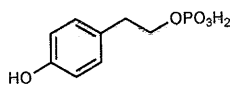


22

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3118HPLC1-1-1.als

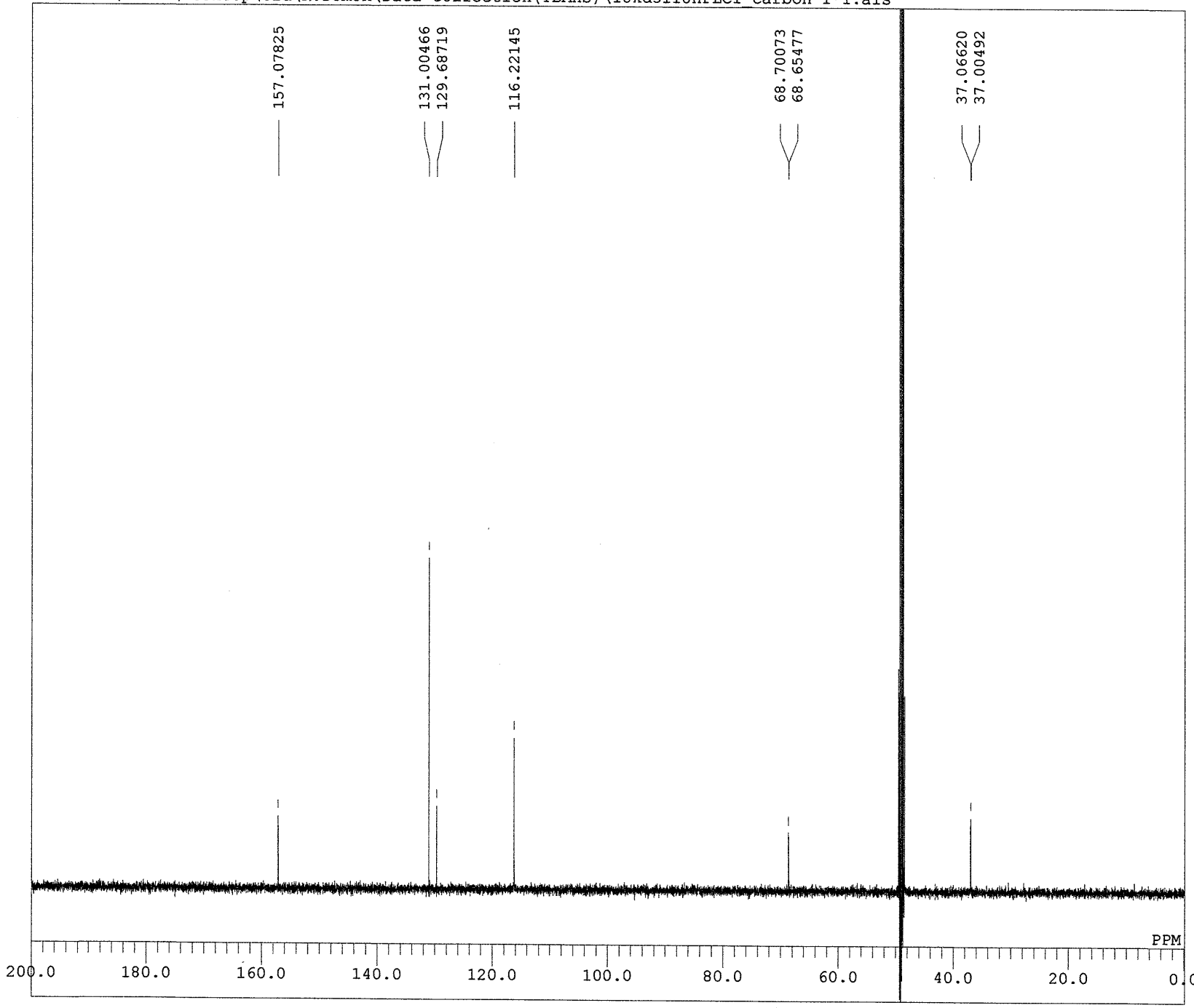



```
DFILE   18kd3118HPLC1-1-1.als
COMNT
DATIM   2018-09-20 01:22:19
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         500.16 MHz
OBSET           2.41 KHz
OBFIN           6.01 Hz
POINT          13107
FREQU        7507.51 Hz
SCANS               7
ACQTM         1.7459 sec
PD            5.0000 sec
PW1             5.55 usec
IRNUC   1H
CTEMP           21.5 c
SLVNT   CD3OD
EXREF           3.30 ppm
BF              0.12 Hz
RGAIN             30
```

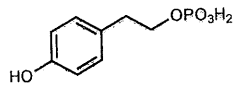


25

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3118HPLC1_carbon-1-1.als



DFILE	18kd3118HPLC1_carbon-1-1.als
COMNT	
DATIM	2018-09-20 02:53:15
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	1.58 KHz
OBFIN	5.95 Hz
POINT	26214
FREQU	50505.05 Hz
SCANS	1952
ACQTM	0.5190 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.2 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60



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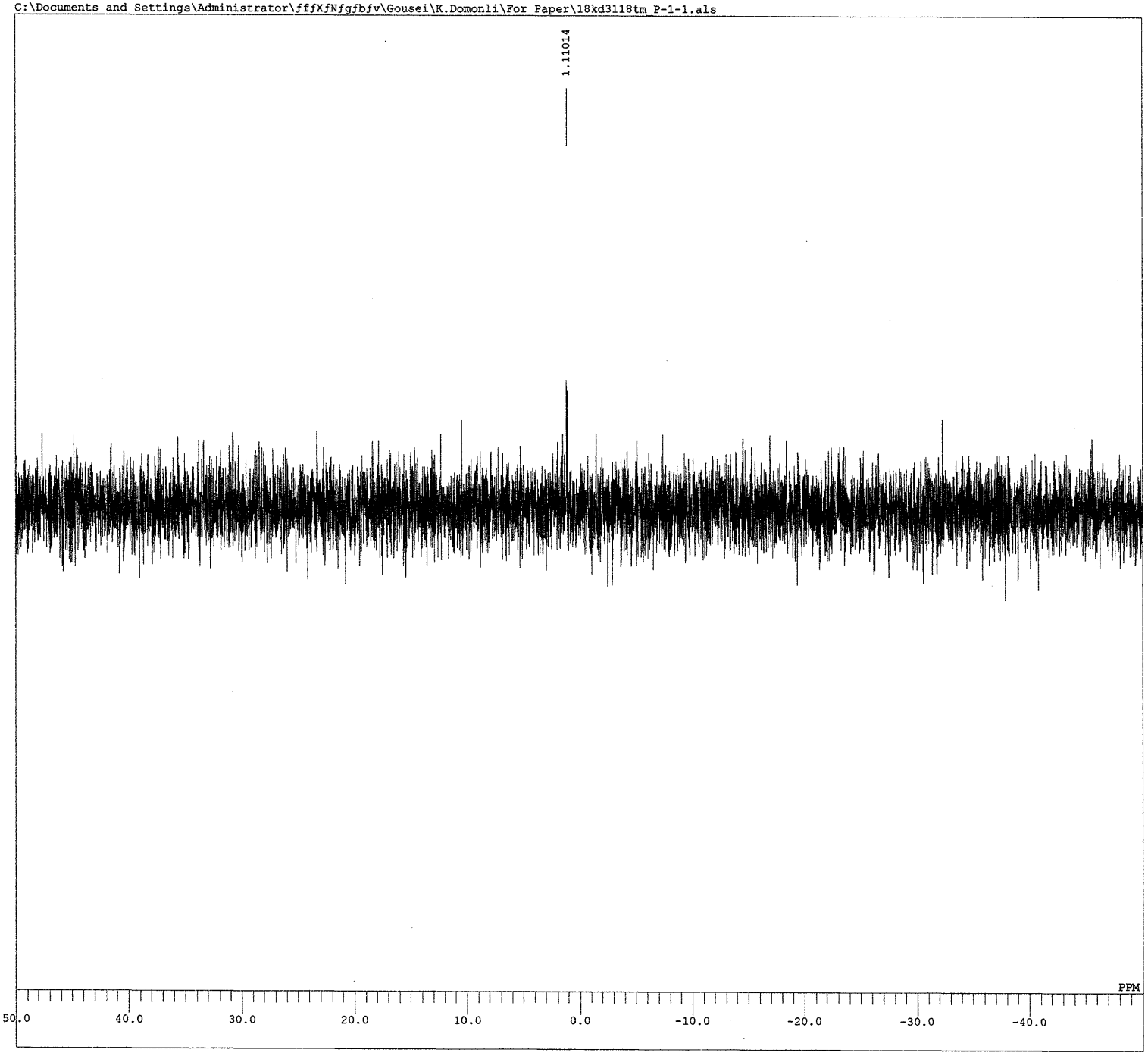
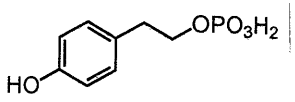
C:\Documents and Settings\Administrator\ffffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3118tm_P-1-1.als

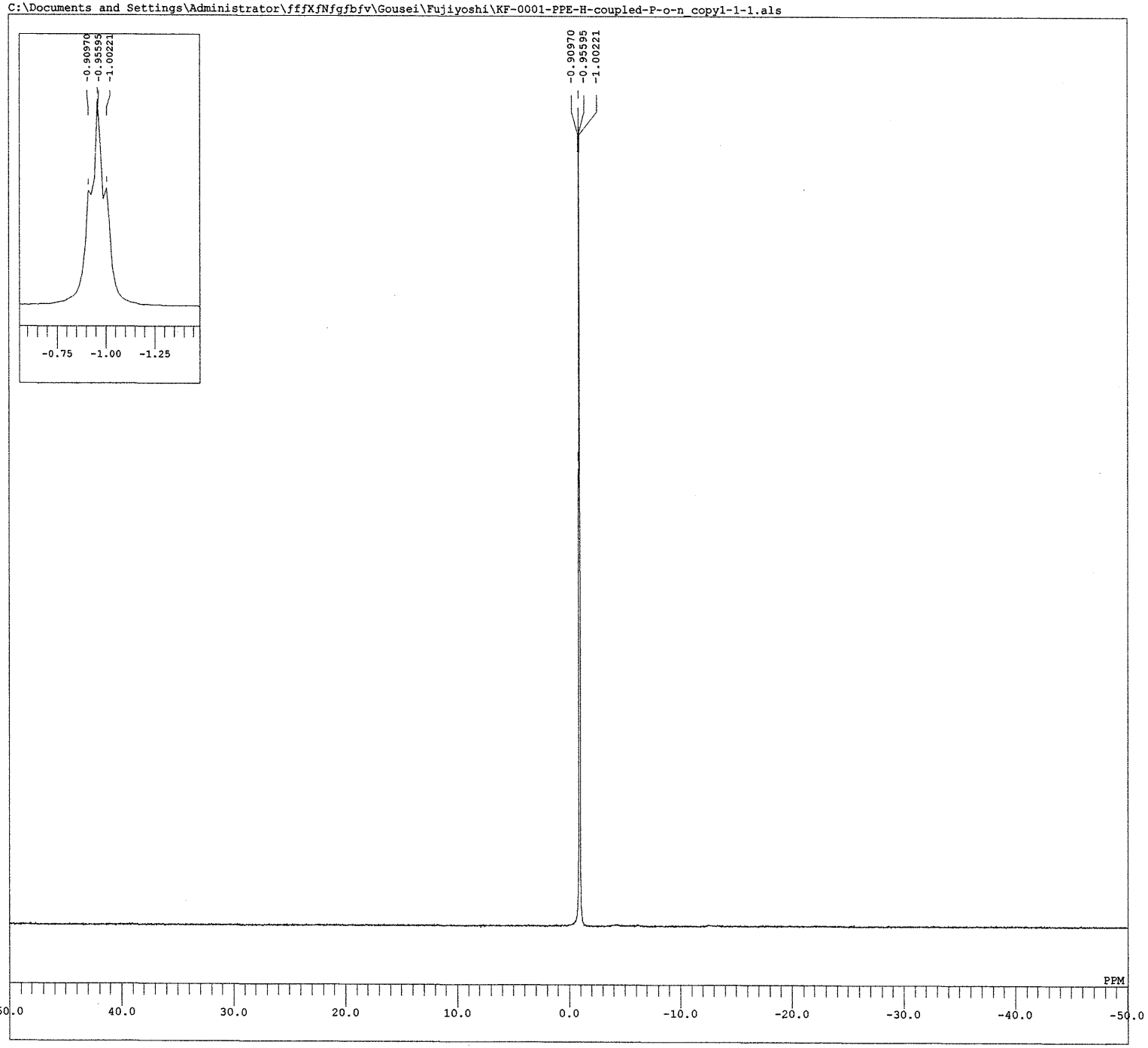



```
DFILE  18kd3118tm_P-1-1.als
COMNT
DATIM  07-03-2019 05:05:07
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            28
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.0 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```

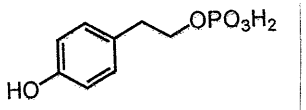


25

C:\Documents and Settings\Administrator\ƒfƒXƒNƒgƒbƒv\Gousei\Fujiyoshi\KF-0001-PPE-H-coupled-P-o-n_copy1-1-1.als

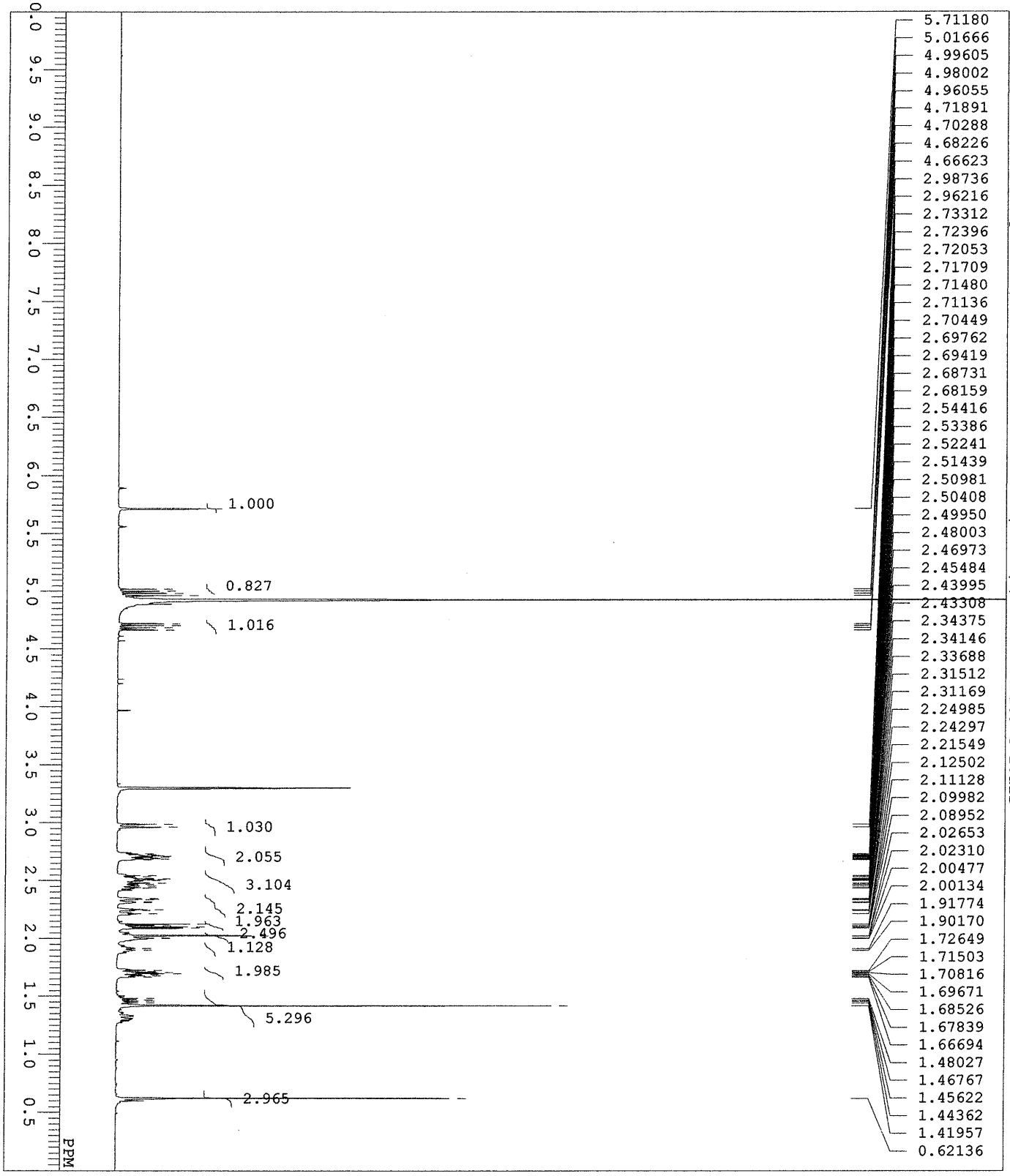


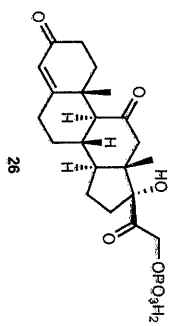

```
DFILE  KF-0001-PPE-H-coupled-P-o-n_copy1-1-1.als
COMNT
DATIM  01-10-2019 22:31:52
OBNUC  31P
EXMOD  single_pulse.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS         16883
ACQTM         0.0000 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  31P
CTEMP          20.6 c
SLVNT  DMSO
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



