Supplementary Data

The synthesis, antiviral, cytostatic and cytotoxic evaluation of a new series of acyclonucleotide analogues with a 1,2,3-triazole linker

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1. General information

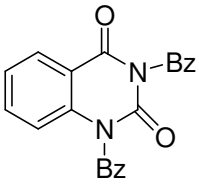
^{1}H NMR were taken in $CDCl_3$, CD_3OD or D_2O on the following spectrometers: Varian Mercury-300 and Bruker Avance III (600 MHz) with TMS as an internal standard; chemical shifts δ in ppm with respect to TMS; coupling constants *J* in Hz. ^{13}C NMR spectra were recorded for $CDCl_3$, CD_3OD or DMSO-d_6 solutions on a Varian Mercury-300 and Bruker Avance III (600 MHz) spectrometer at 75.5 and 150.5 MHz, respectively. ^{31}P NMR spectra were taken in $CDCl_3$, CD_3OD or D_2O on Varian Mercury-300 at 121.5 MHz.

IR spectral data were measured on an Infinity MI-60 FT-IR spectrometer. Melting points were determined on a Boetius apparatus and are uncorrected. Elemental analyses were performed by the Microanalytical Laboratory of this Faculty on a Perkin Elmer PE 2400 CHNS analyzer.

The following adsorbents were used: column chromatography, Merck silica gel 60 (70-230 mesh); analytical TLC, Merck TLC plastic sheets silica gel 60 F_{254}. TLC plates were developed in chloroform–methanol solvent systems. Visualisation of spots was effected with iodine vapours. All solvents were purified by methods described in the literature.

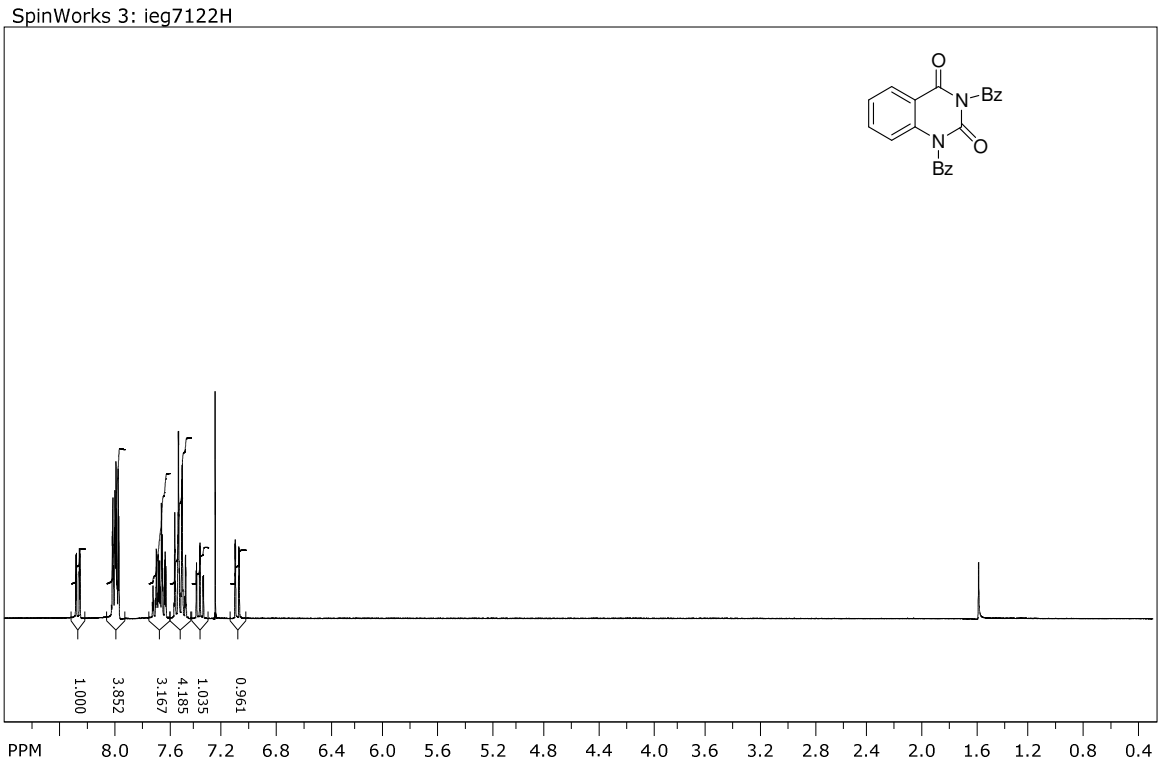
All microwave irradiation experiments were carried out in microwave reactor Plazmartonika RM 800. The reaction carried out in 50 mL glass vial.

2. Characterization of intemediates and representative compound



1,3-Dibenzoylquinazoline-2,4-dione **28**. White powder; m.p.: 159–160°C; IR (KBr): ν = 3040 1753, 1723; 1674, 1605, 1472, 974; 866; 753, 688 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.28 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H, H5); 8.02–7.98 (m, 4H, 4×*o*-CH); 7.73–7.63 (m, 3H, 2×*p*-CH, H7); 7.56–7.48 (m, 4H, 4×*m*-CH); 7.36 (dt, *J* = 7.9 Hz, *J* = 0.7 Hz, 1H, H6); 7.10 (d, *J* = 8.4 Hz, 1H, H8); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 169.2; 167.8; 160.9; 147.9; 138.6; 136.1; 135.7; 135.3; 131.8; 131.4; 130.6; 130.5; 129.5; 129.3; 129.1; 124.8; 115.2; 114.9; Anal. Calcd. for $C_{22}H_{14}N_2O_4$: C, 71.35; H, 3.81; N, 7.56. Found: C, 71.49; H, 3.76; N, 7.44.

^{1}H NMR



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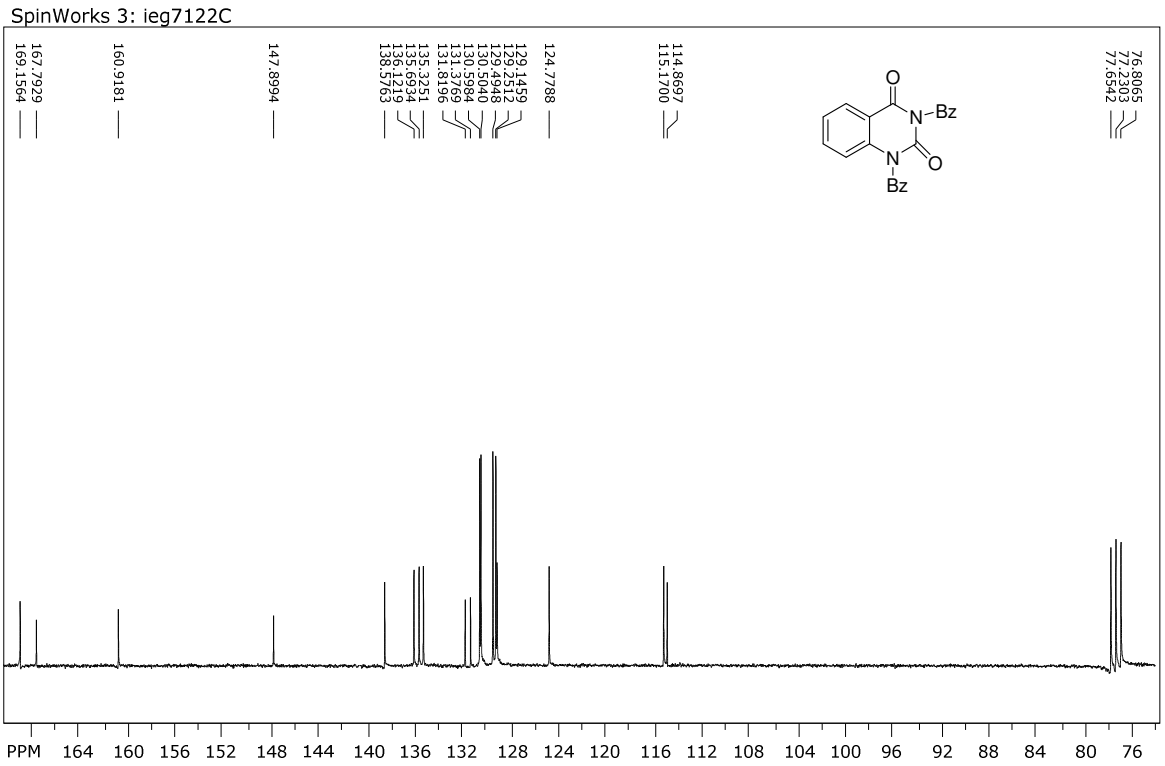
^{13}C NMR



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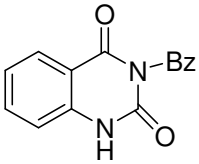
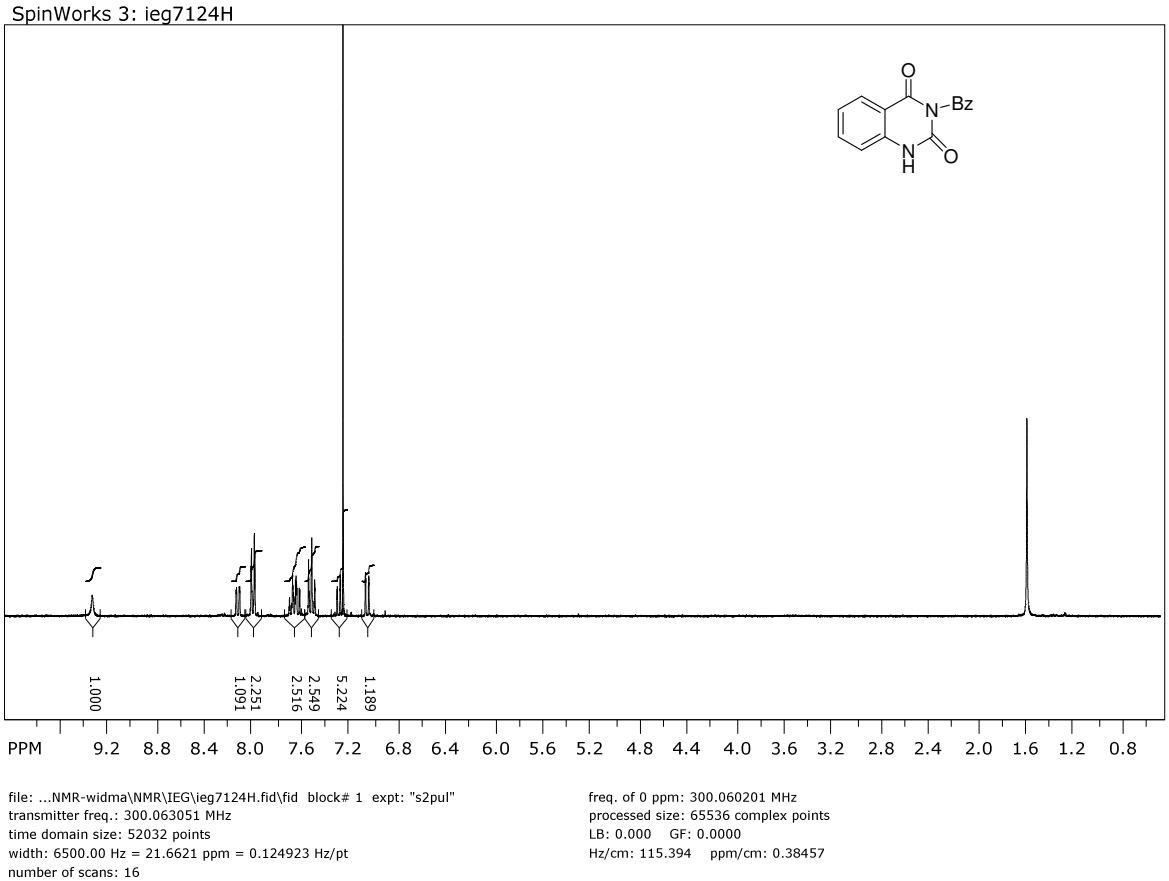