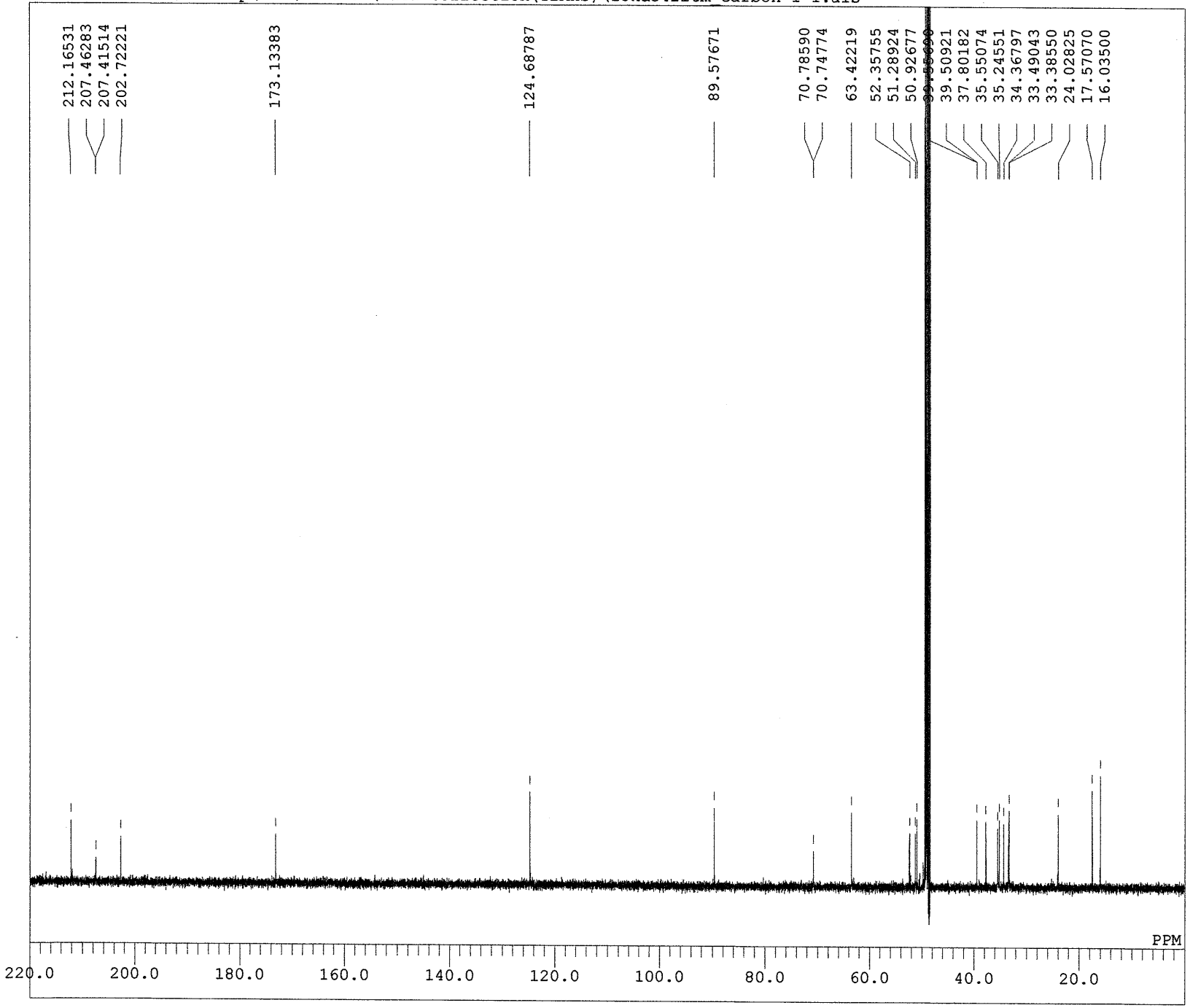
25

^{1}H coupled ^{31}P NMR

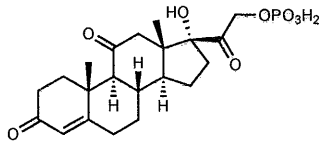

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3171HPLC5-1-1.als
5.71180
5.01666
4.99605
4.98002
4.96055
4.71891
4.70288
4.68226
4.66623
2.98736
2.96216
2.73312
2.72396
2.72053
2.71709
2.71480
2.71136
2.70449
2.69762
2.69419
2.68731
2.68159
2.54416
2.53386
2.52241
2.51439
2.50981
2.50408
2.49950
2.48003
2.46973
2.45484
2.43995
2.43308
2.34375
2.34146
2.33688
2.31512
2.31169
2.24985
2.24297
2.21549
2.12502
2.11128
2.09982
2.08952
2.02653
2.02310
2.00477
2.00134
1.91774
1.90170
1.72649
1.71503
1.70816
1.69671
1.68526
1.67839
1.66694
1.48027
1.46767
1.45622
1.44362
1.41957
0.62136
1.000
0.827
1.016
1.030
2.055
3.104
2.145
1.963
2.496
1.128
1.985
5.296
2.965
PPM
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
DFILE 18kd3171HPLC5-1-1.als
COMNT
DATIM 2018-09-30 20:24:17
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 30


26
HO
OPO3H2

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3422tm_carbon-1-1.als

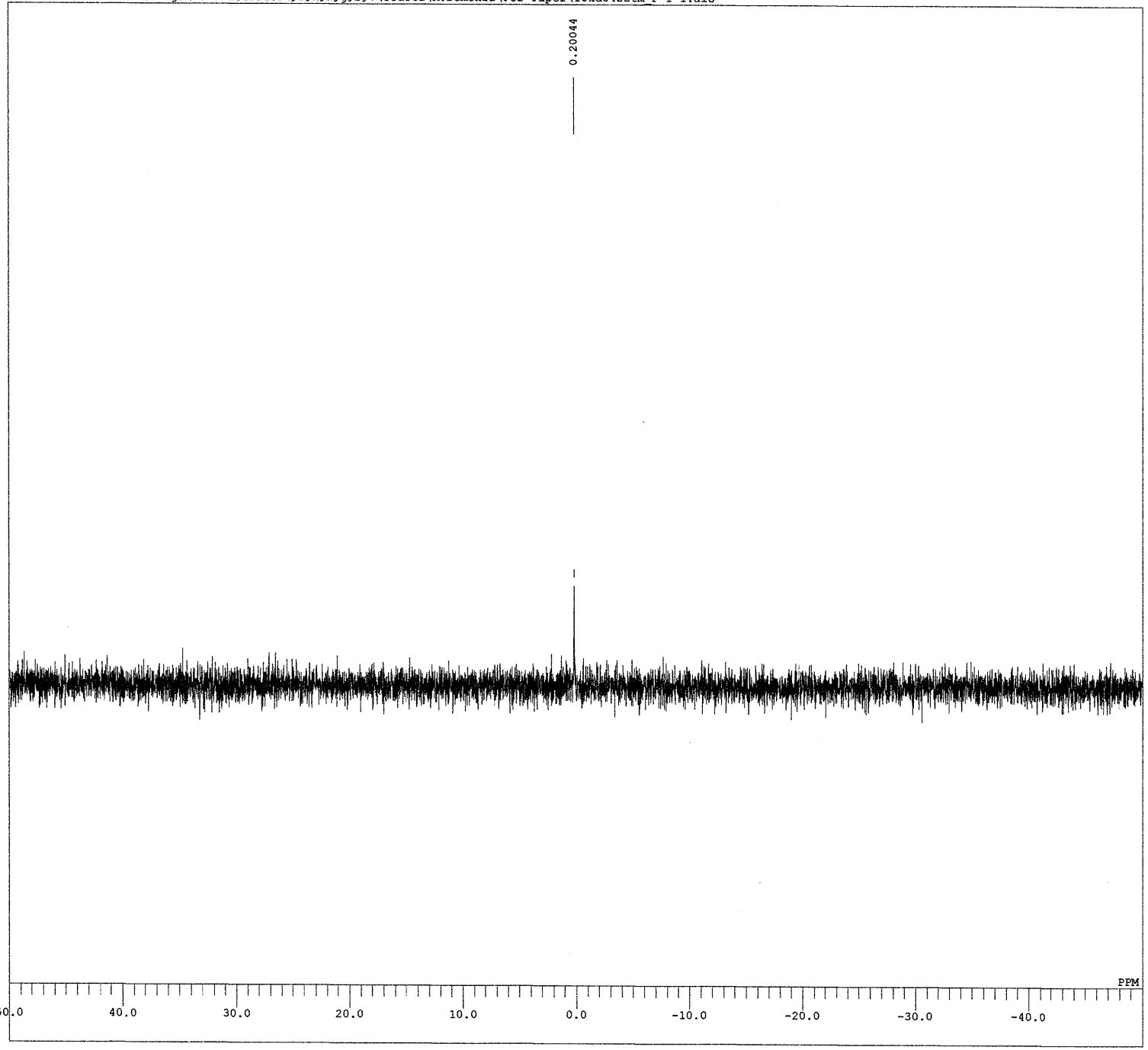


DFILE	18kd3422tm_carbon-1-1.als
COMNT	
DATIM	2019-03-20 01:07:39
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	9877
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	21.9 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

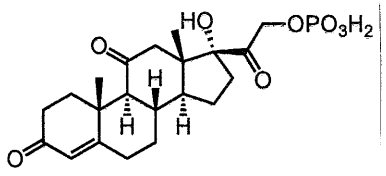


26

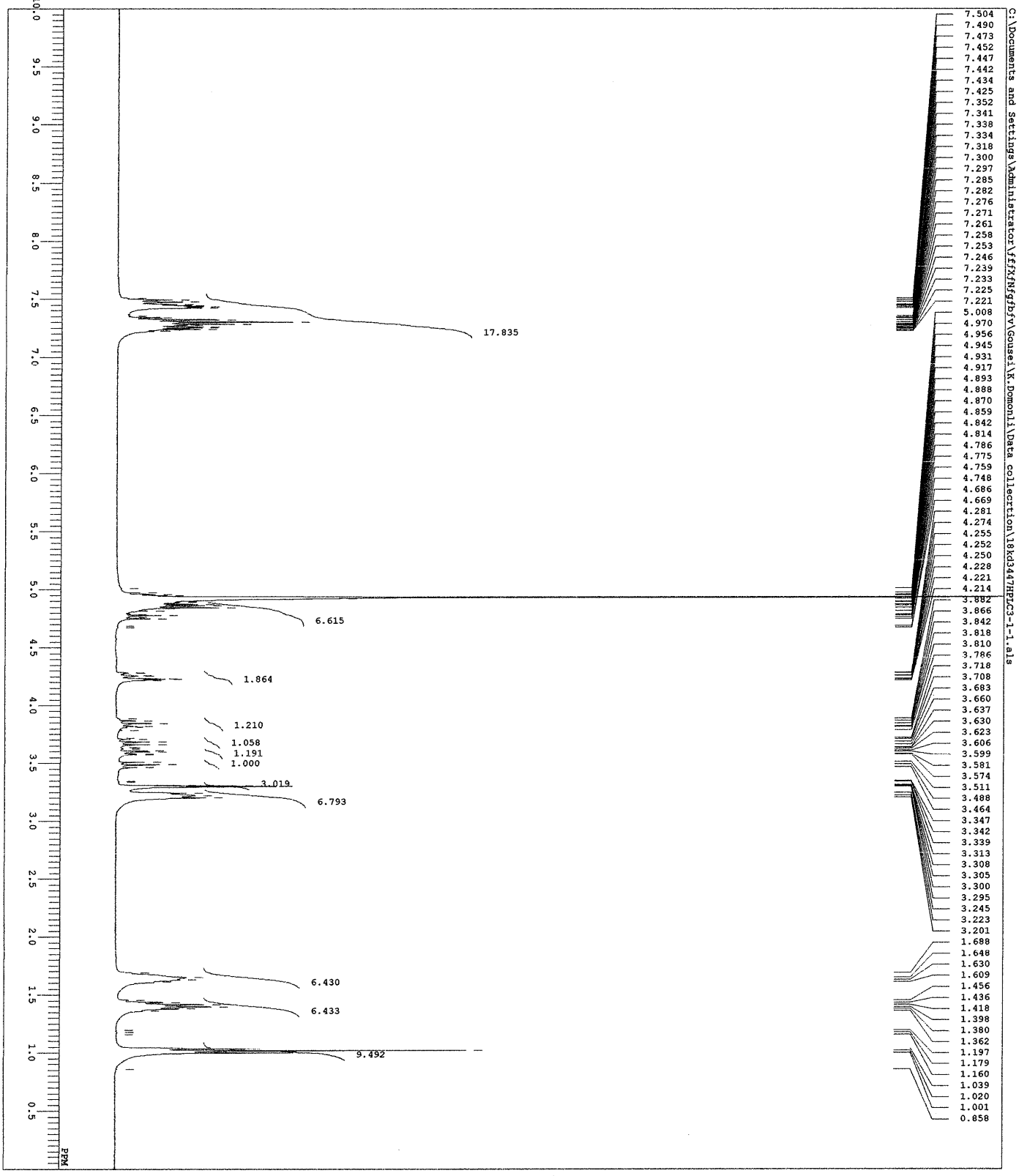
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3422tm_P-1-1.als



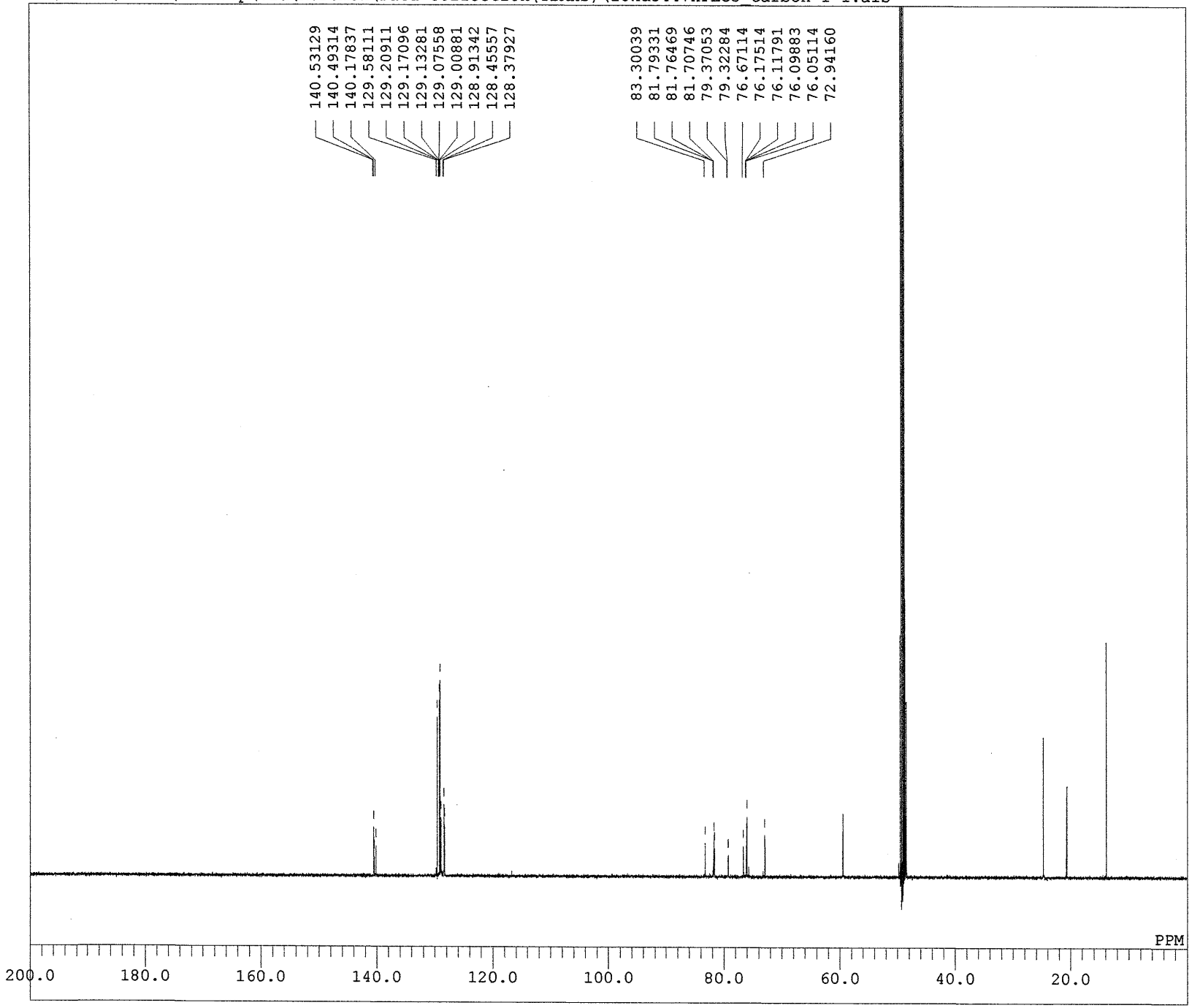

```
DFILE  18kd3422tm_P-1-1.als
COMNT
DATIM  07-03-2019 05:10:35
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            13
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP           20.1 c
SLVNT  CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



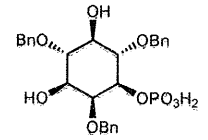
26


C:\Documents and Settings\administrator\ffjfNfgfbfr\Gousei\K.Domonli\Data collection\18kd3447HPLC3-1-1.als
7.504
7.490
7.473
7.452
7.447
7.442
7.434
7.425
7.352
7.341
7.338
7.334
7.318
7.300
7.297
7.285
7.282
7.276
7.271
7.261
7.258
7.253
7.246
7.239
7.233
7.225
7.221
5.008
4.970
4.956
4.945
4.931
4.917
4.893
4.888
4.870
4.859
4.842
4.814
4.786
4.775
4.759
4.748
4.686
4.669
4.281
4.274
4.255
4.252
4.250
4.228
4.221
4.214
3.882
3.866
3.842
3.818
3.810
3.786
3.718
3.708
3.683
3.660
3.637
3.630
3.623
3.606
3.599
3.581
3.574
3.511
3.488
3.464
3.347
3.342
3.339
3.313
3.308
3.305
3.300
3.295
3.245
3.223
3.201
1.688
1.648
1.630
1.609
1.456
1.436
1.418
1.398
1.380
1.362
1.197
1.179
1.160
1.039
1.020
1.001
0.858
17.835
6.615
1.864
1.210
1.058
1.191
1.000
3.019
6.793
6.430
6.433
9.492
PPM
DFILE 18kd3447HPLC3-1-1.als
COMNT
DATIM 05-03-2019 03:23:52
OBNUC 1H
EXMOD proton.jxp
OBFRQ 391.78 MHz
OBSET 8.51 KHz
OBFIN 3.34 Hz
POINT 13107
FREQU 5882.35 Hz
SCANS 8
ACQTM 2.2282 sec
PD 5.0000 sec
PW1 5.22 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 32
BnO
OH
HO
OBn
OBn
OPO3H2
27 (rac)

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3447HPLC3_carbon-1-1.als

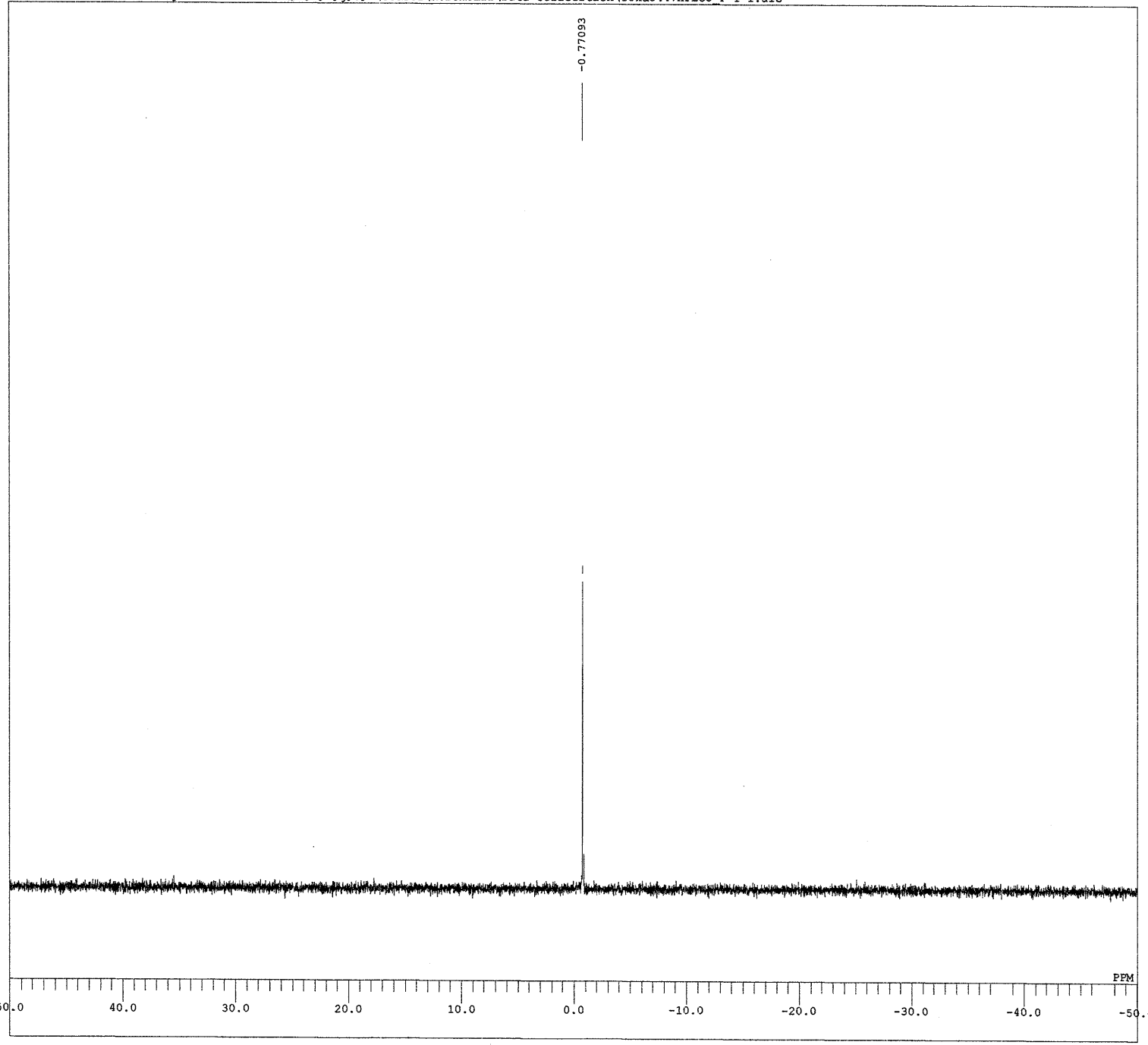


DFILE	18kd3447HPLC3_carbon-1-1.als
COMNT	
DATIM	2019-03-06 03:27:44
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	125.77 MHz
OBSET	7.87 KHz
OBFIN	4.21 Hz
POINT	26214
FREQU	31446.54 Hz
SCANS	10000
ACQTM	0.8336 sec
PD	2.0000 sec
PW1	3.40 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CD3OD
EXREF	49.00 ppm
BF	0.12 Hz
RGAIN	60

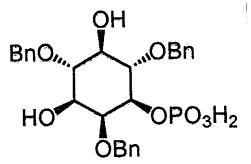


27 (rac)

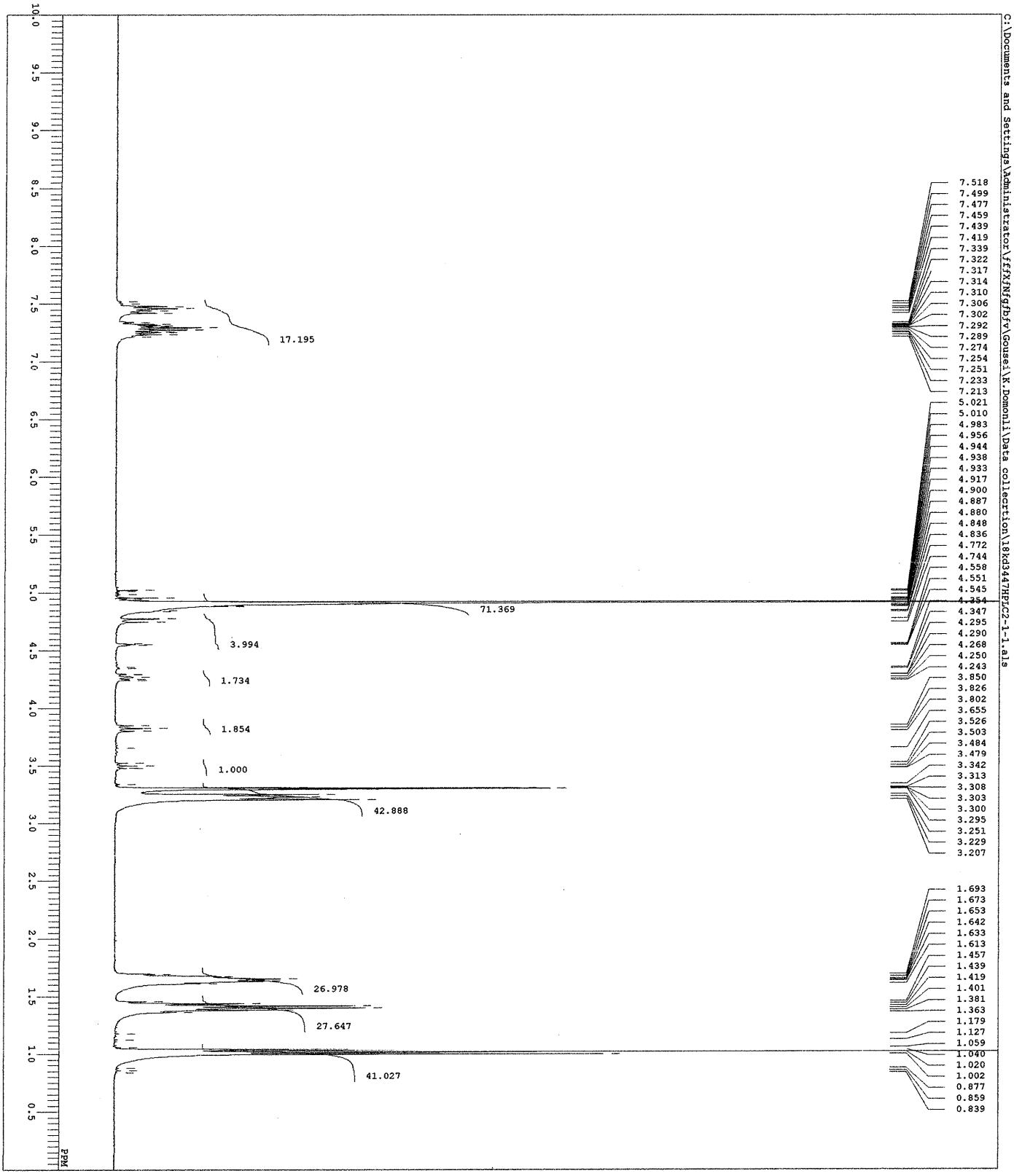
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd3447HPLC3_P-1-1.als

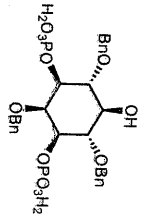



```
DFILE  18kd3447HPLC3_P-1-1.als
COMNT
DATIM  05-03-2019 03:40:21
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            15
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP           20.1 c
SLVNT  CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```

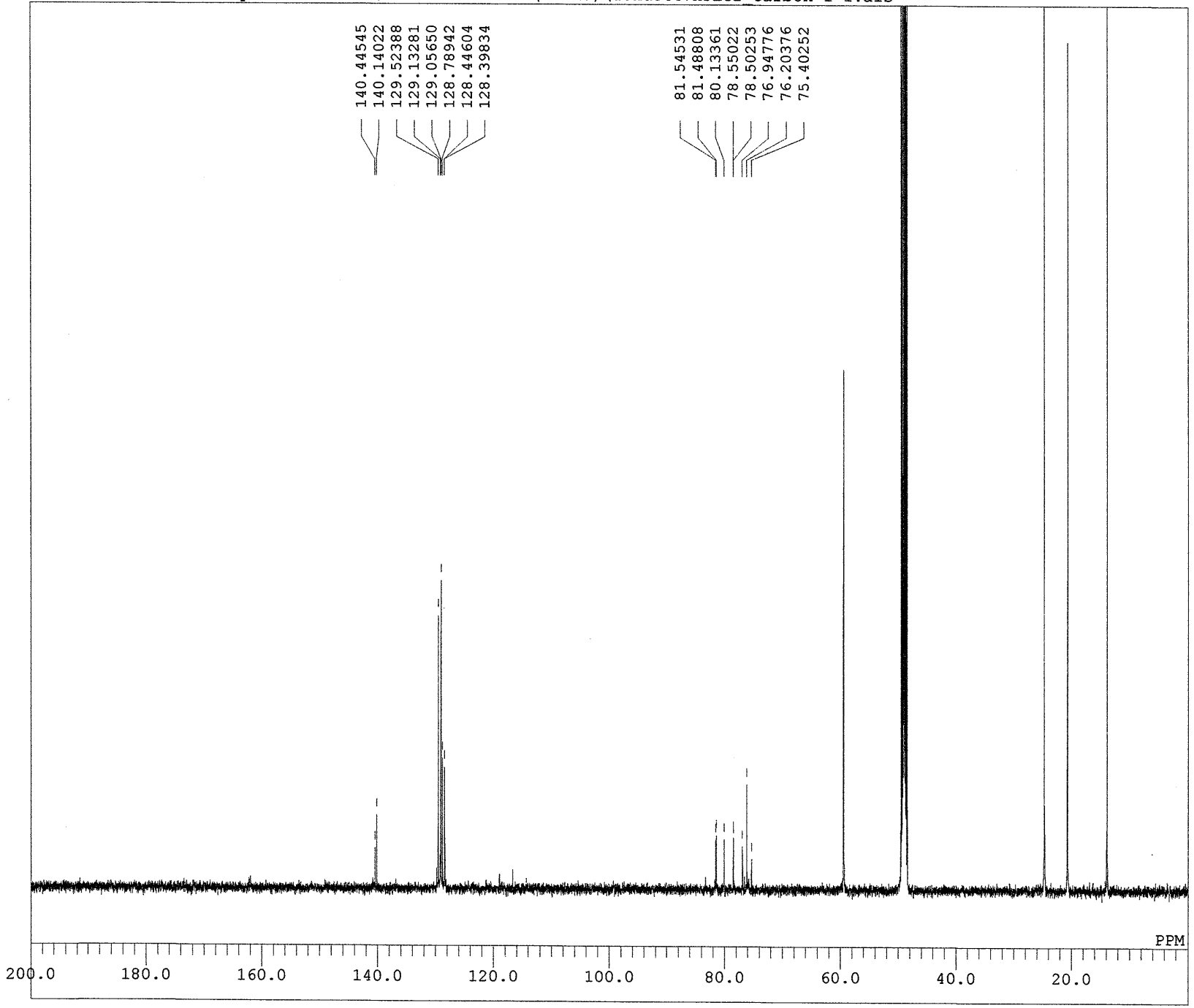


27 (rac)

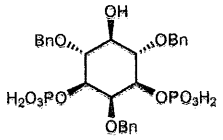

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\Data collecrtion\18kd3447HPLC2-1-1.als
17.195
71.369
3.994
1.734
1.854
1.000
42.888
26.978
27.647
41.027
PPM
DFILE 18kd3447HPLC2-1-1.als
COMNT
DATIM 05-03-2019 03:30:56
OBNUC 1H
EXMOD proton.jxp
OBFRQ 391.78 MHz
OBSET 8.51 KHz
OBFIN 3.34 Hz
POINT 13107
FREQU 5882.35 Hz
SCANS 5
ACQTM 2.2282 sec
PD 5.0000 sec
PW1 5.22 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 36


H2O3PO
BnO
OH
OBn
OBn
OPO3H2

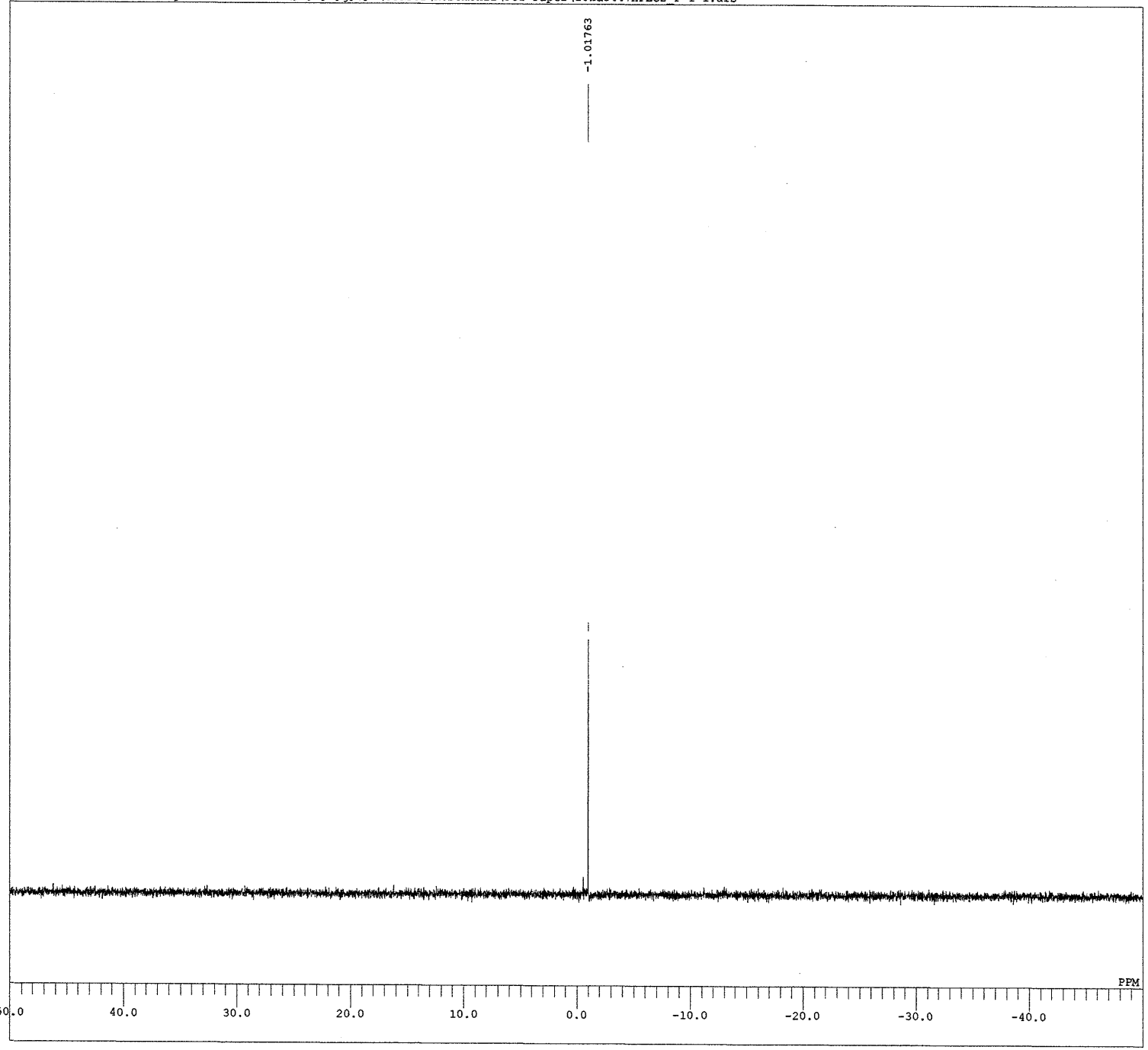
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3447HPLC2_carbon-1-1.als



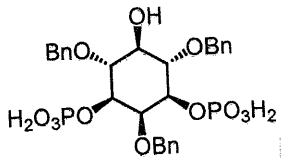
DFILE 18kd3447HPLC2_carbon-1-1.als
COMNT
DATIM 2019-03-16 13:33:22
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 125.77 MHz
OBSET 7.87 KHz
OBFIN 4.21 Hz
POINT 26214
FREQU 31446.54 Hz
SCANS 20000
ACQTM 0.8336 sec
PD 2.0000 sec
PW1 3.40 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CD3OD
EXREF 49.00 ppm
BF 1.20 Hz
RGAIN 60



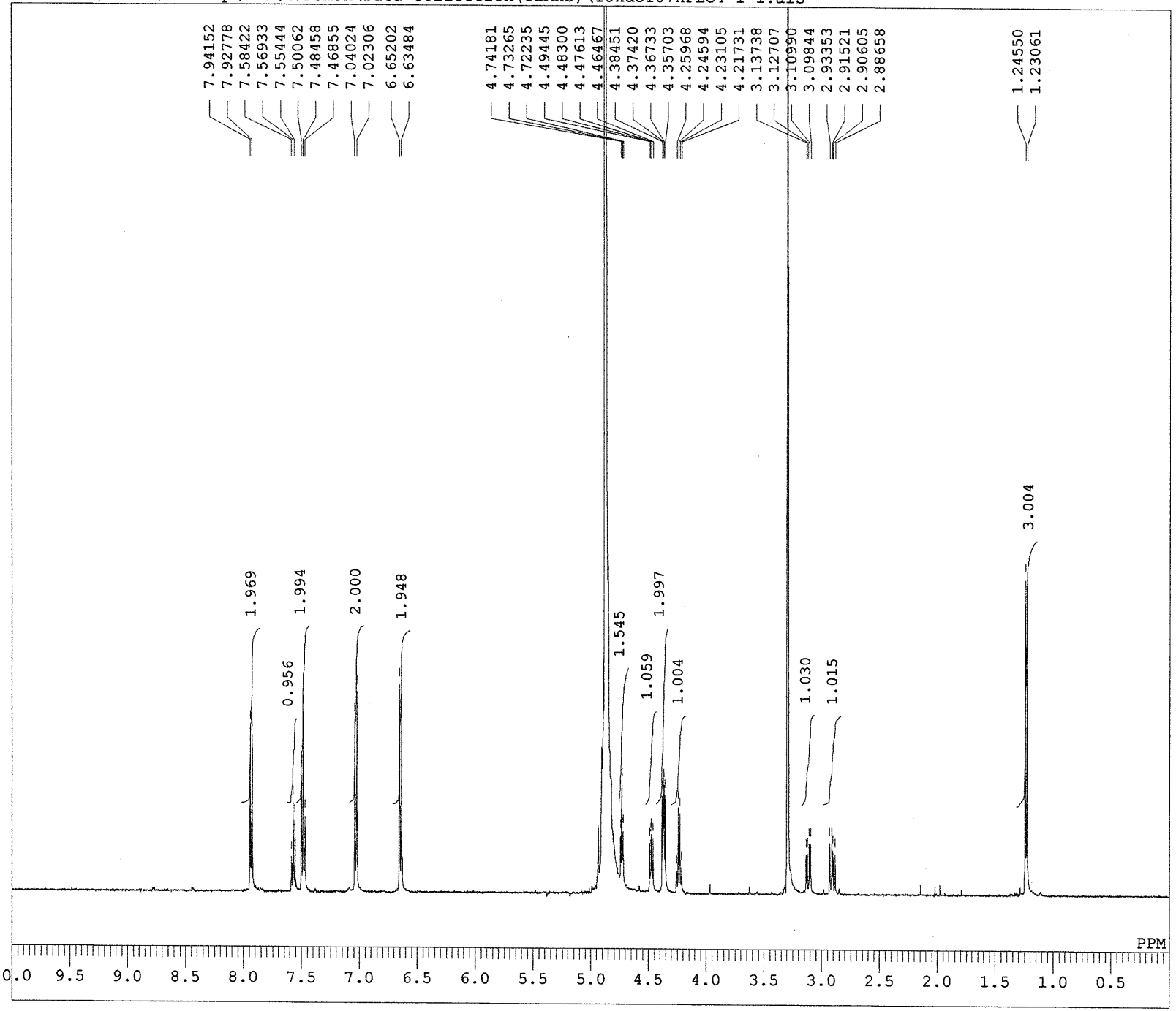
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3447HPLC2_P-1-1.als