N^3-Benzoylquinazoline-2,4-dione **29**. White needles; m.p.: 209–211°C; IR (KBr): ν = 3436, 3063, 2937, 1753, 1707, 1668, 1400, 760, 687 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 9.34 (brs, 1H, NH); 8.13 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H); 8.03–7.99 (m, 2H, 2×*o*-CH); 7.71–7.62 (m, 2H); 7.55–7.49 (m, 2H); 7.29 (dd, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H); 7.31 (ddd, *J* = 8.2 Hz, *J* = 0.9 Hz, *J* = 0.5 Hz, 1H); ^{13}C NMR (151 MHz, DMSO-d_6): δ = 170.3; 162.3; 149.3; 140.9; 136.4; 135.9; 132.0; 130.9; 129.9; 127.7; 123.6; 116.4; 114.3; Anal. Calcd. for $C_{15}H_{10}N_2O_3$: C, 67.67; H, 3.79; N, 10.52. Found: C, 67.48; H, 3.91; N, 10.45.

^1H NMR



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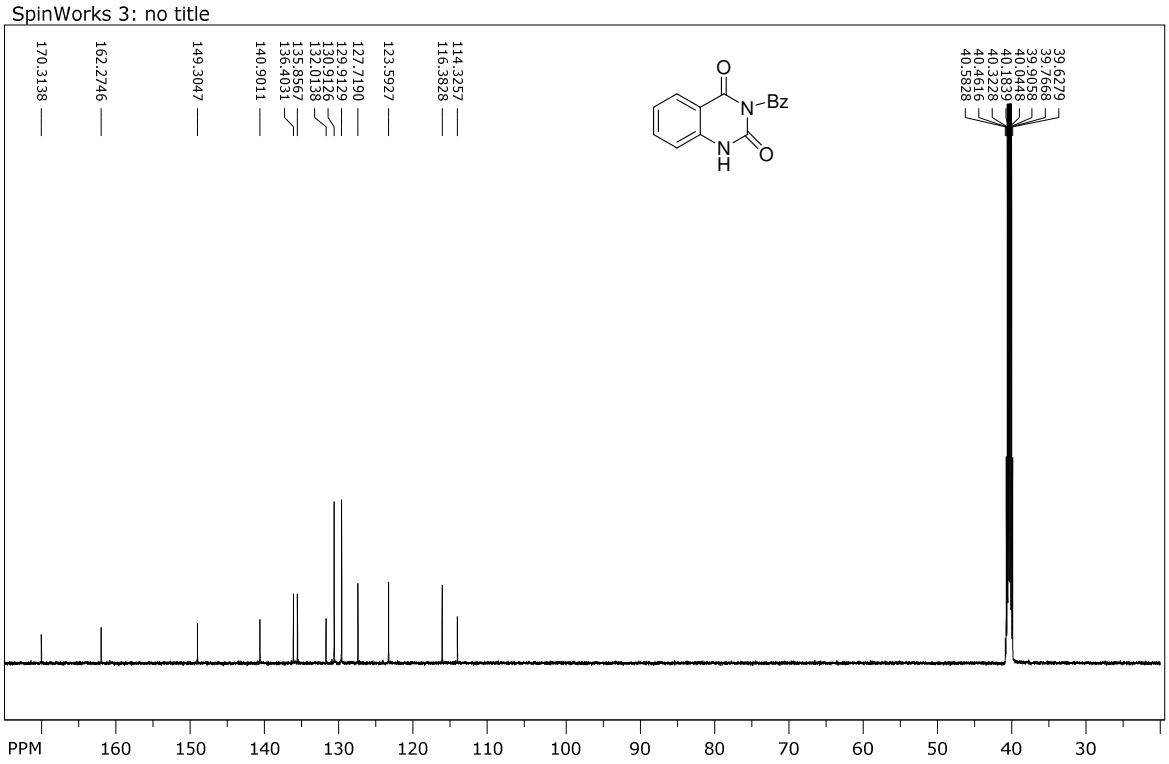
^{13}C NMR



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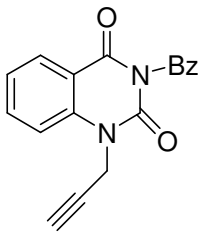
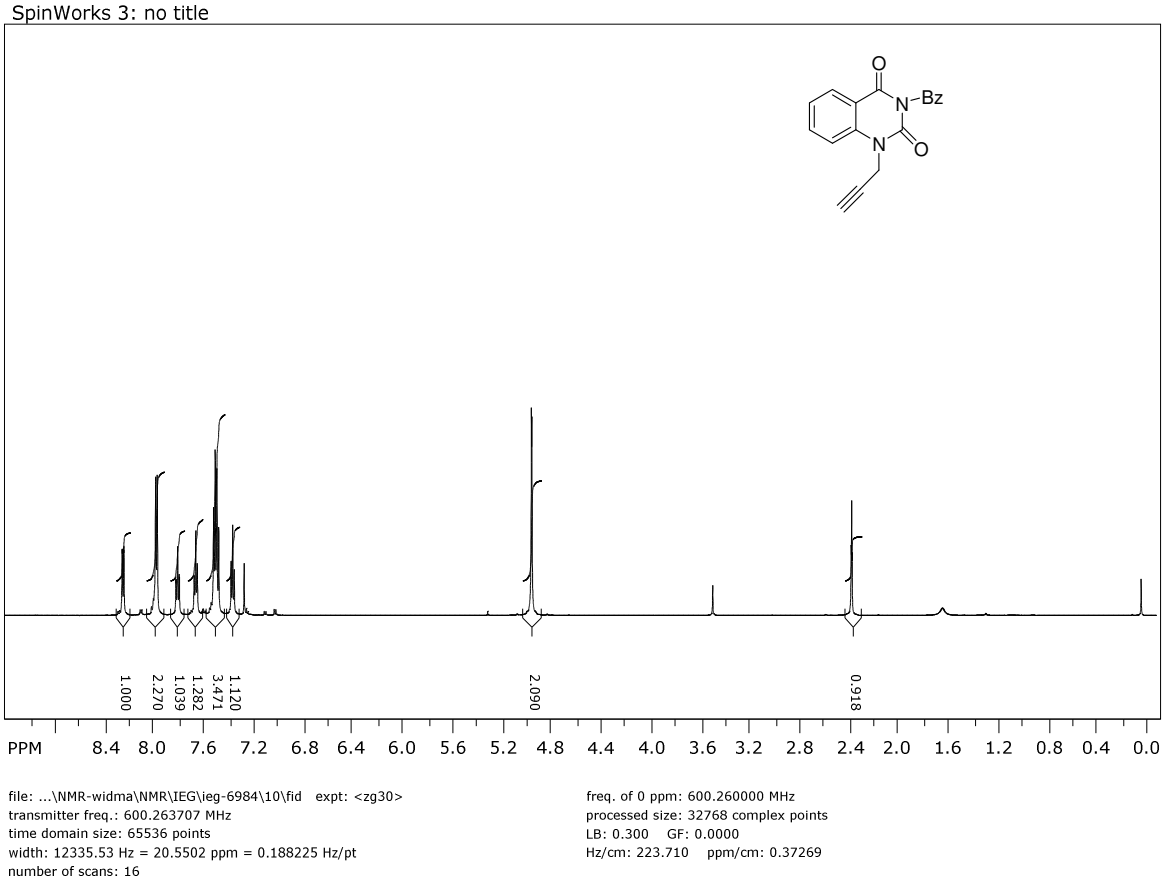


N^3-Benzoyl-N^1-propargylquinazoline-2,4-dione **19e**. White powder; m.p.: 180–182°C; IR (KBr): ν = 3256, 3002, 2925, 1751, 1697, 1659, 1482, 756, 684 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.26 (dd, *J* = 7.9 Hz, *J* = 1.3 Hz, 1H, H5); 8.12–7.99 (m, 2H, 2×*o*-CH); 7.83 (dt, *J* = 7.3 Hz, *J* = 1.4 Hz, 1H, H7); 7.69–7.67 (m, 1H, *p*-CH); 7.54–7.50 (m, 3H, 2×*m*-CH, H8); 7.31 (brt, *J* = 7.6 Hz, 1H); 4.96 (d, *J* = 2.5 Hz, 2H, CH≡CCH_2); 3.74 (t, *J* = 2.5 Hz, 1H, C*H*≡CCH_2); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 168.4 (s, C=O); 160.9 (s, C=O); 148.8 (s, C=O); 139.6; 136.1; 135.1; 131.7; 130.5; 129.2; 129.2; 123.9; 115.8; 114.7; 73.8; 32.8; Anal. Calcd. for $C_{18}H_{12}N_2O_3$: C, 71.05; H, 3.97; N, 9.21. Found: C, 70.92; H, 4.05; N, 9.14.