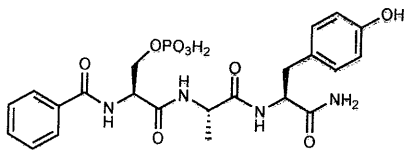

```
DFILE  18kd3447HPLC2_P-1-1.als
COMNT
DATIM  05-03-2019 03:33:58
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            29
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP           20.1 c
SLVNT  CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3107HPLC4-1-1.als

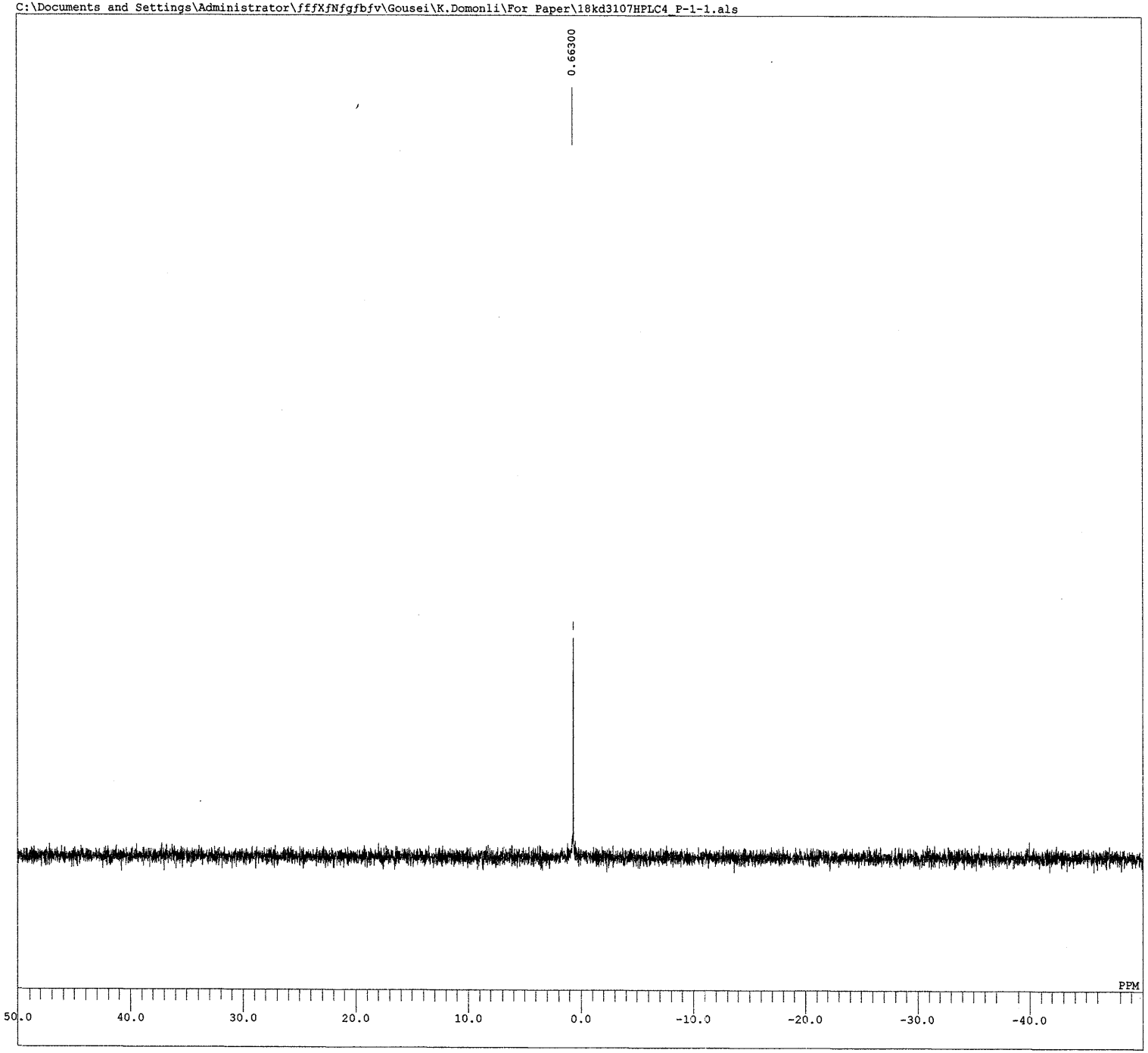


DFILE	18kd3107HPLC4-1-1.als
COMNT	
DATIM	2018-09-17 06:04:53
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	7
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.6 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30

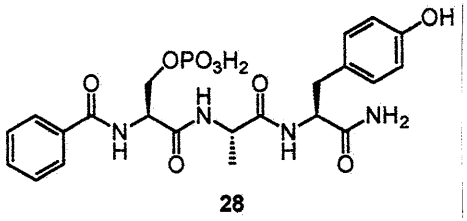


28

C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3107HPLC4_P-1-1.als

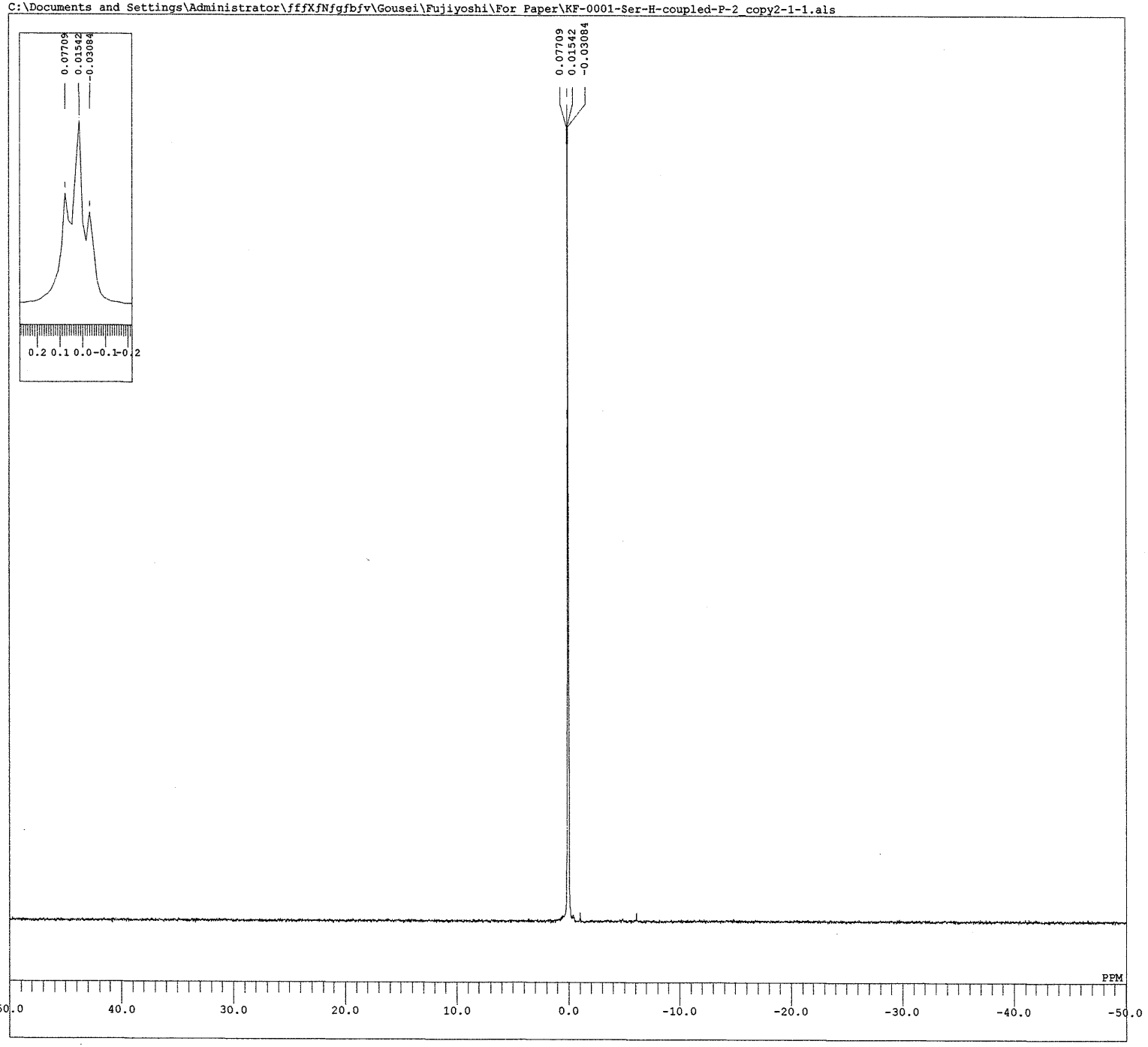



```
DFILE   18kd3107HPLC4_P-1-1.als
COMNT
DATIM   18-09-2018 09:45:45
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS             52
ACQTM          0.4089 sec
PD             2.0000 sec
PW1              4.80 usec
IRNUC   1H
CTEMP            20.2 c
SLVNT   CD3OD
EXREF            0.00 ppm
BF               0.12 Hz
RGAIN              56
```

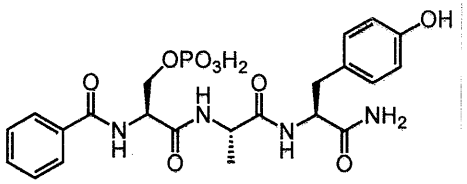


28

C:\Documents and Settings\Administrator\ƒfƒXƒNƒgƒbƒv\Gousei\Fujiyoshi\For Paper\KF-0001-Ser-H-coupled-P-2_copy2-1-1.als

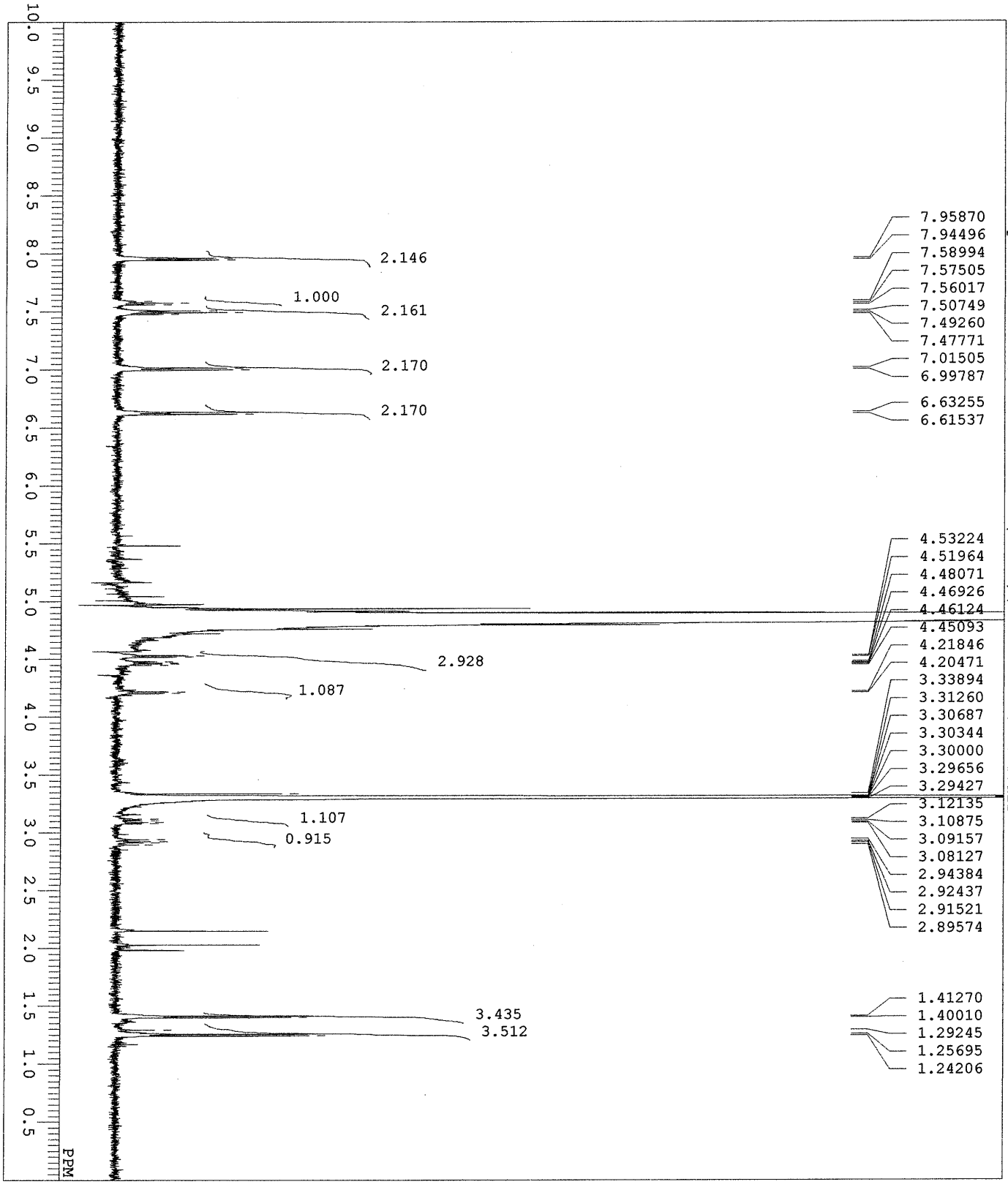