^1H NMR



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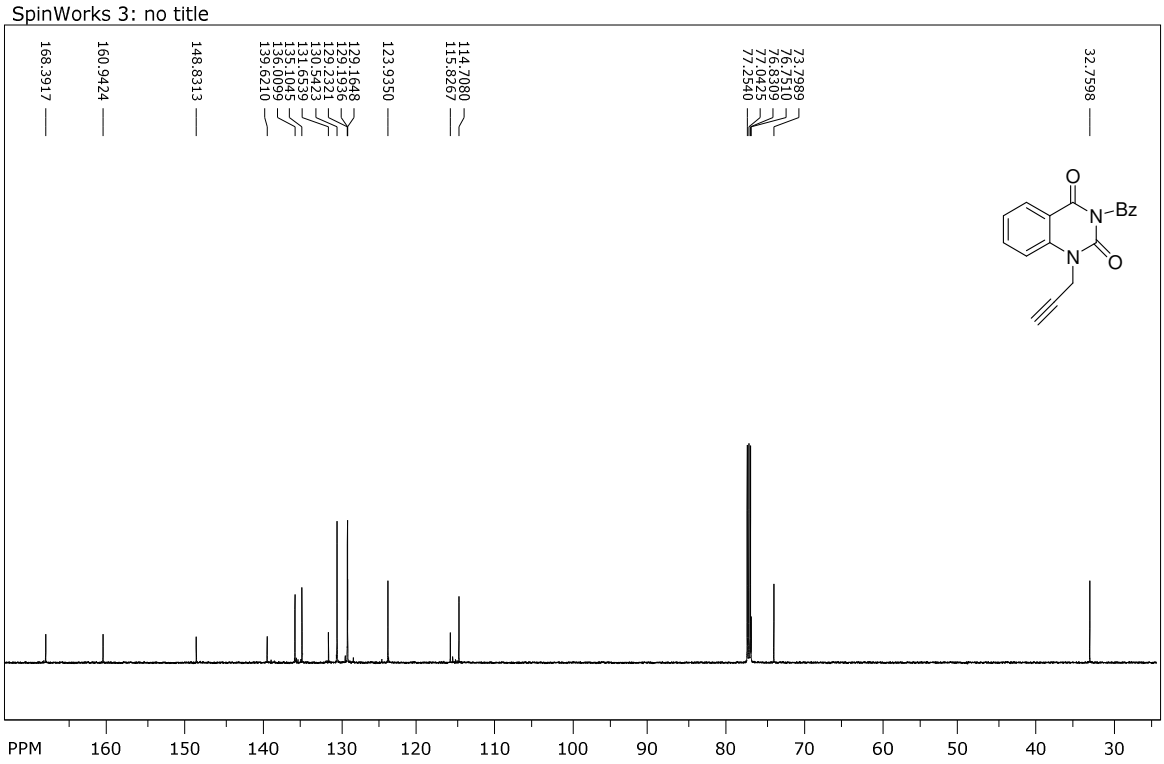
^{13}C NMR



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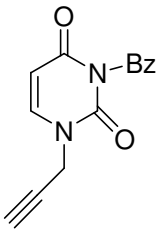
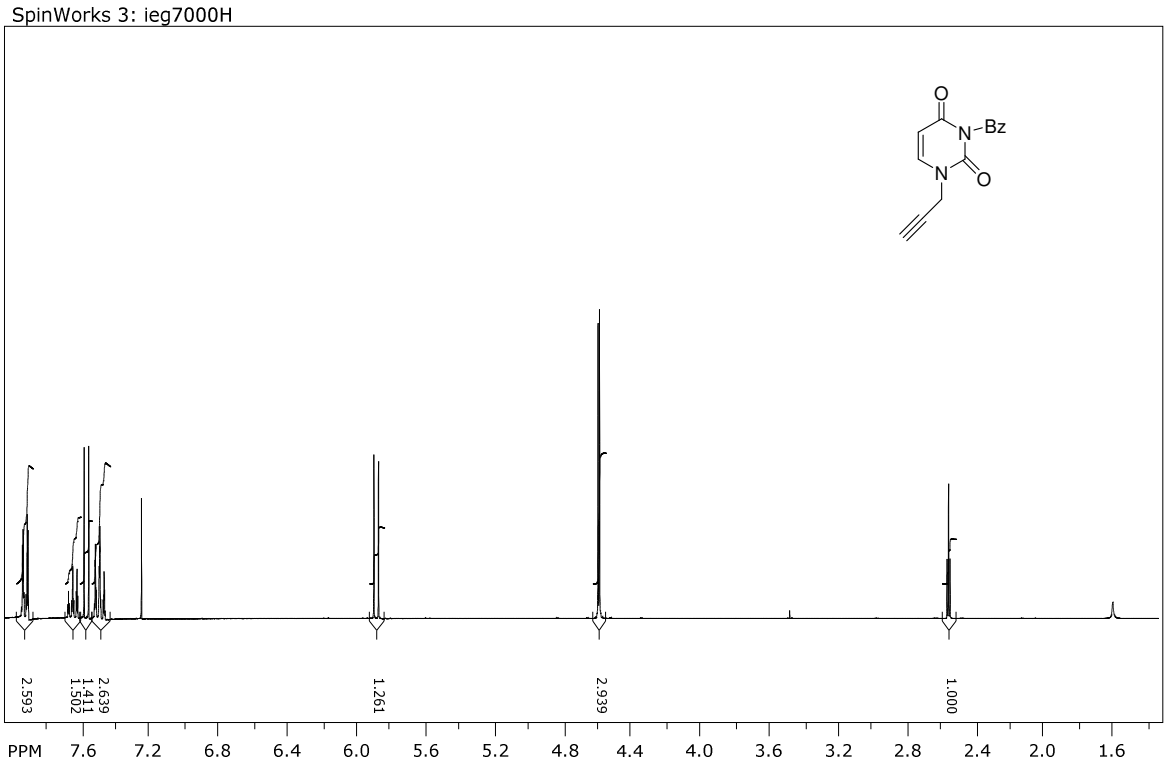


N^3-Benzoyl-N^1-propargyluracil **19m**. White solid, m.p.: 139–140°C; ^{1}H NMR (300 MHz, $CDCl_3$): 7.95–7.92 (m, 2H, 2×*o*-CH); 7.69–7.63 (m, 1H, *p*-CH); 7.58 (d, *J* = 8.1 Hz, 1H, *H*C=CH); 7.55–7.48 (m, 2H, *m*-CH); 5.89 (d, *J* = 8.1 Hz, 1H, *H*C=CH); 4.59 (d, *J* = 2.6 Hz, 2H, CH≡CCH_2); 2.55 (t, *J* = 2.6 Hz, 1H, C*H*≡CCH_2).

^{1}H NMR



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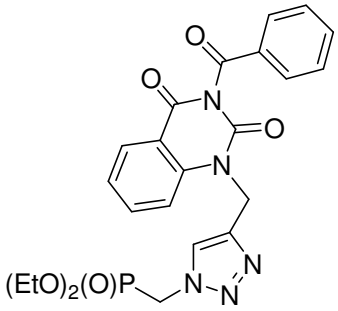
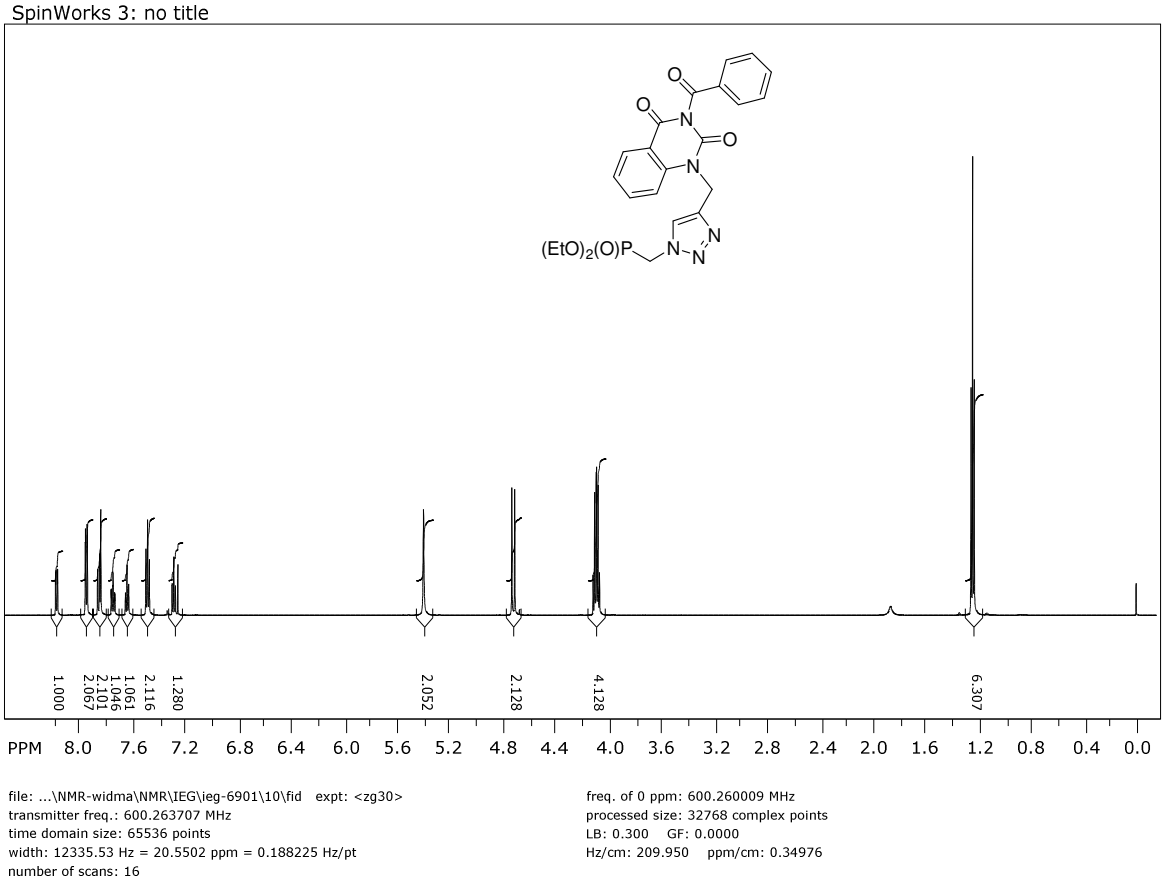
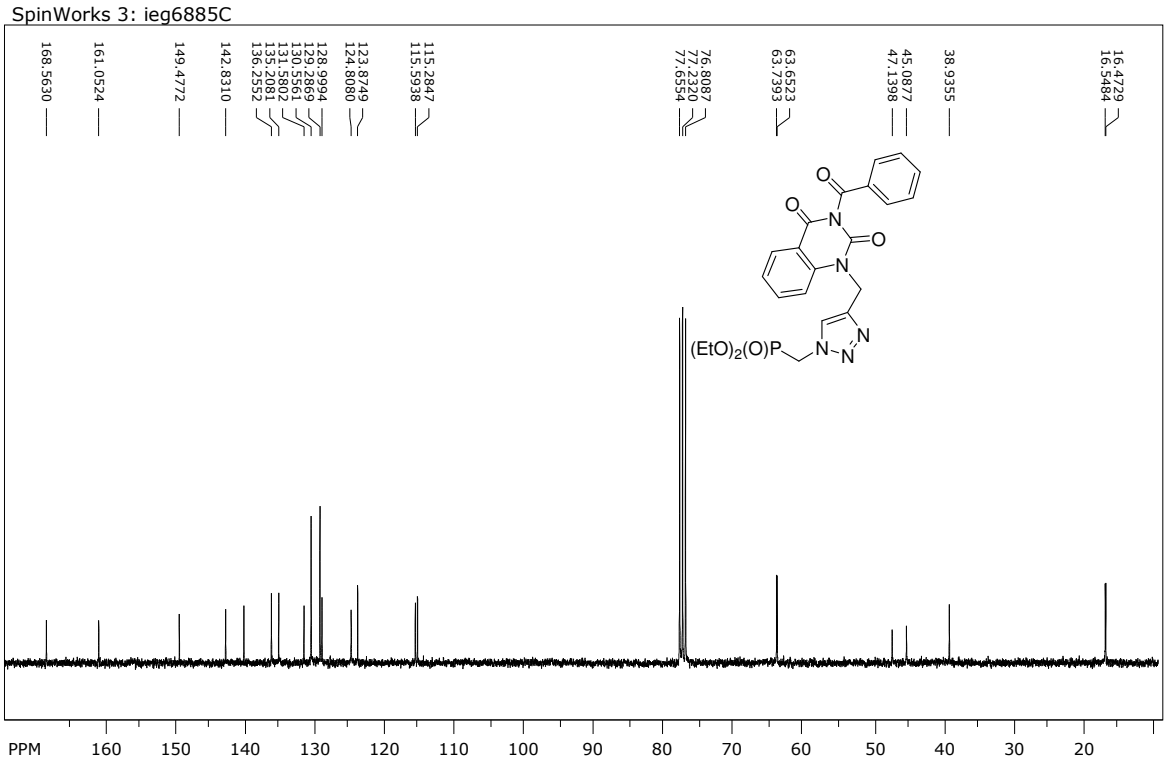


Diethyl {4-[(3-benzoyl-2,4-dioxoquinazolin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20e**. Colourless oil; IR (film): ν = 3030, 2982, 1750, 1700, 1662, 1021, 757, 671 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.20 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H, H5); 7.99–7.95 (m, 2H, 2×*o*-CH); 7.88 (brd, *J* = 8.5 Hz, 1H, H8); 7.86 (s, 1H, *H*C5′); 7.76 (ddd, *J* = 8.5 Hz, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H, H7); 7.68–7.64 (m, 1H, *p*-CH); 7.52–7.49 (m, 2H, 2×*m*-CH); 7.31 (dt, *J* = 7.9 Hz, *J* = 0.6 Hz, 1H, H6); 5.42 (s, 2H, CH_2); 4.73 (d, *J* = 13.1 Hz, 2H, PCH_2); 4.17–4.06 (m, 4H, 2×POC$H_2$$CH_3$); 1.25 (t, *J* = 7.2 Hz, 3H, $POCH_2CH_3$); 1.24 (t, *J* = 7.2 Hz, 3H, $POCH_2CH_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.6 (s, C=O); 161.1 (s, C=O); 149.5 (s, C=O); 142.8 (s, H*C*=C); 140.2; 136.2; 135.2; 131.6; 130.6; 129.4; 129.0; 124.8 (s, HC=*C*); 123.9; 115.6; 115.3; 63.7 (d, *J* = 6.5 Hz, POC); 46.1 (d, *J* = 154.9 Hz, PC); 38.9; 16.5 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.49 ppm. Anal. Calcd. for $C_{23}H_{24}N_5O_6P$: C, 55.53; H, 4.86; N, 14.08. Found: C, 55.24; H, 4.73; N, 13.86.

^1H NMR



^{13}C NMR



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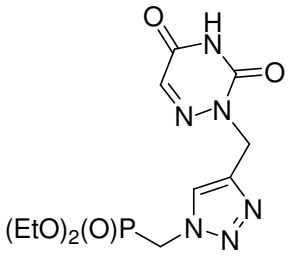
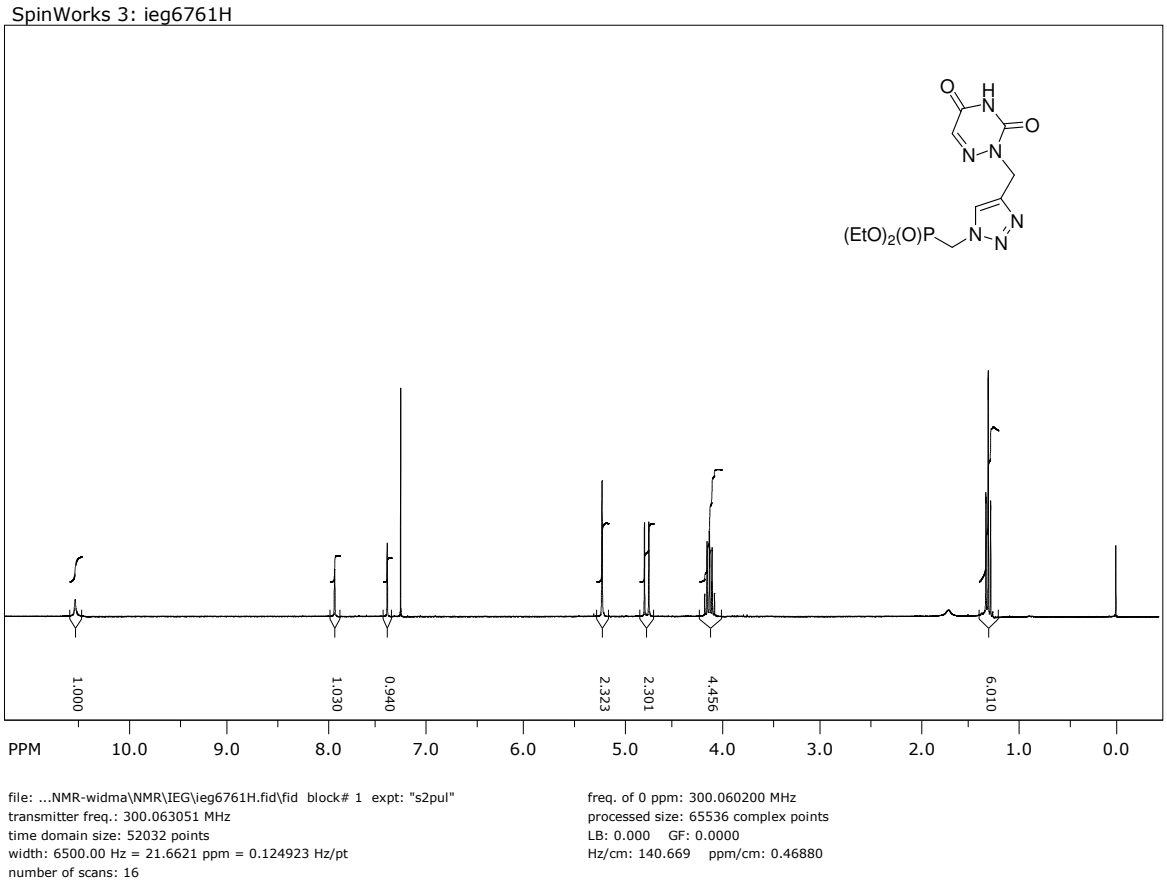


Diethyl {4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20f**. White solid; m.p.: 139–140°C; IR (KBr): ν = 3344, 2988, 1697,1668, 1235, 1025 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 10.6 (s, 1H, NH); 7.94 (s, 1H); 7.40 (s, 1H); 5.22 (s, 2H, CH_2); 4.76 (d, *J* = 13.3 Hz, 2H, PC*H*$_2$); 4.18–4.07 (m, 4H, 2×POC*H*$_2$CH$_3$); 1.30 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.29 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.9 (s, C=O); 149.1 (C=O); 142.2 (s, H*C*=C); 134.8 (s, HC=N); 125.1 (s, HC=*C*); 63.9 (d, *J* = 6.6 Hz, POC); 46.0 (d, *J* = 155.5 Hz, PC); 34.7; 16.5 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.83 ppm. Anal. Calcd. for $C_{11}H_{17}N_6O_5P$: C, 38.38; H, 4.98; N, 24.41. Found: C, 38.15; H, 5.08; N, 24.53.

^1H NMR



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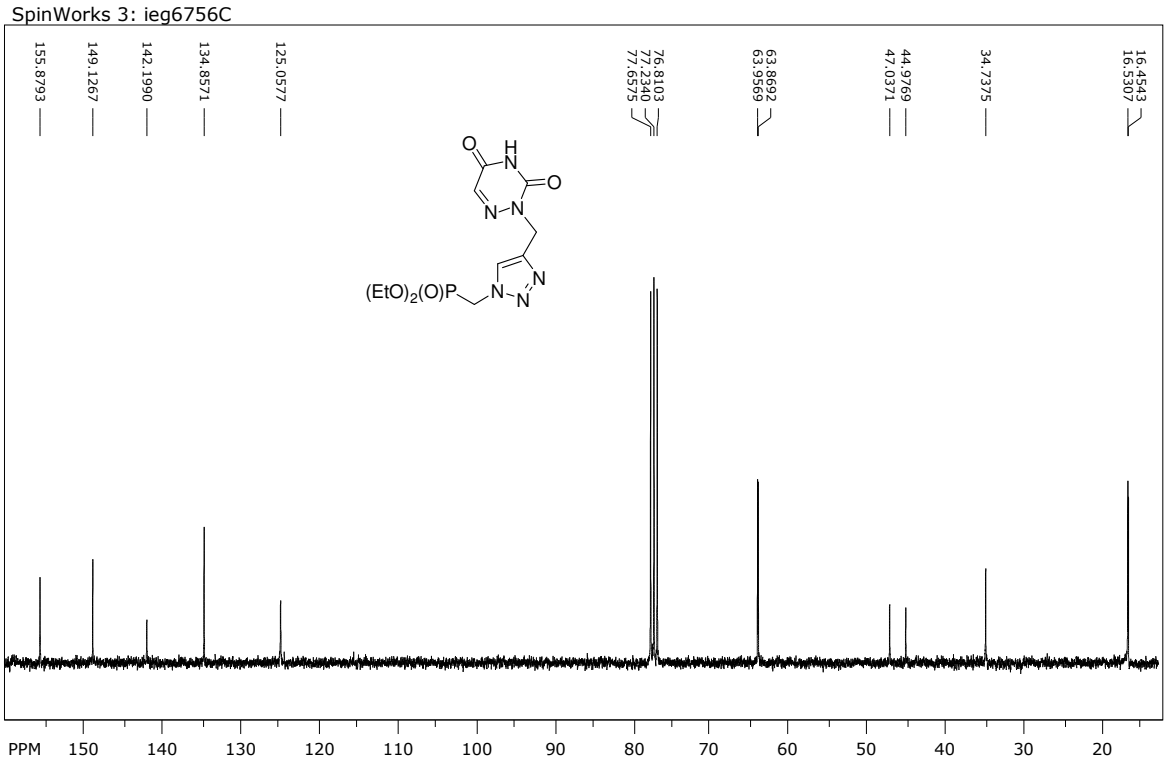
^{13}C NMR