```
DFILE  KF-0001-Ser-H-coupled-P-2_copy2-1-1.als
COMNT
DATIM  24-10-2019 23:36:23
OBNUC  31P
EXMOD  single_pulse.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS         16986
ACQTM        0.0000 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  31P
CTEMP         20.7 c
SLVNT  DMSO
EXREF          0.00 ppm
BF             1.20 Hz
RGAIN            56
```

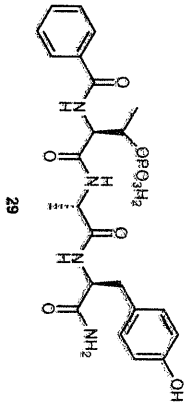


28

^{1}H coupled ^{31}P NMR



DFILE 18kd3154HPLC7-1-1.als
COMNT
DATIM 2018-09-29 21:10:27
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 30



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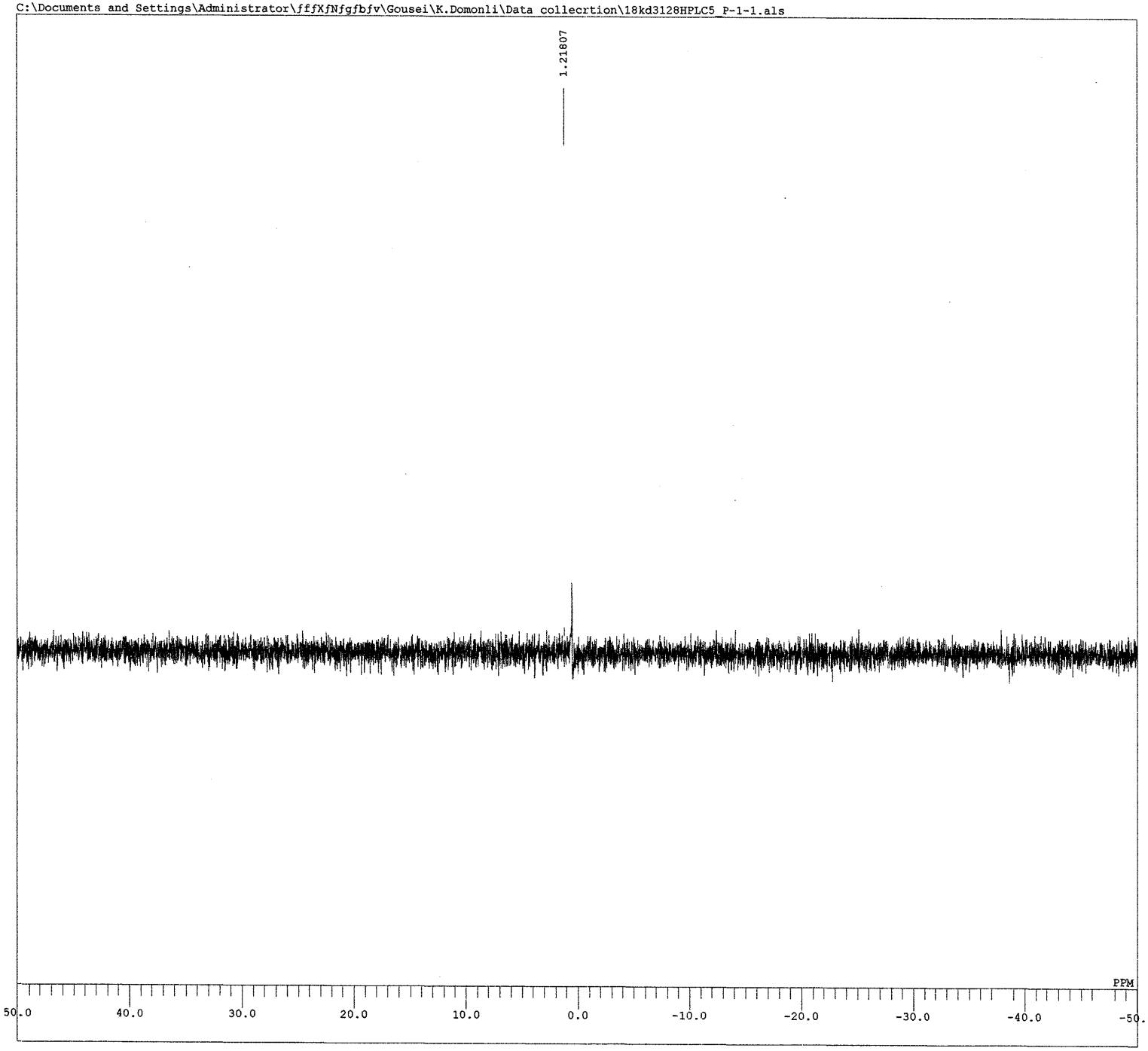
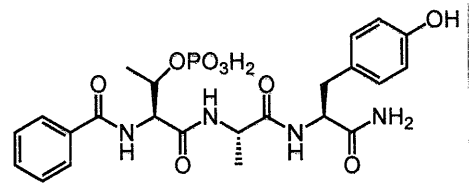
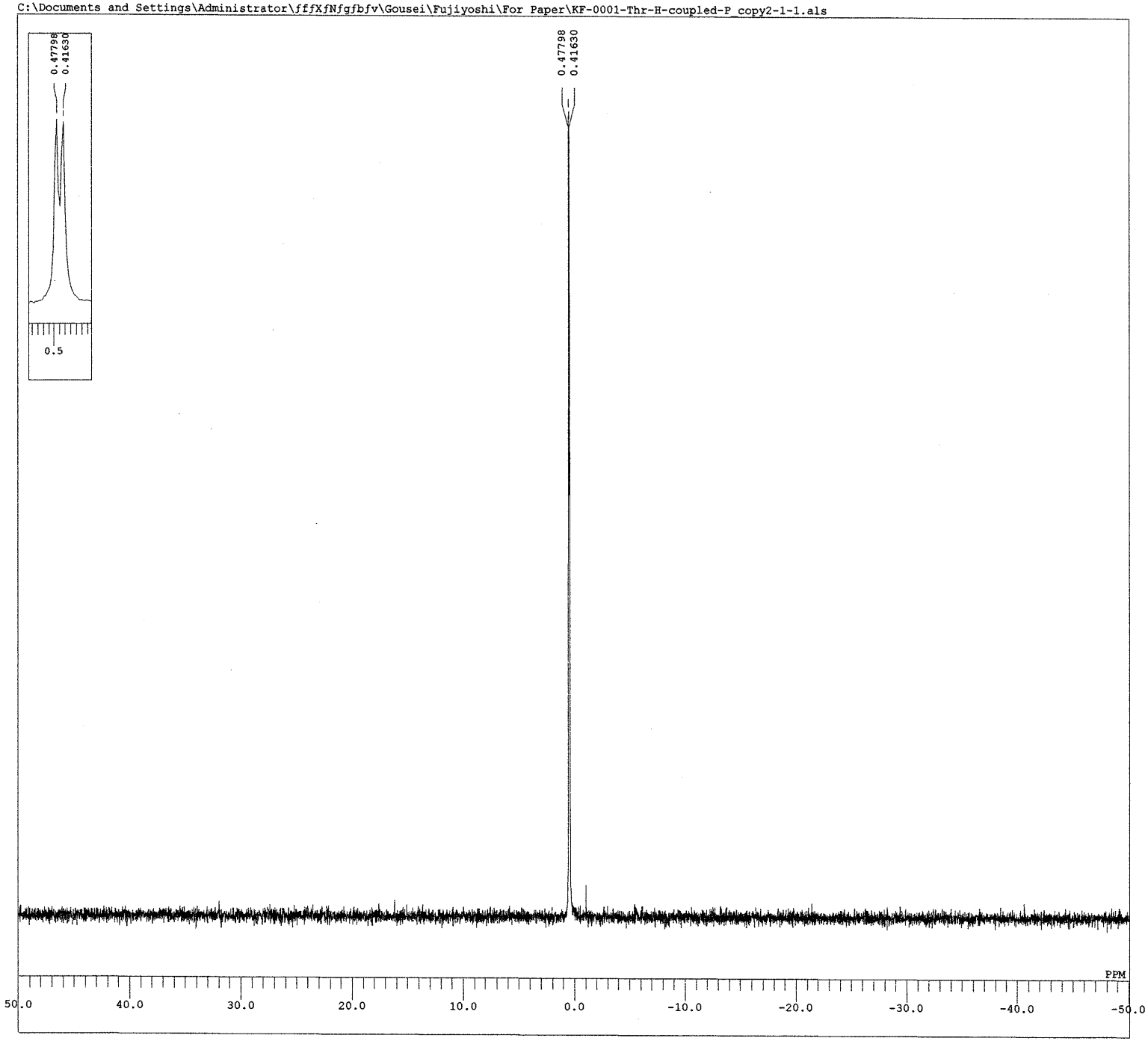


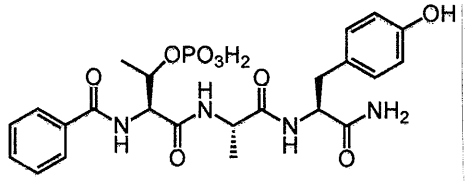

```
DFILE   18kd3128HPLC5_P-1-1.als
COMNT
DATIM   20-09-2018 08:28:17
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS           1014
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC   1H
CTEMP           20.3 c
SLVNT   DMSO
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



29



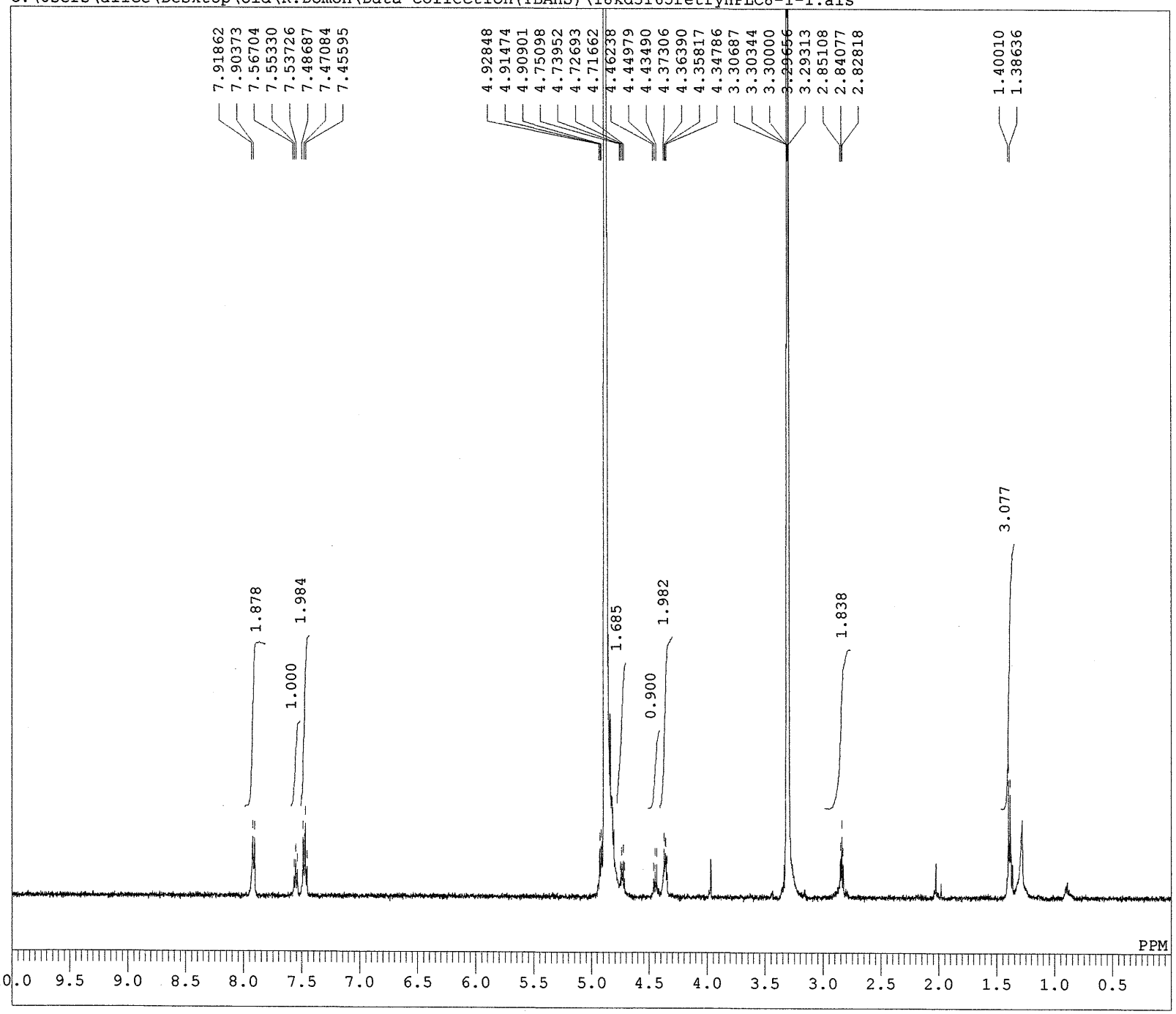

```
DFILE  KF-0001-Thr-H-coupled-P_copy2-1-1.als
COMNT
DATIM  28-09-2019 22:39:48
OBNUC  31P
EXMOD  single_pulse.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS         20863
ACQTM         0.0000 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  31P
CTEMP          20.7 c
SLVNT  DMSO
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



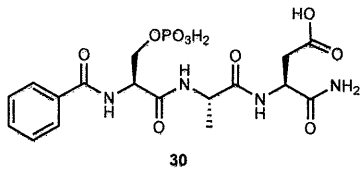
29

^{1}H coupled ^{31}P NMR

C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3165retryHPLC8-1-1.als



DFILE	18kd3165retryHPLC8-1-1.als
COMNT	
DATIM	2018-09-28 20:57:52
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	8
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	32



30

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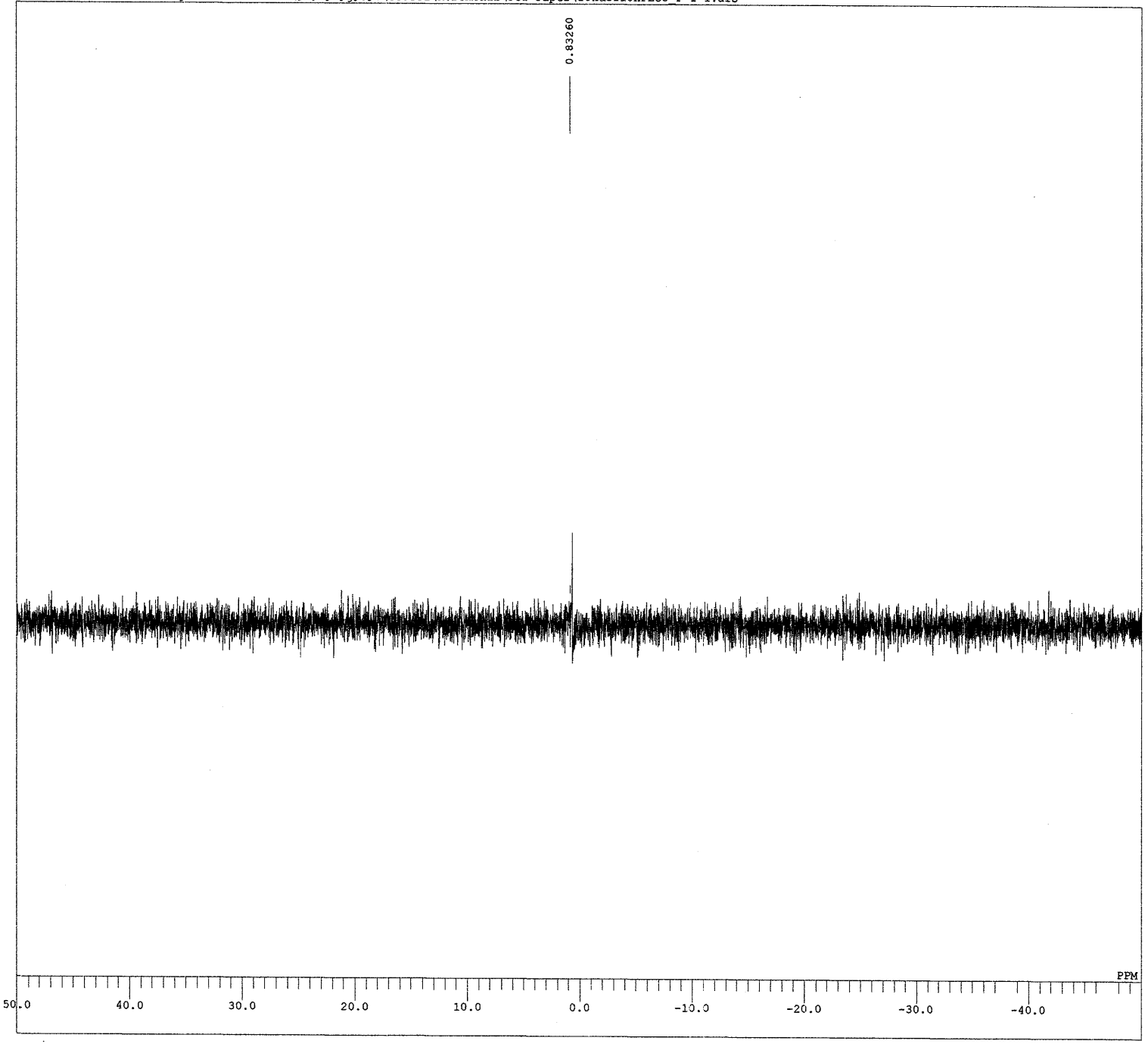
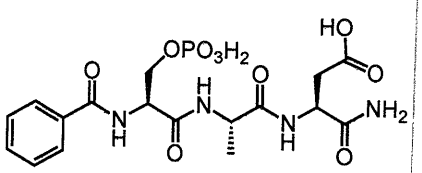
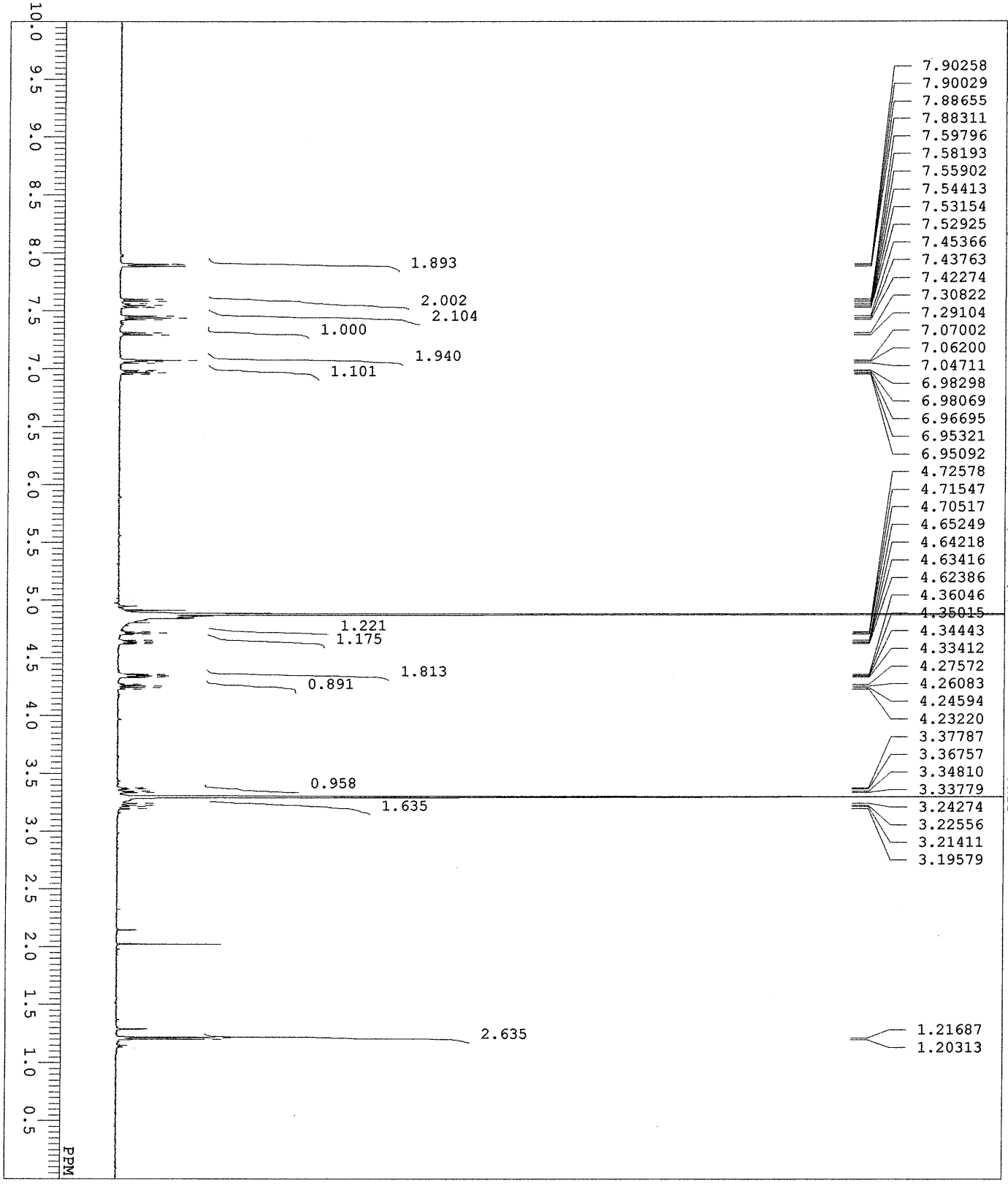


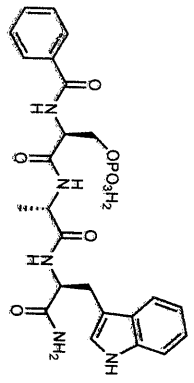

```
DFILE   18kd3110HPLC5_P-1-1.als
COMNT
DATIM   18-09-2018 09:17:33
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS            539
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC   1H
CTEMP           20.4 c
SLVNT   CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



30



DFILE 18kd3166HPLC2-1-1.als
COMNT
DATIM 2018-09-28 18:13:05
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 30