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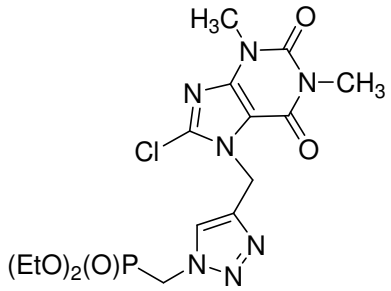
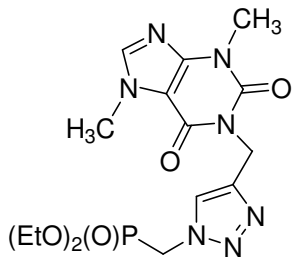
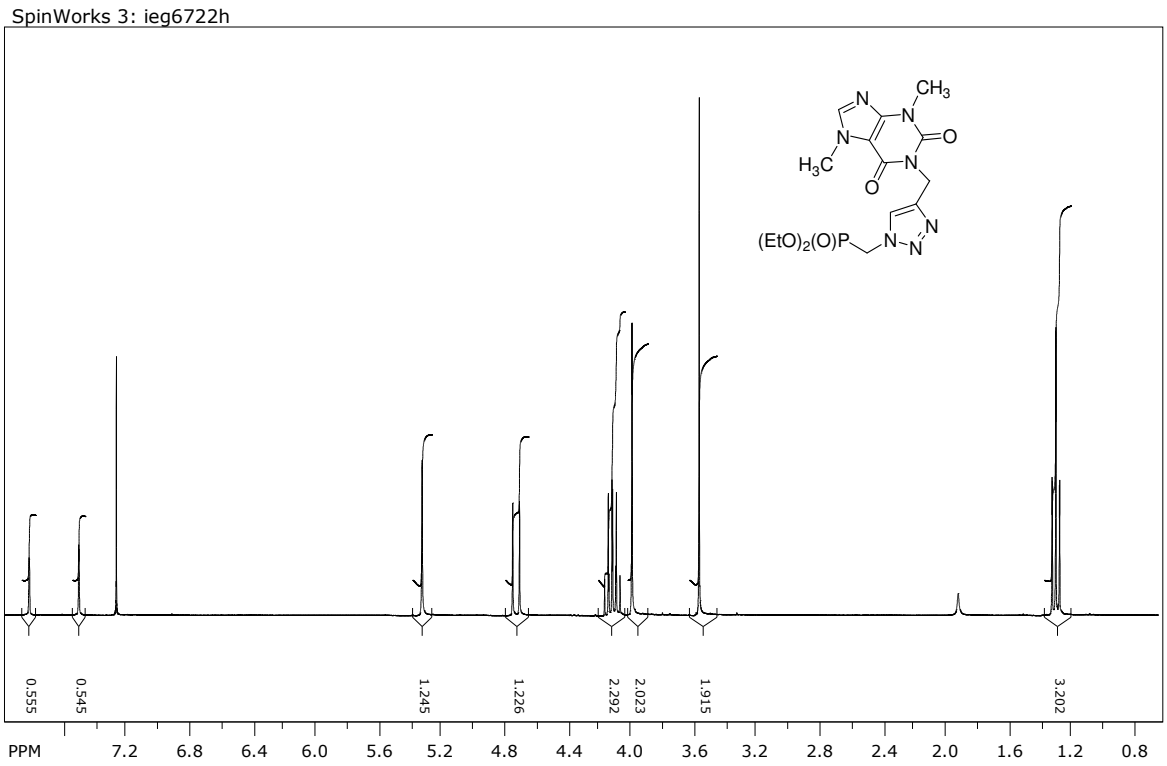


Diethyl {4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20g**. White solid; m.p.: 156–157°C; IR (KBr): ν = 2996, 2955, 1707, 1667, 1251, 1025, 757 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.98 (s, 1H, *H*C5′); 5.65 (s, 2H, CH_2); 4.74 (d, *J* = 13.1 Hz, 2H, PC*H*$_2$); 4.18–4.07 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.54 (s, 3H, CH_3); 3.40 (s, 3H, CH_3); 1.30 (t, *J* = 7.2 Hz, 3H, POCH$_2$C*H*$_3$); 1.28 (t, *J* = 7.2 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.3 (s, C=O); 151.1 (s, C=O); 147.3; 142.0; 138.9; 124.5; 107.5; 63.7 (d, *J* = 6.5 Hz, POC); 46.0 (d, *J* = 154.9 Hz, PC); 41.0; 30.0; 28.1; 16.4 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.48 ppm. Anal. Calcd. for $C_{15}H_{21}ClN_7O_5P$: C, 40.41; H, 4.75; N, 21.99. Found: C, 40.58; H, 4.55; N, 22.07.



Diethyl {4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20h**. White solid; m.p.: 139–140°C; IR (KBr): ν = 2984, 2944, 2830, 1706, 1663, 1237, 1028 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.83 (s, 1H); 7.52 (s, 1H); 5.33 (s, 2H, CH_2); 4.73 (d, *J* = 13.1 Hz, 2H, PC*H*$_2$); 4.17–4.06 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.99 (s, 3H, CH_3); 3.56 (s, 3H, CH_3); 1.29 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); 1.28 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.7 (s, C=O); 151.2 (s, C=O); 148.9; 144.0; 141.7; 124.3; 107.7; 63.6 (d, *J* = 6.6 Hz, POC); 45.9 (d, *J* = 154.9 Hz, PC); 36.1; 33.8; 29.9; 16.5 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.84 ppm. Anal. Calcd. for $C_{15}H_{22}N_7O_5P$: C, 43.80; H, 5.39; N, 23.84. Found: C, 44.02; H, 5.54; N, 23.99.

^{1}H NMR



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number of scans: 16

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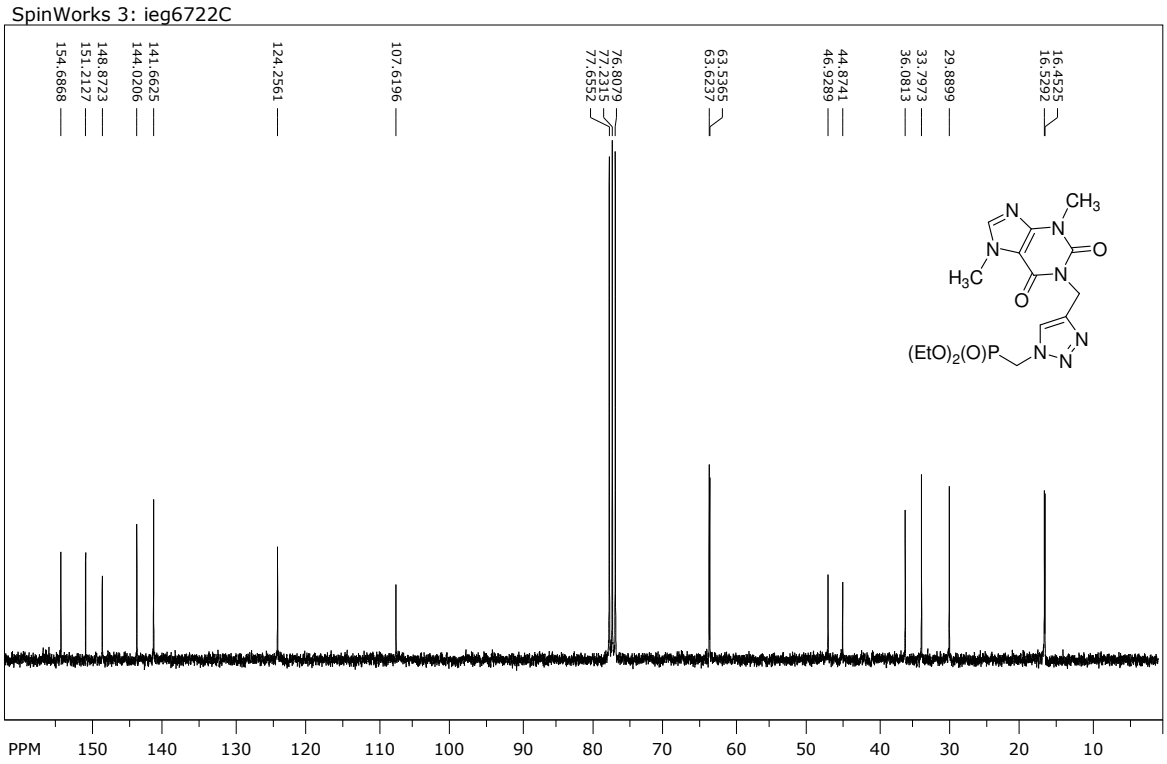
LB: 0.000 GF: 0.0000
Hz/cm: 88.262 ppm/cm: 0.29414

^{13}C NMR



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number of scans: 688

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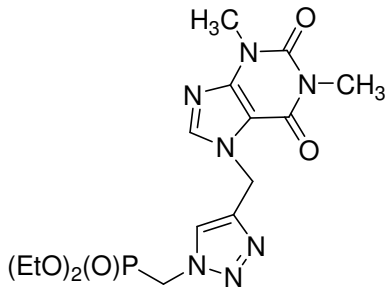
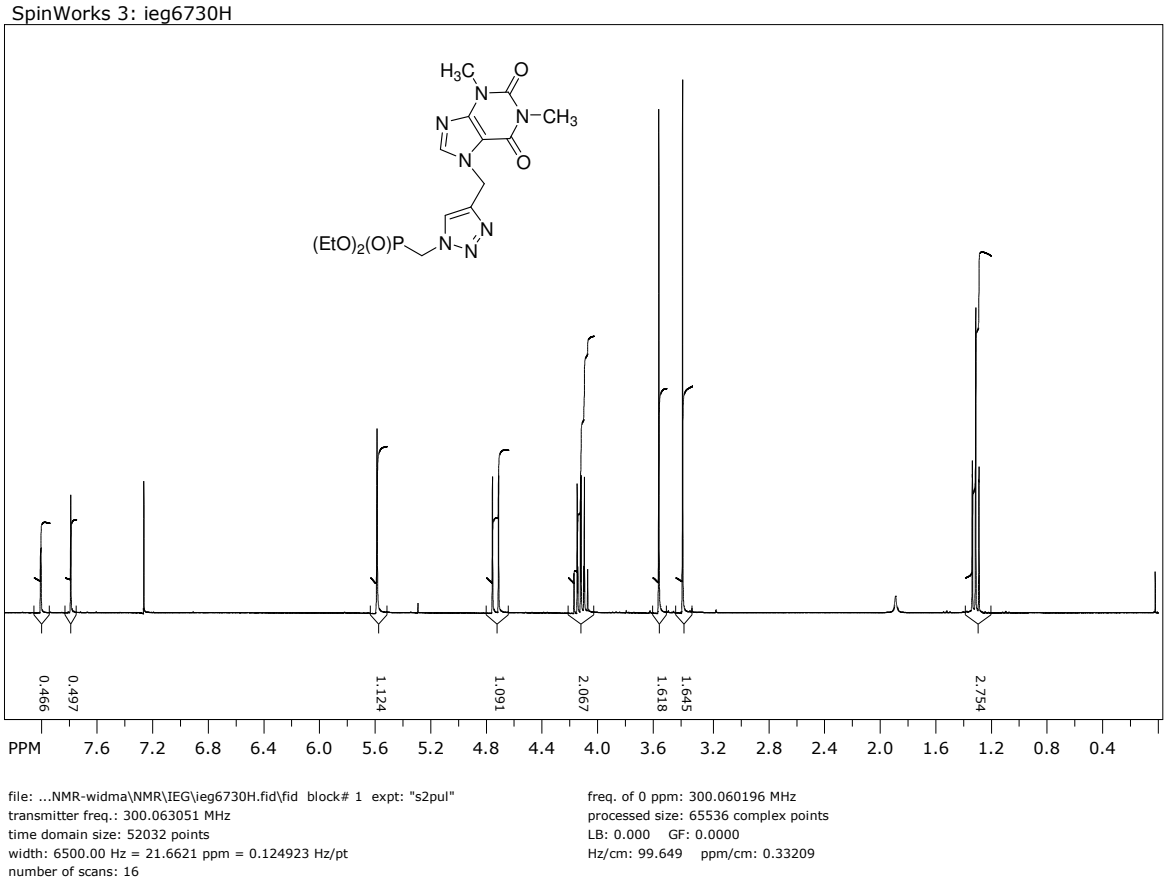
processed size: 131072 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 489.150 ppm/cm: 6.48244



Diethyl {4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20i**. White solid; m.p.: 105–108°C; IR (KBr): ν = 2994, 2945, 1705, 1660, 1244, 1026 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.02 (s, 1H); 7.80 (s, 1H); 5.60 (s, 2H, CH_2); 4.74 (d, *J* = 13.1 Hz, 2H, PC*H*$_2$); 4.18–4.08 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.57 (s, 3H, CH_3); 3.40 (s, 3H, CH_3); 1.29 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.28 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.3 (s, C=O); 151.6 (s, C=O); 149.0; 142.6; 141.3; 124.7; 106.5; 63.7 (d, *J* = 6.6 Hz, POC); 46.2 (d, *J* = 154.9 Hz, PC); 41.7; 30.0; 28.2; 16.5 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.50 ppm. Anal. Calcd. for $C_{15}H_{22}N_7O_5P$: C, 43.80; H, 5.39; N, 23.84. Found: C, 43.78; H, 5.45; N, 24.00.

^{1}HNMR



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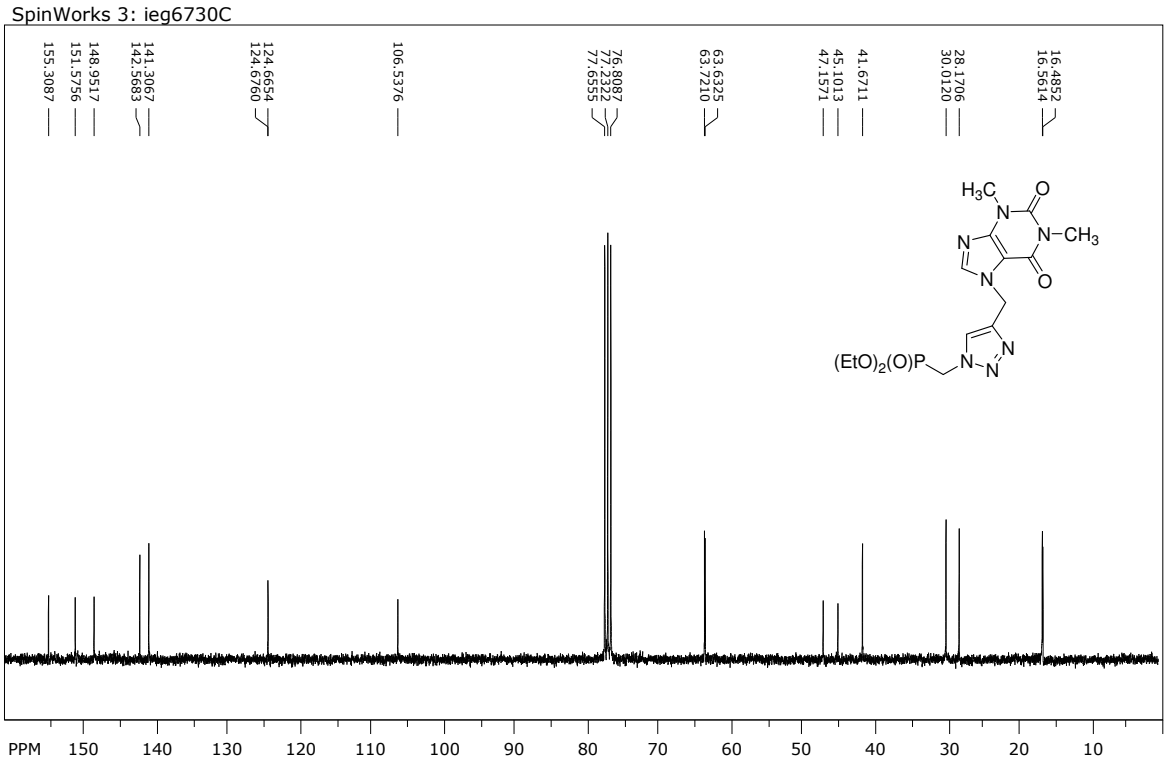
time domain size: 52032 points
width: 6500.00 Hz = 21.6621 ppm = 0.124923 Hz/pt
number of scans: 16

freq. of 0 ppm: 300.060196 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 99.649 ppm/cm: 0.33209

^{13}C NMR



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number of scans: 576

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processed size: 131072 complex points
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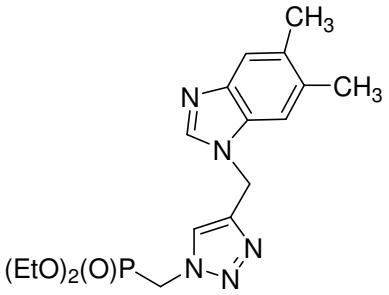
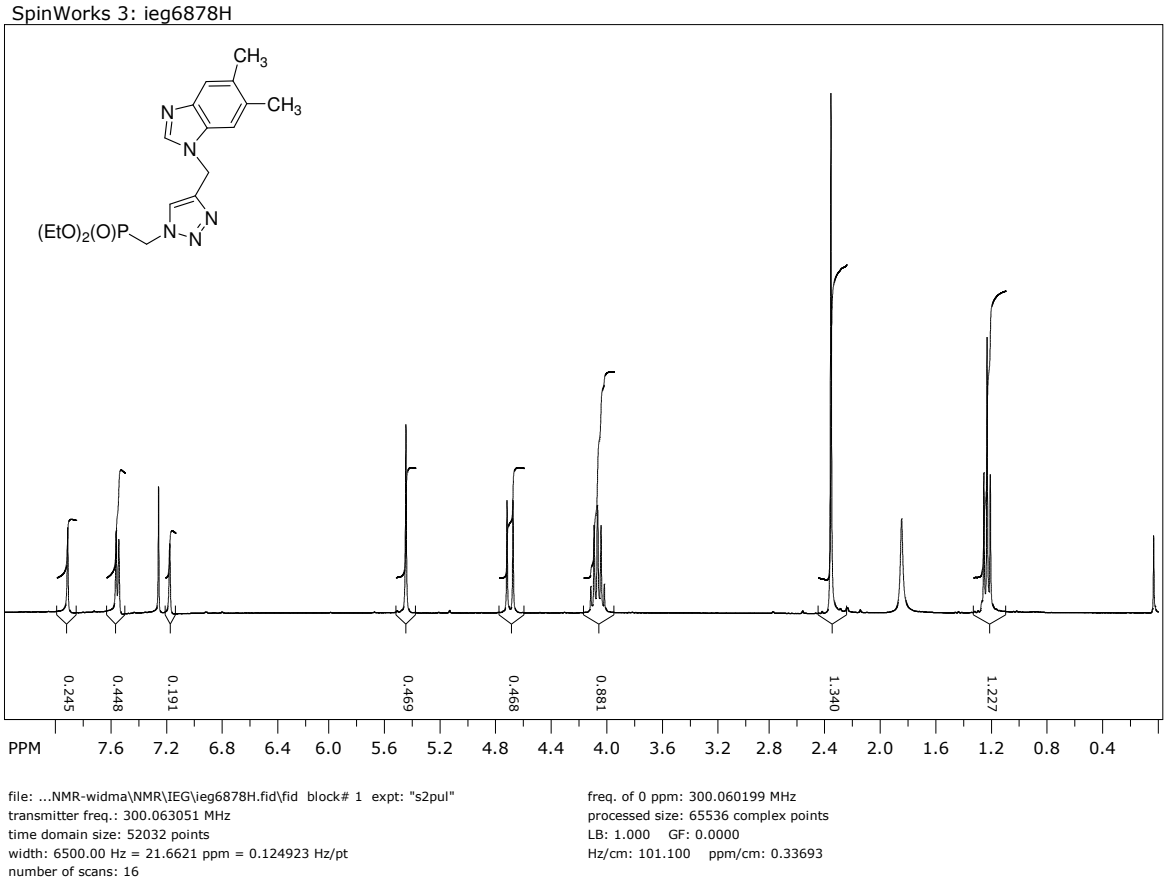
Hz/cm: 486.160 ppm/cm: 6.44282