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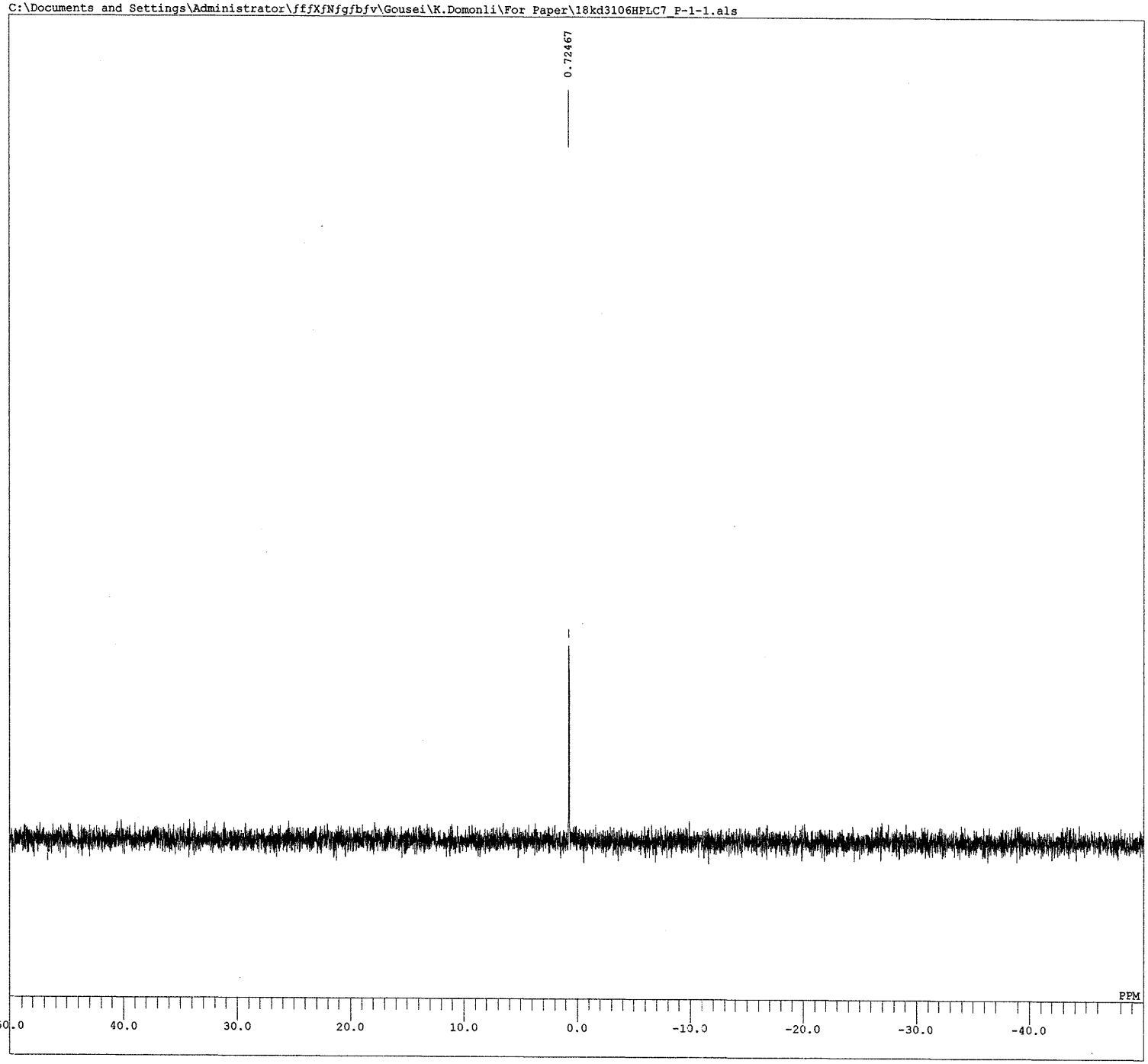
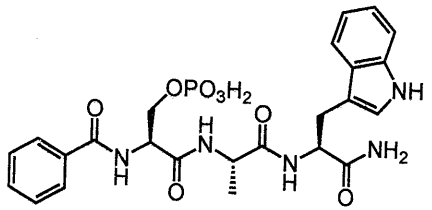
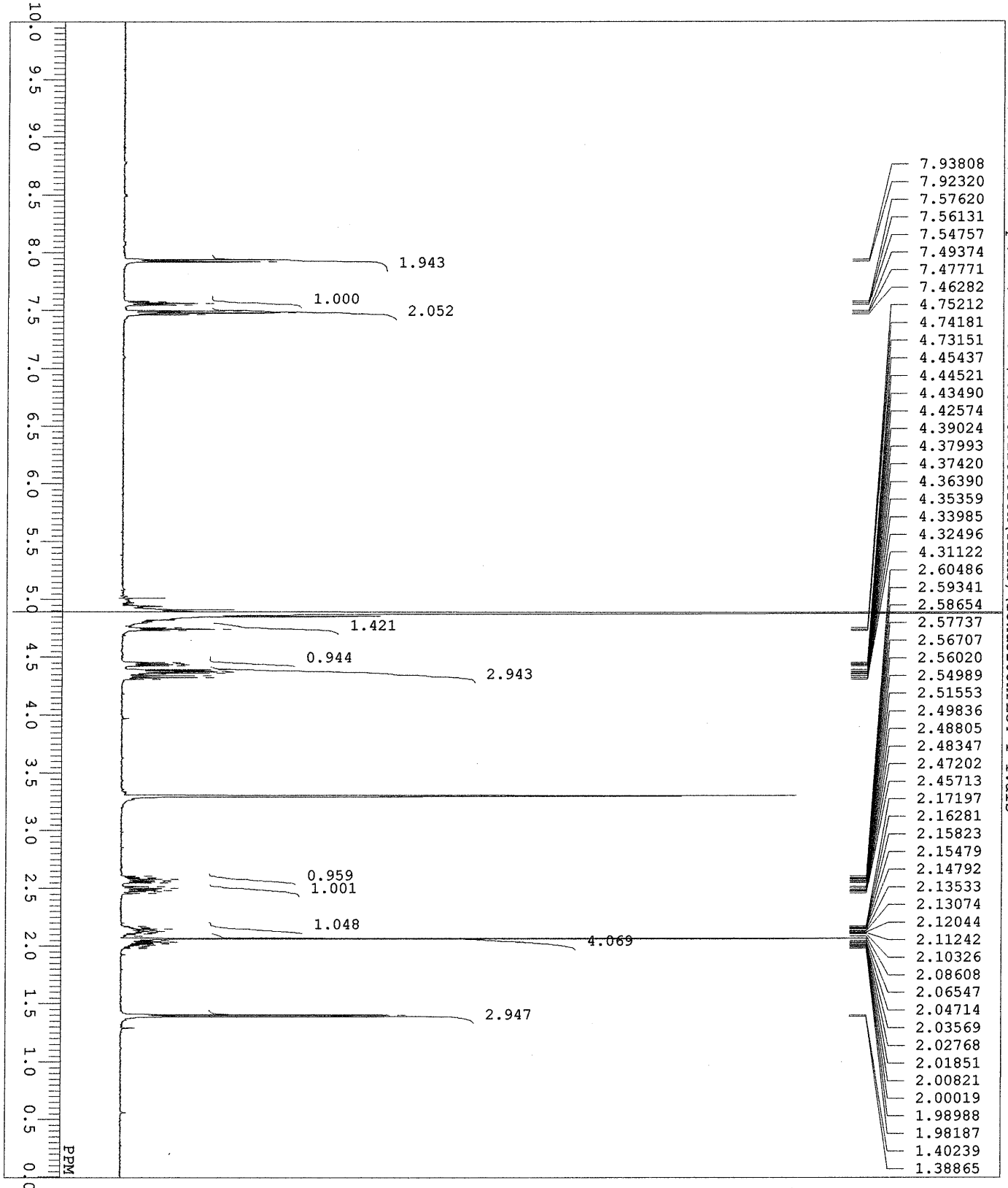


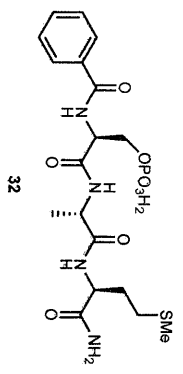

```
DFILE  18kd3106HPLC7_P-1-1.als
COMNT
DATIM  18-09-2018 09:41:24
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            26
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP         20.3 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



31



DFILE 18kd3108HPLC4-1-1.als
COMNT
DATIM 2018-09-17 06:07:40
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 5
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 30



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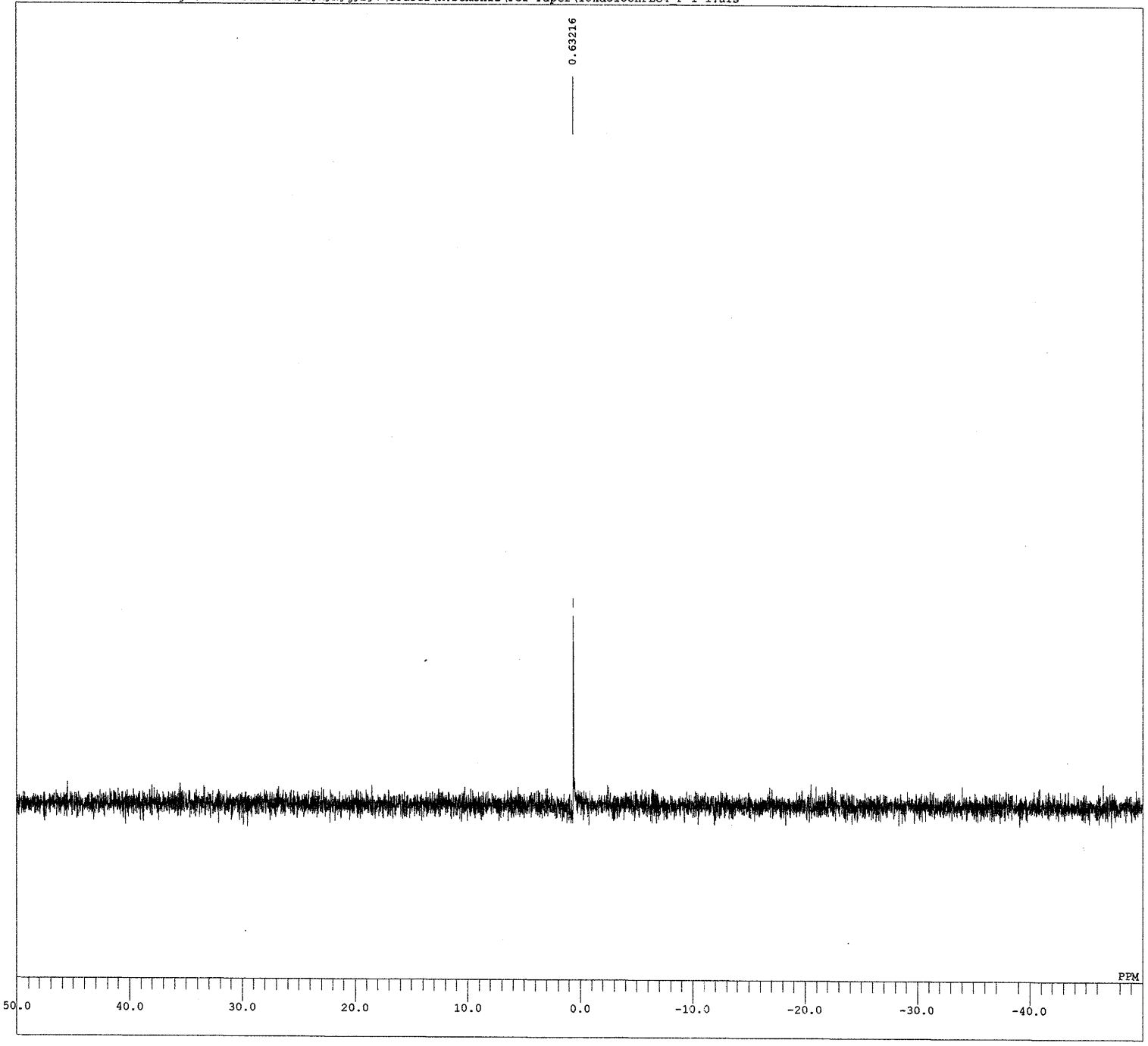
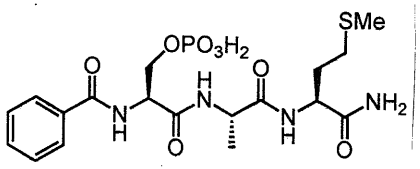
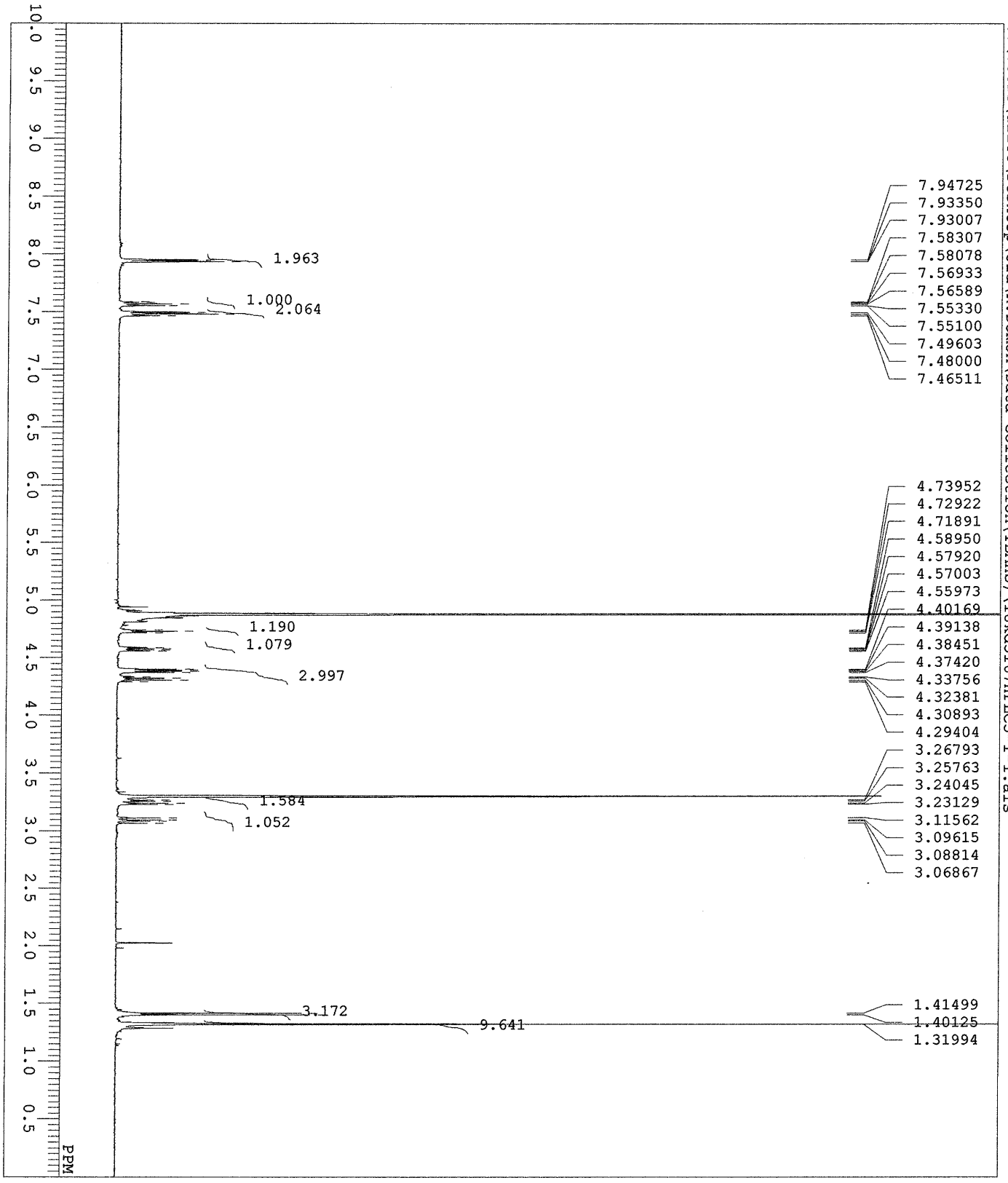


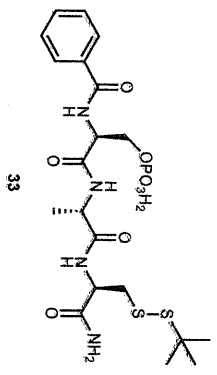

```
DFILE  18kd3108HPLC4_P-1-1.als
COMNT
DATIM  18-09-2018 09:50:17
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             6
ACQTM        0.4089 sec
PD           2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP         20.2 c
SLVNT  CD3OD
EXREF         0.00 ppm
BF            0.12 Hz
RGAIN           56
```



32



DFILE 18kd317HPLC5-1-1.als
COMNT
DATIM 2018-09-28 18:16:32
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.12 Hz
RGAIN 30



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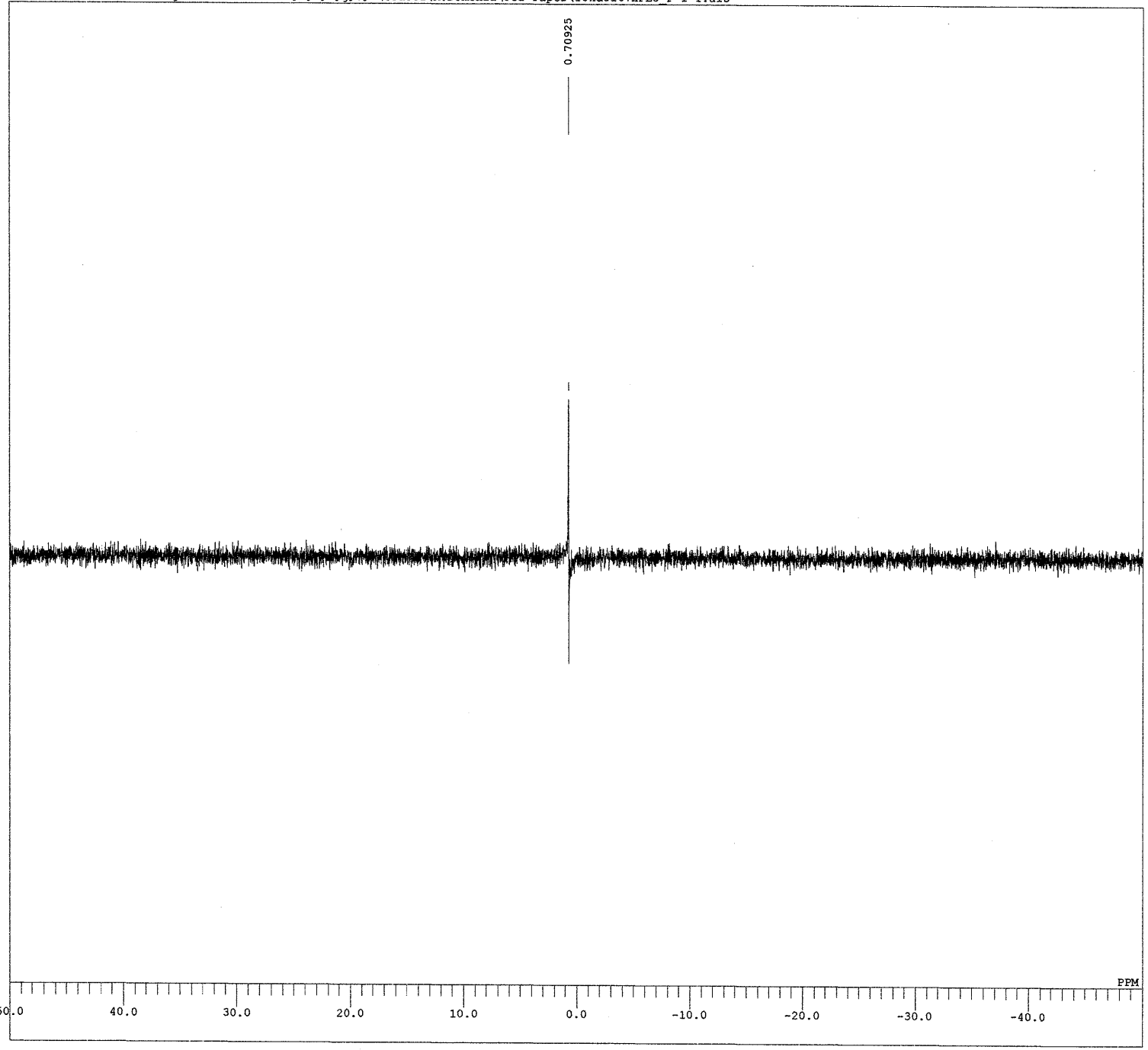
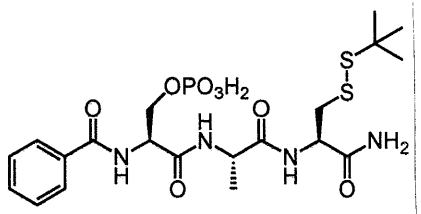



```
DFILE  18kd3167HPL5_P-1-1.als
COMNT
DATIM  28-09-2018 18:58:16
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS             8
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP          20.3 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
```



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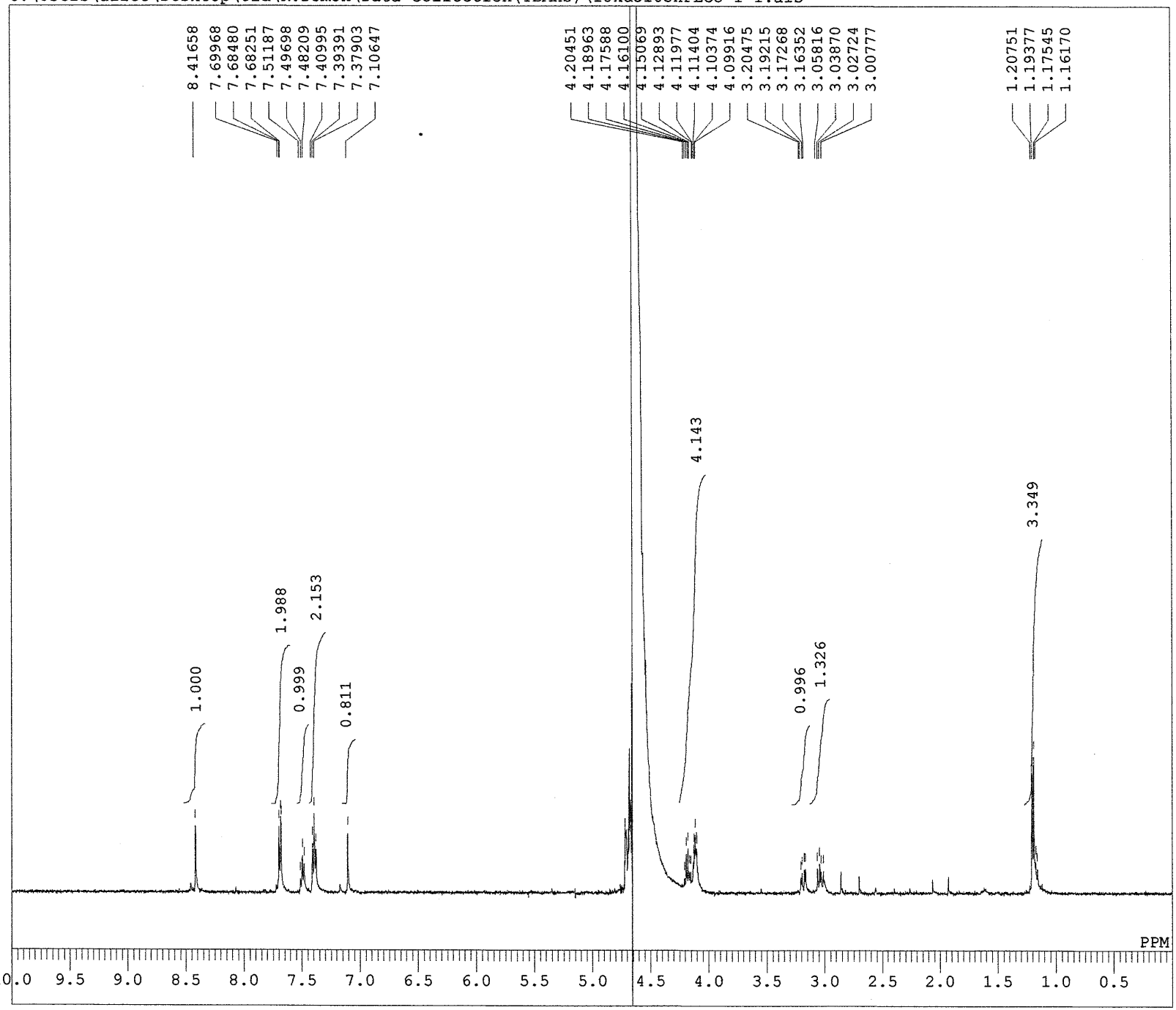
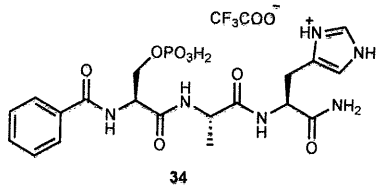
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3103HPLC3-1-1.als



DFILE	18kd3103HPLC3-1-1.als
COMNT	
DATIM	2018-09-07 13:43:39
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	20
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.5 c
SLVNT	D2O
EXREF	4.65 ppm
BF	0.12 Hz
RGAIN	30



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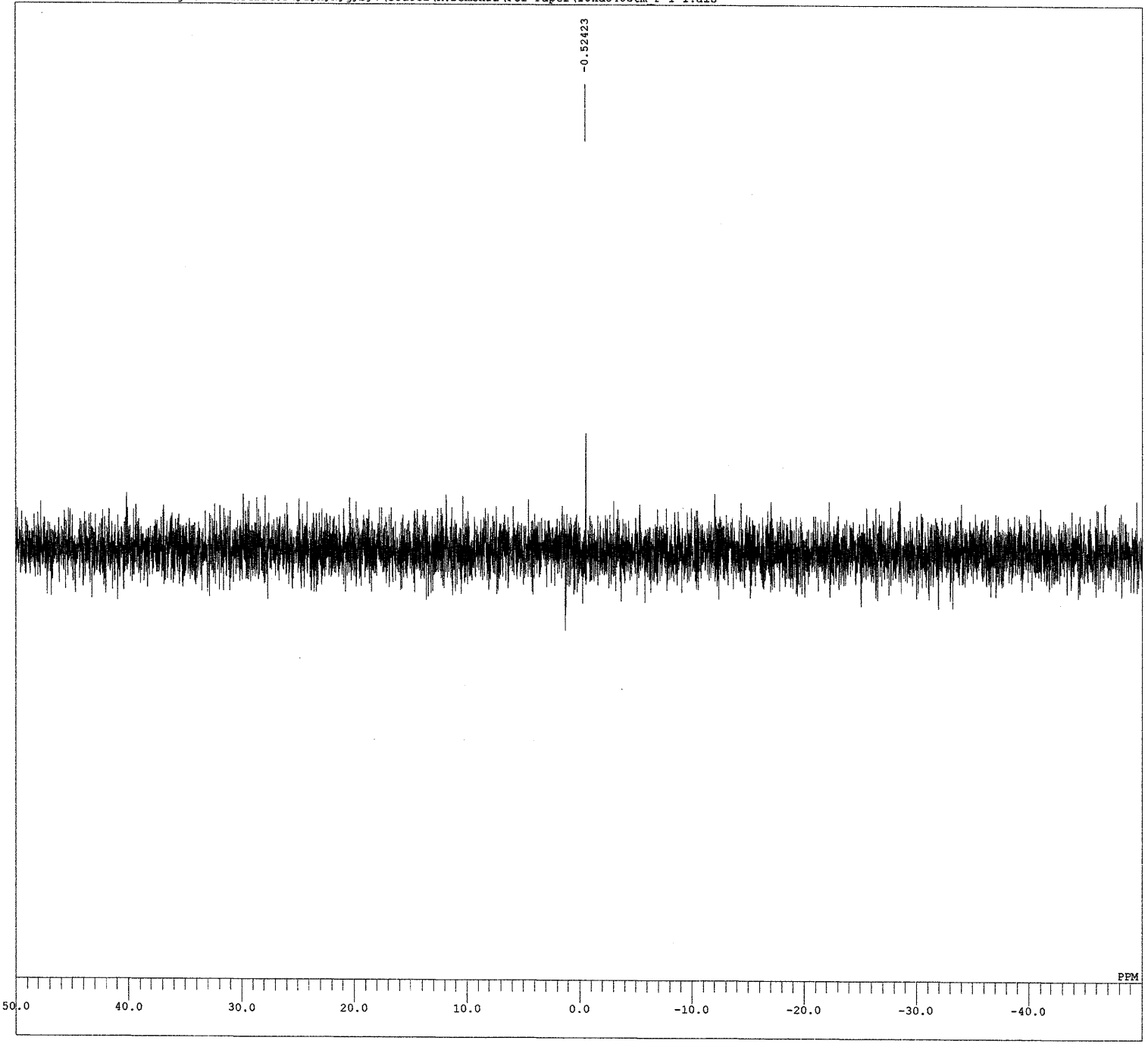
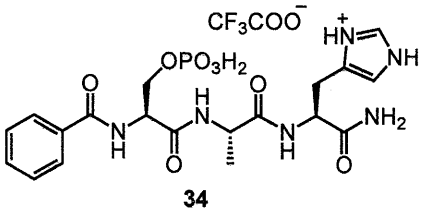
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3403tm_P-1-1.als




```
DFILE  18kd3403tm_P-1-1.als
COMNT
DATIM  07-03-2019 04:55:01
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            37
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP         20.0 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            54
```



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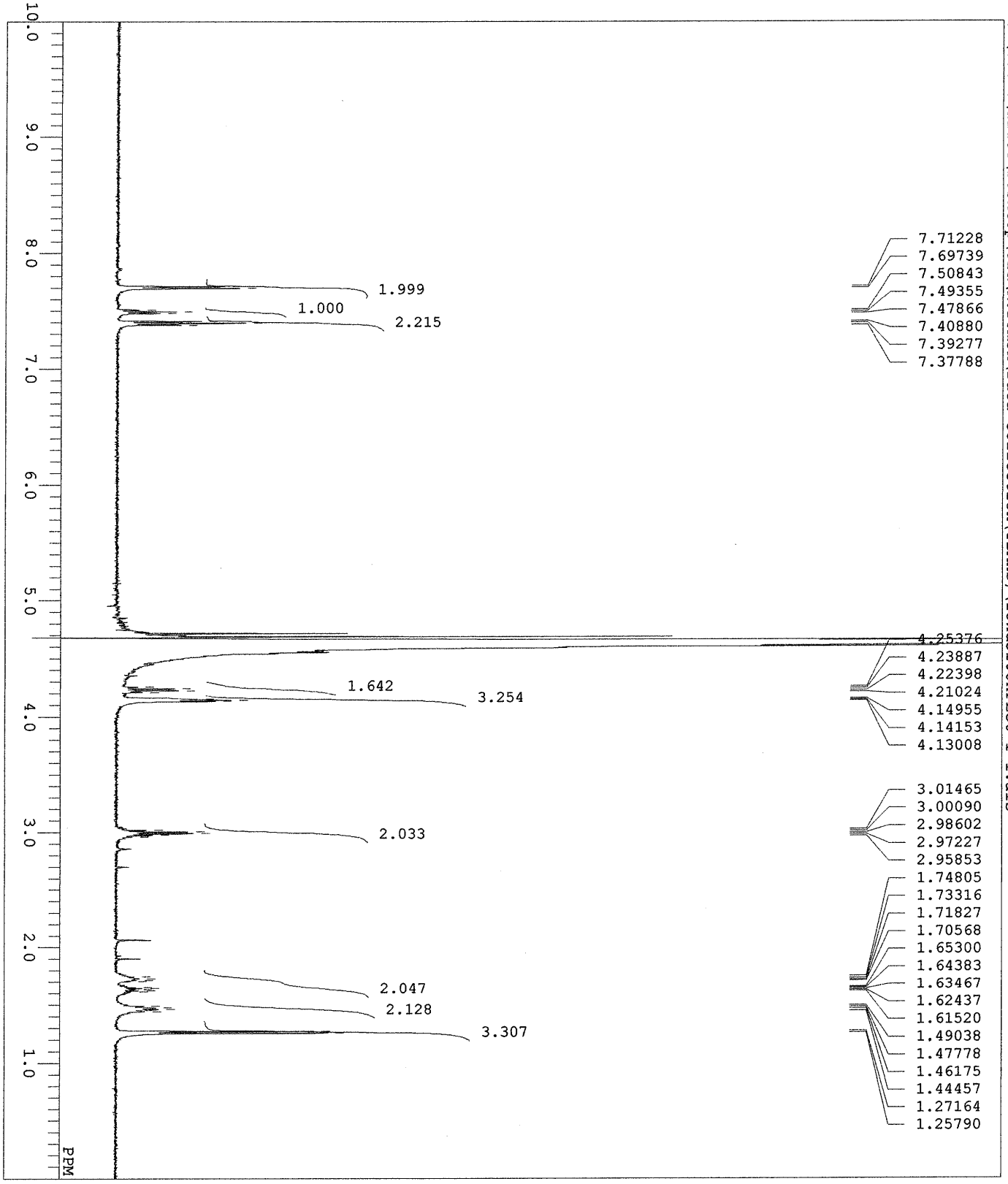
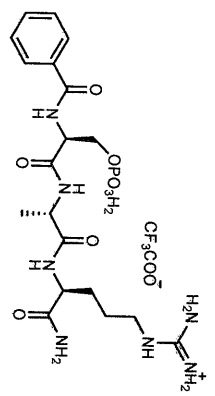


DFILE 18kd3100HPLC6-1-1.als
COMNT
DATIM 2018-09-06 05:34:36
OBNUC 1H
EXMOD proton.jxp
OBFRQ 500.16 MHz
OBSET 2.41 KHz
OBFIN 6.01 Hz
POINT 13107
FREQU 7507.51 Hz
SCANS 8
ACQTM 1.7459 sec
PD 5.0000 sec
PW1 5.55 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT D2O
EXREF 4.65 ppm
BF 0.12 Hz
RGAIN 30



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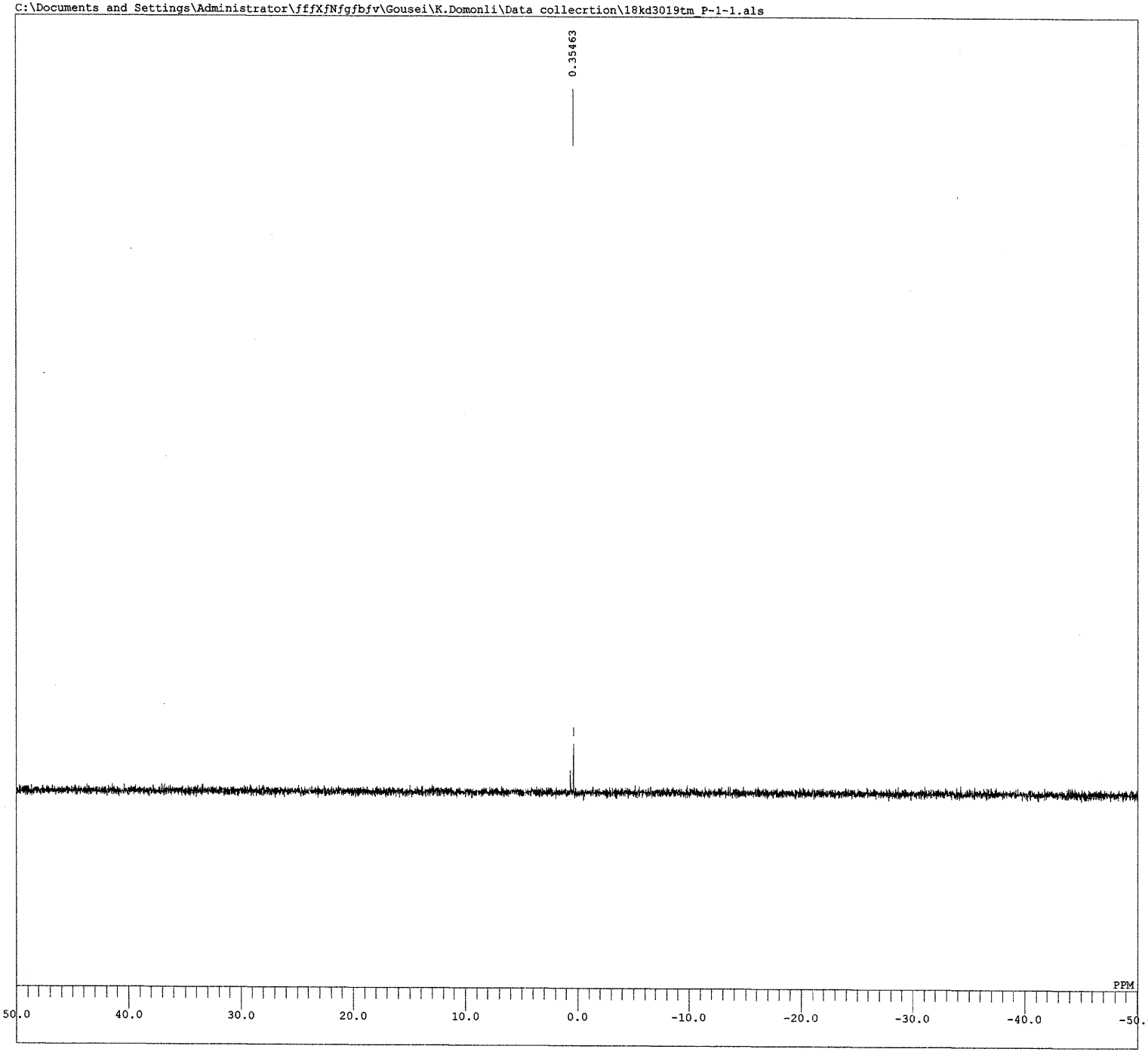
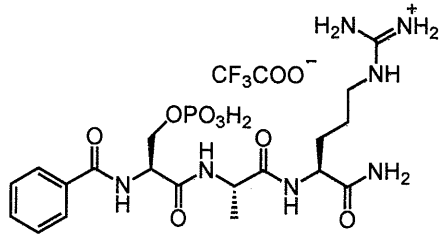