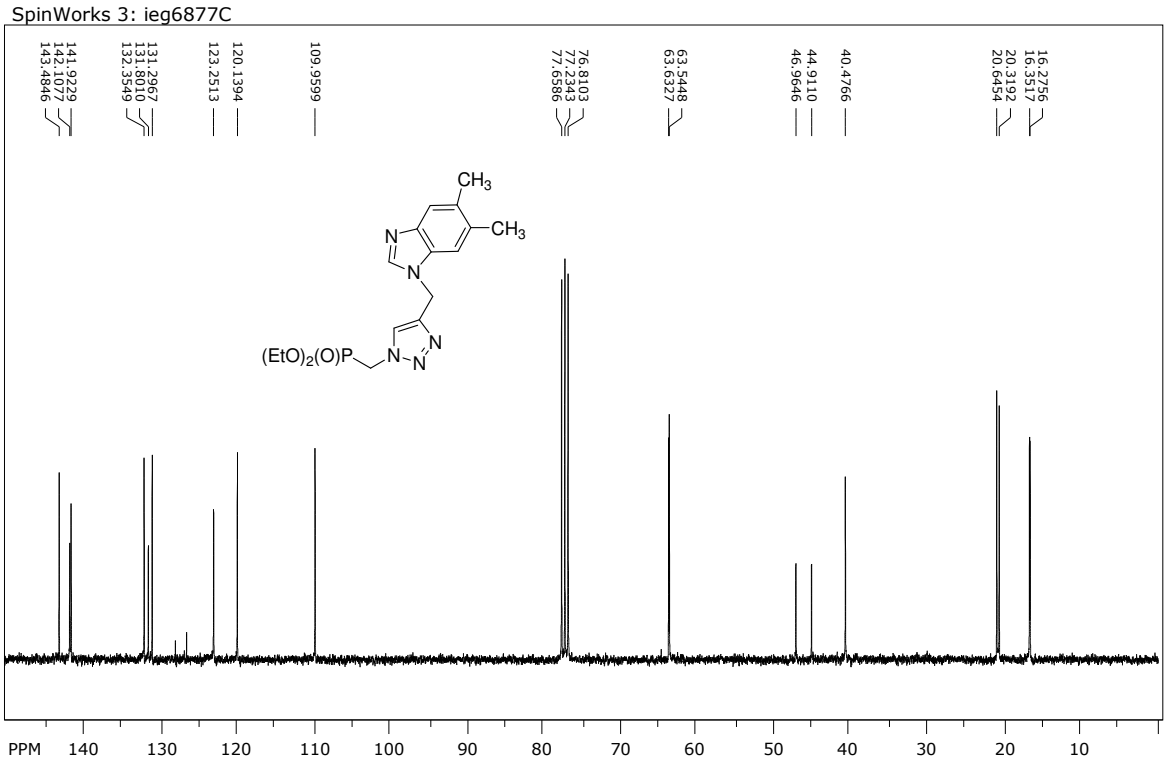


Diethyl {4-[(5,6-dimethylbenzimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20j**. White powder; m.p.: 100–102°C; IR (KBr): ν = 3004, 2960, 2945, 1025, 846, 757 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.93 (s, 1H); 7.52 (s, 1H); 7.56 (s, 1H); 7.18 (s, 1H); 5.46 (s, 2H, CH_2); 4.69 (d, *J* = 13.3 Hz, 2H, PC*H*$_2$); 4.11–4.01 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.36 (s, 6H, 2×CH_3); 1.22 (t, *J* = 7.2 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 143.5; 142.1; 141.9; 132.4; 131.8; 131.3; 123.3; 120.1; 110.0; 63.6 (d, *J* = 6.6 Hz, POC); 46.0 (d, *J* = 154.9 Hz, PC); 40.5; 20.6; 20.3; 16.3 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.52 ppm. Anal. Calcd. for $C_{17}H_{24}N_5O_3P$: C, 54.11; H, 6.41; N, 18.56. Found: C, 53.97; H, 6.38; N, 18.44.

^{1}H NMR



^{13}C NMR



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number of scans: 800

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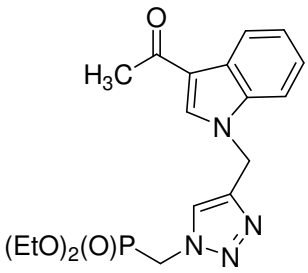
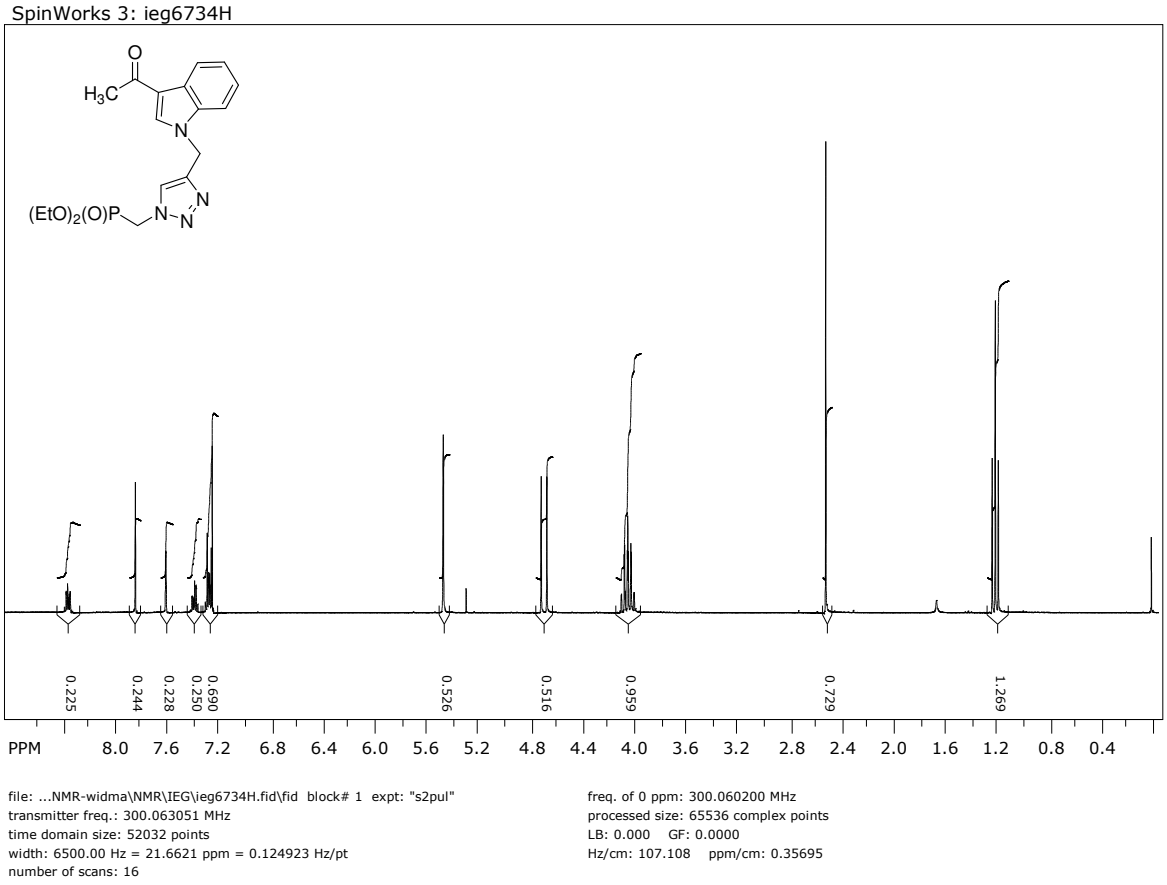
processed size: 131072 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 456.261 ppm/cm: 6.04658



Diethyl {4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20k**. White solid; m.p.: 128–129°C; IR (KBr): ν = 3004, 2960, 2945, 1025, 846, 757 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.42–8.34 (m, 1H); 7.86 (s, 1H, *H*C5′); 7.62 (s, 1H); 7.45–7.36 (m, 1H); 7.33–7.24 (m, 2H); 5.48 (s, 2H, CH_2); 4.70 (d, *J* = 13.3 Hz, 2H, PC*H*$_2$); 4.10–4.00 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.25 (s, 3H, CH_3); 1.21 (t, *J* = 6.9 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 192.9 (s, C=O); 143.6; 136.6; 134.6; 126.6; 123.7; 123.3; 123.0; 122.9; 117.9; 109.9; 63.8 (d, *J* = 6.5 Hz, POC); 46.3 (d, *J* = 155.4 Hz, PC); 42.7; 27.9 (s, CH_3); 16.5 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.51 ppm. Anal. Calcd. for $C_{18}H_{23}N_4O_4P$: C, 55.38; H, 5.94; N, 14.35. Found: C, 55.12; H, 6.09; N, 14.44.

^{1}H NMR



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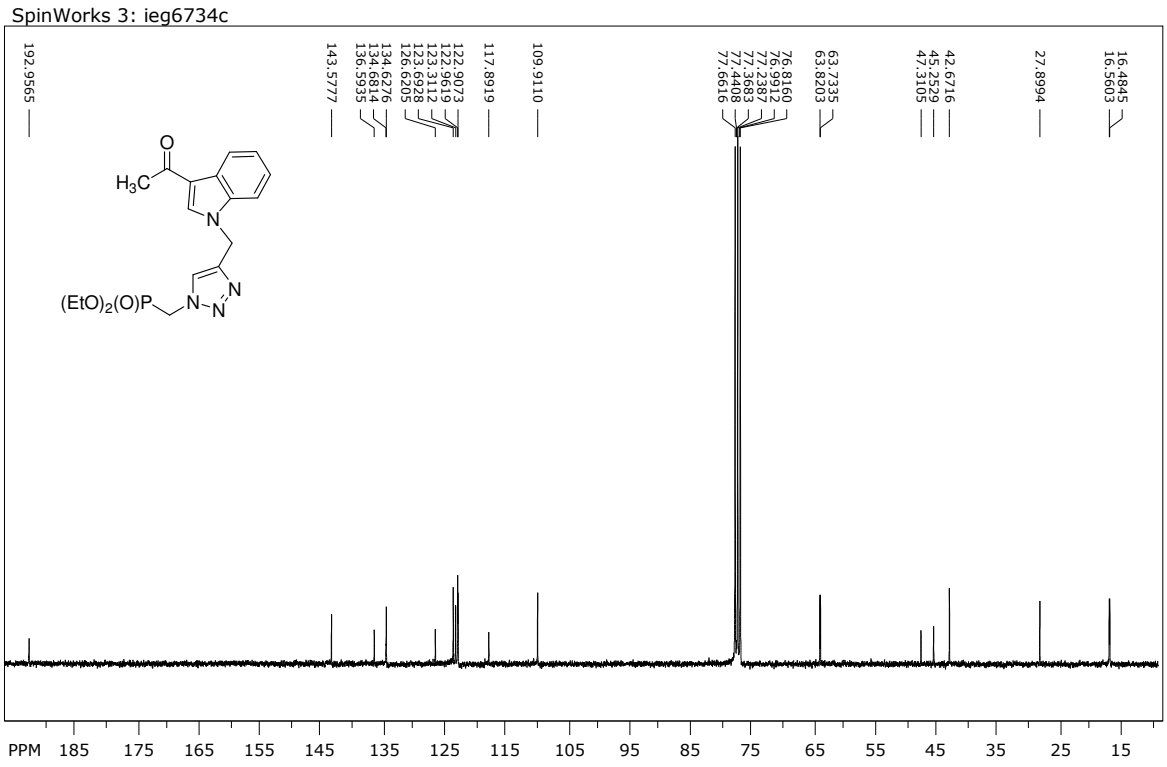
number of scans: 16

freq. of 0 ppm: 300.060200 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 107.108 ppm/cm: 0.35695