```
DFILE   18kd3019tm_P-1-1.als
COMNT
DATIM   06-03-2019 14:41:25
OBNUC   31P
EXMOD   carbon.jxp
OBFRQ         158.59 MHz
OBSET           7.99 KHz
OBFIN           9.23 Hz
POINT          26214
FREQU       64102.56 Hz
SCANS             11
ACQTM          0.4089 sec
PD             2.0000 sec
PW1              4.80 usec
IRNUC   1H
CTEMP           19.8 c
SLVNT   CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



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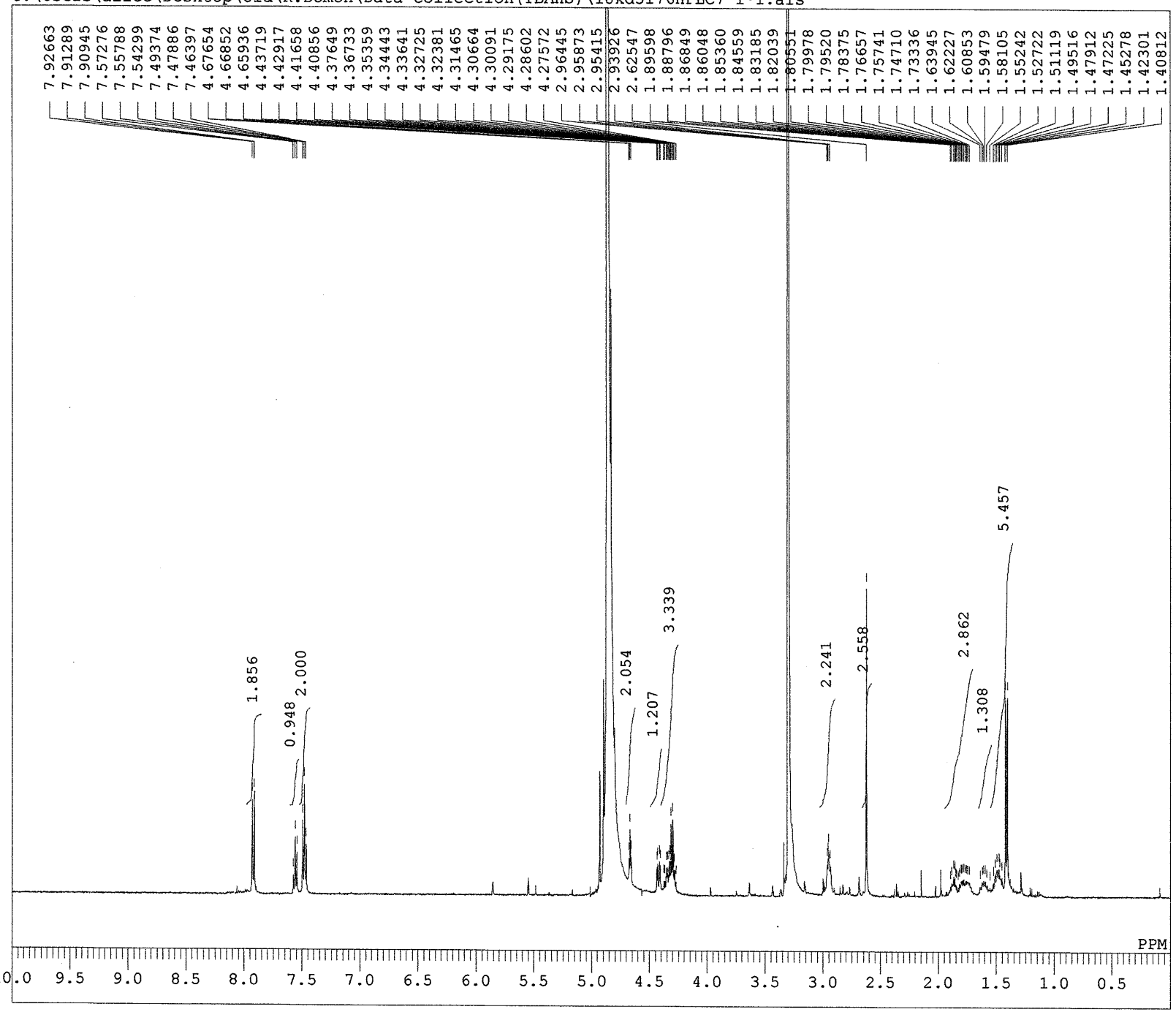
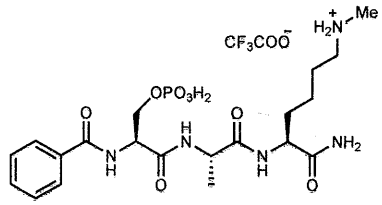
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3176HPLC7-1-1.als



DFILE	18kd3176HPLC7-1-1.als
COMNT	
DATIM	2018-10-02 14:51:45
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	195
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.8 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30



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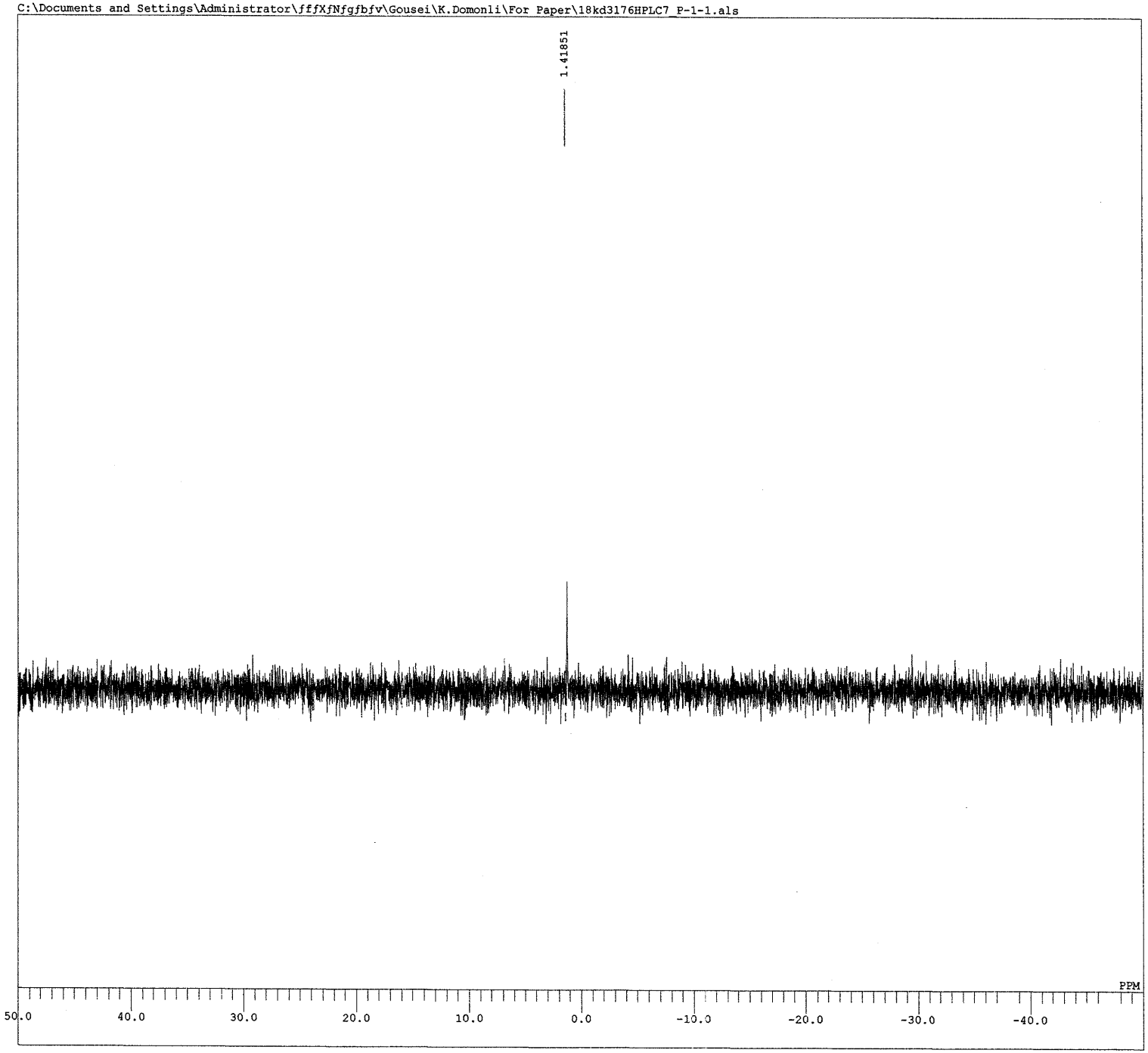
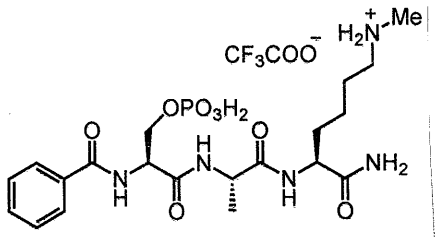
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3176HPLC7_P-1-1.als




```
DFILE  18kd3176HPLC7_P-1-1.als
COMNT
DATIM  03-10-2018 21:53:46
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            77
ACQTM         0.4089 sec
PD            2.0000 sec
PW1             4.80 usec
IRNUC  1H
CTEMP           20.2 c
SLVNT  CD3OD
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             56
```



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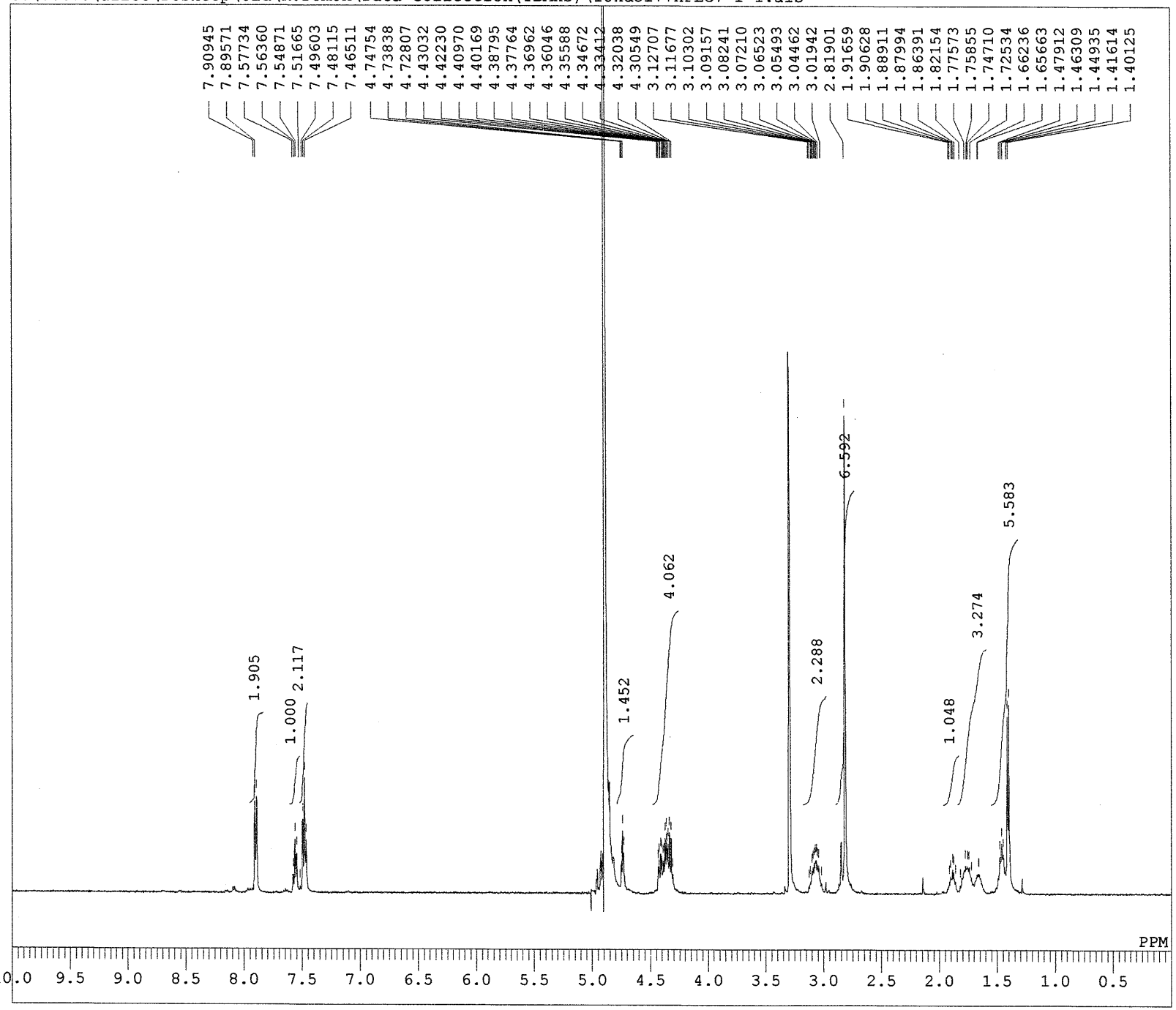
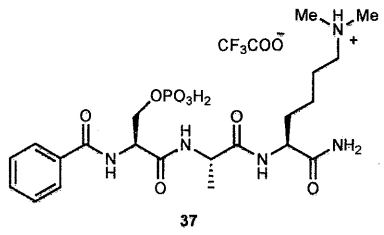
C:\Users\alice\Desktop\Old\K.Domon\Data collection(TBAHS)\18kd3177HPLC7-1-1.als



DFILE	18kd3177HPLC7-1-1.als
COMNT	
DATIM	2018-10-01 04:25:33
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	500.16 MHz
OBSET	2.41 KHz
OBFIN	6.01 Hz
POINT	13107
FREQU	7507.51 Hz
SCANS	5
ACQTM	1.7459 sec
PD	5.0000 sec
PW1	5.55 usec
IRNUC	1H
CTEMP	21.7 c
SLVNT	CD3OD
EXREF	3.30 ppm
BF	0.12 Hz
RGAIN	30



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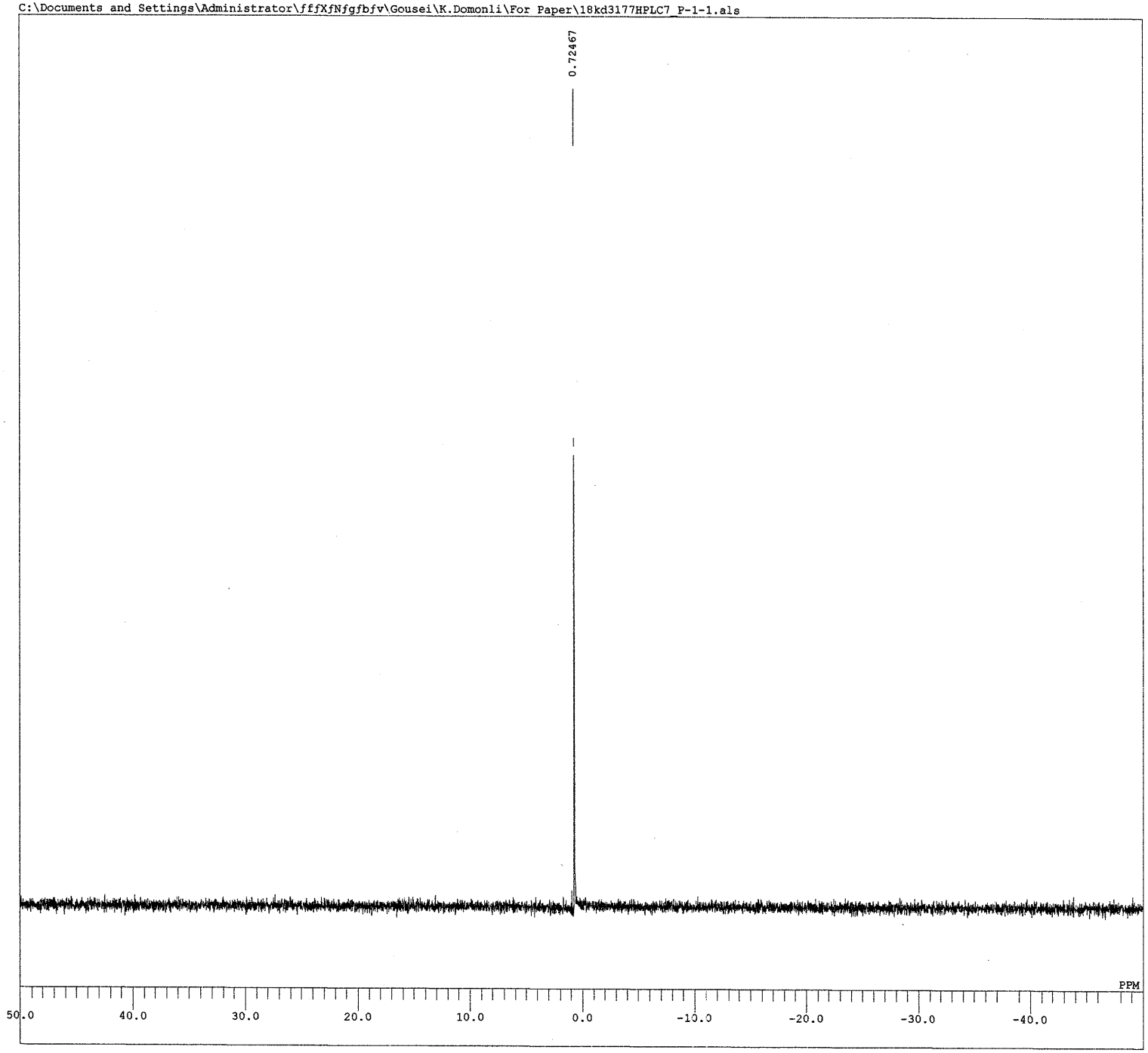
C:\Documents and Settings\Administrator\ffXfNfgfbfv\Gousei\K.Domonli\For Paper\18kd3177HPLC7_P-1-1.als

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DFILE  18kd3177HPLC7_P-1-1.als
COMNT
DATIM  03-10-2018 22:00:37
OBNUC  31P
EXMOD  carbon.jxp
OBFRQ        158.59 MHz
OBSET          7.99 KHz
OBFIN          9.23 Hz
POINT         26214
FREQU      64102.56 Hz
SCANS            84
ACQTM        0.4089 sec
PD           2.0000 sec
PW1            4.80 usec
IRNUC  1H
CTEMP          20.3 c
SLVNT  CD3OD
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            56
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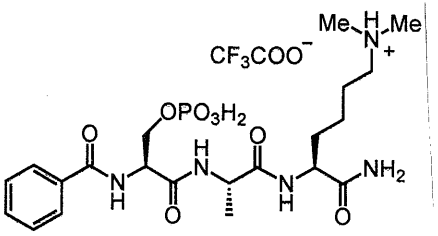

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