^{13}C NMR



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transmitter freq.: 75.457729 MHz
time domain size: 68096 points
width: 18761.73 Hz = 248.6389 ppm = 0.275519 Hz/pt
number of scans: 5000

freq. of 0 ppm: 75.450184 MHz
processed size: 131072 complex points
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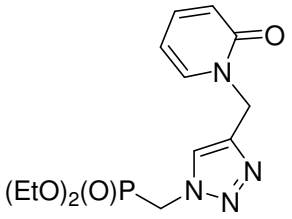
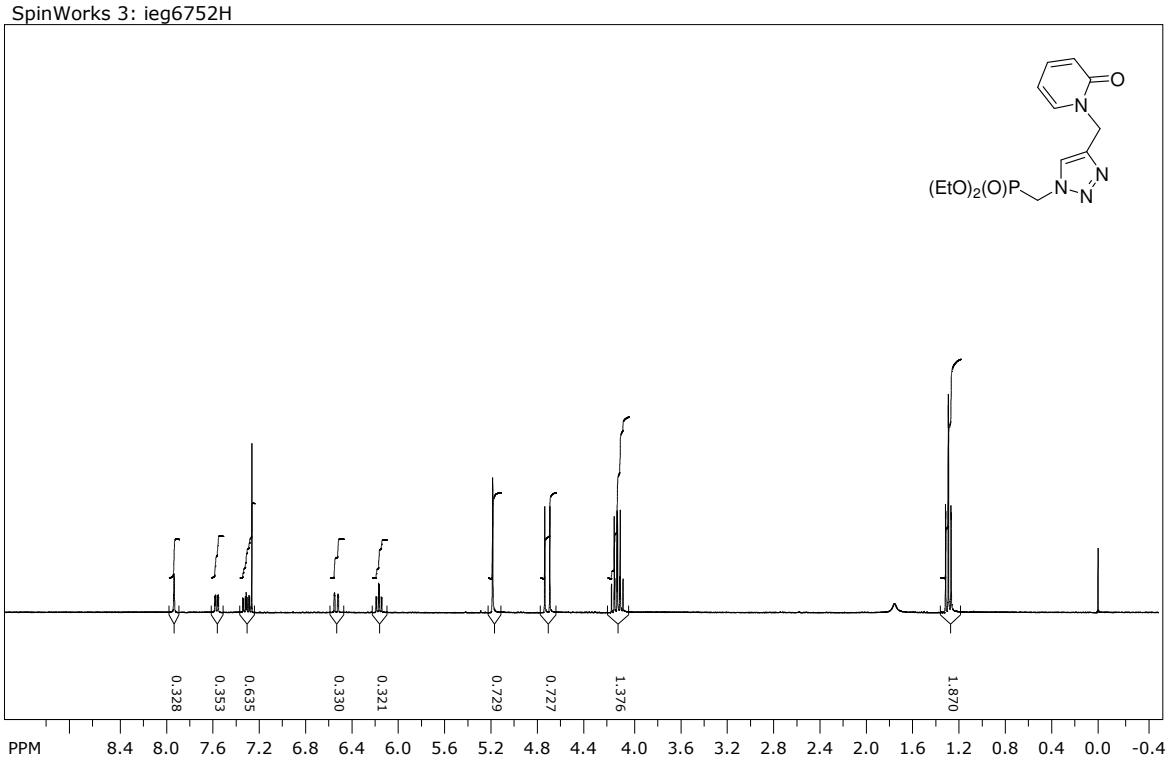
Hz/cm: 568.682 ppm/cm: 7.53643



Diethyl {4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}methylphosphonate **20l**. Brown solid; m.p.: 82–85°C; IR (KBr): ν = 3080, 2985, 2935, 1660, 1025, 978 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.93 (s, 1H); 7.56 (dd, *J* = 6.7 Hz, *J* = 1.9 Hz, 1H); 7.31 (ddd, *J* = 9.2 Hz, *J* = 6.7 Hz, *J* = 1.9 Hz, 1H); 6.59 (d, *J* = 9.2 Hz, 1H); 6.17 (dt, *J* = 6.7 Hz, *J* = 1.2 Hz, 1H); 5.20 (s, 2H, CH_2); 4.73 (d, *J* = 13.1 Hz, 2H, PCH_2); 4.18–4.07 (m, 4H, 2×POC$H_2$$CH_3$); 1.29 (t, *J* = 6.9 Hz, 3H, $POCH_2CH_3$); 1.28 (t, *J* = 6.9 Hz, 3H, $POCH_2CH_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.1 (s, C=O); 142.9 (s, H*C*=C); 139.9; 137.6; 124.9 (s, HC=*C*); 120.6; 106.4; 63.5 (d, *J* = 6.7 Hz, POC); 45.8 (d, *J* = 154.5 Hz, PC); 44.4; 16.3 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 16.62 ppm. Anal. Calcd. for $C_{13}H_{19}N_4O_4P$: C, 47.85; H, 5.87; N, 17.17. Found: C, 48.01; H, 6.00; N, 17.25.

^{1}H NMR



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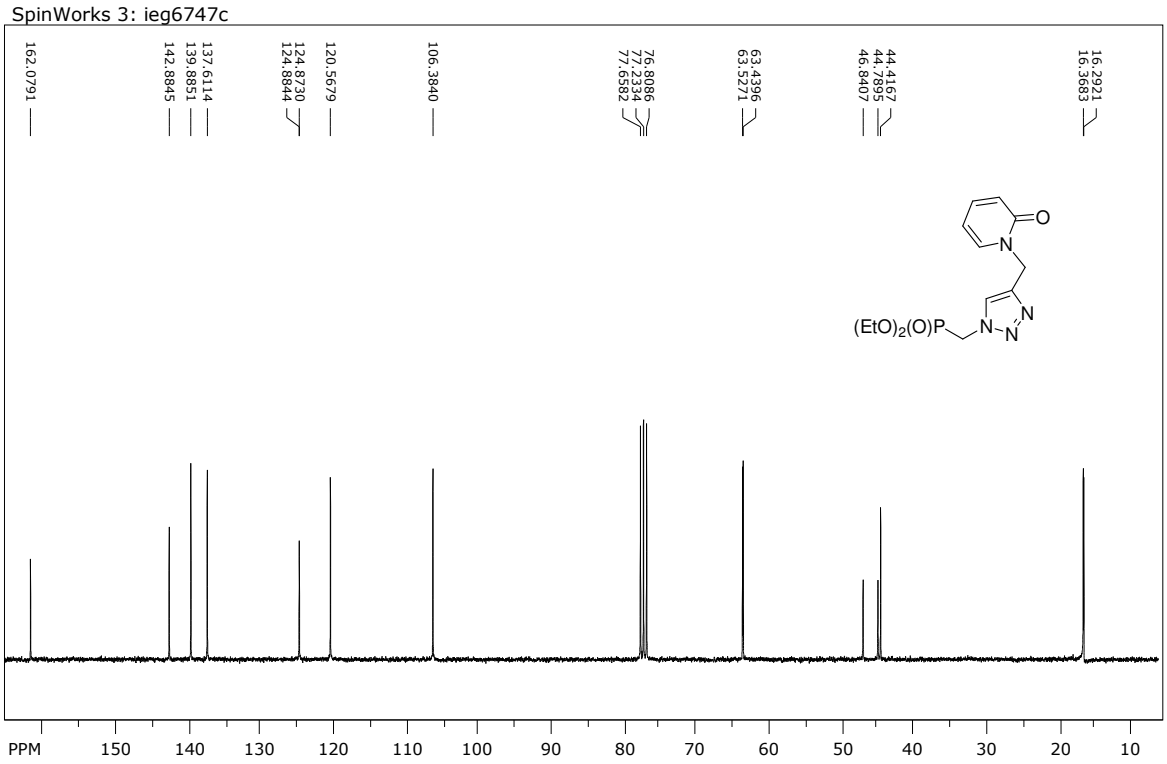
number of scans: 16

freq. of 0 ppm: 300.060200 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 118.916 ppm/cm: 0.39630

^{13}C NMR



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number of scans: 976

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processed size: 131072 complex points
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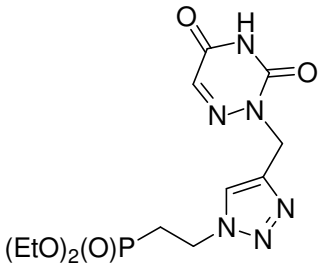
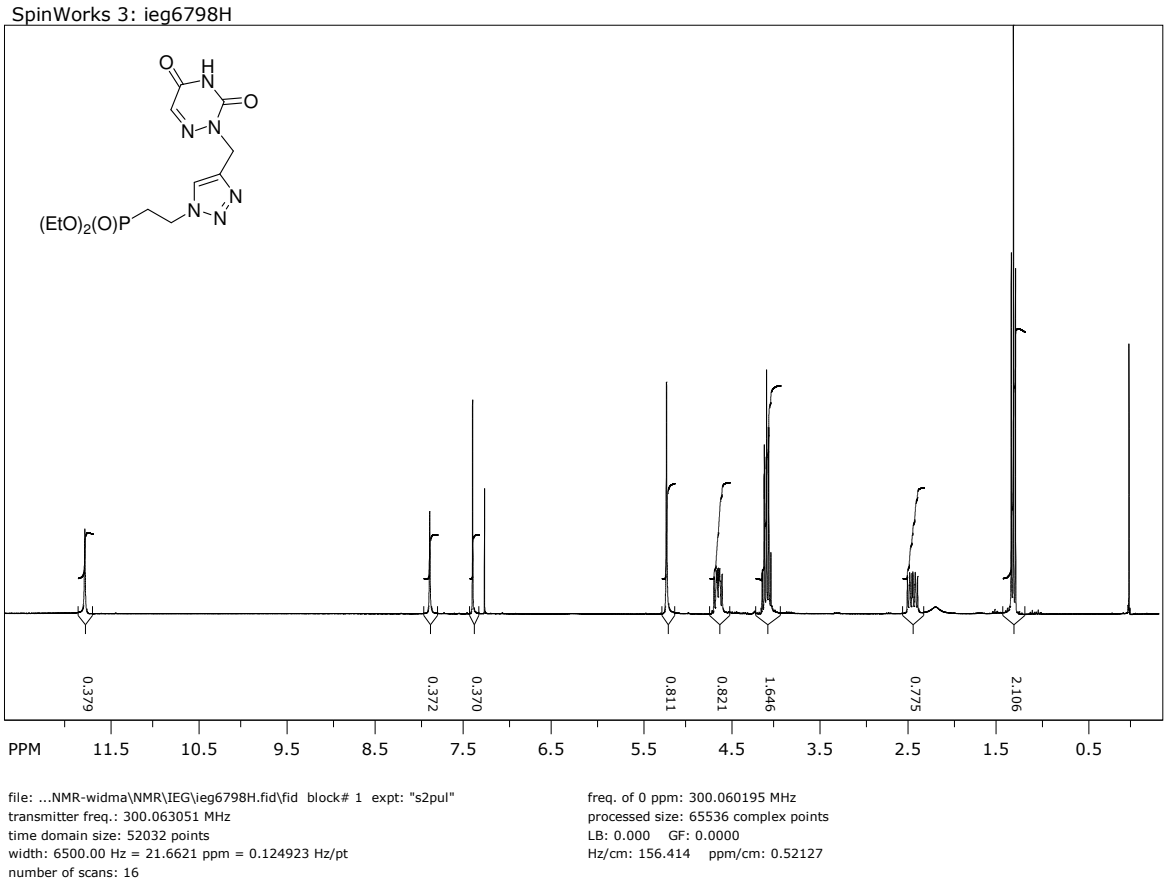
Hz/cm: 481.975 ppm/cm: 6.38734



Diethyl 2-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21f**. White solid; m.p.: 119– 121°C; IR (KBr): ν = 3301, 2999, 2985, 1688, 1220, 1045 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 11.80 (s, 1H, NH); 7.90 (s, 1H); 7.41 (s, 1H); 5.22 (s, 2H, CH_2); 4.68–4.50 (m, 2H, PCH_2); 4.16–4.04 (m, 4H, 2×POCH_2CH$_3$); 2.78–2.62 (m, 2H, PCCH_2); 1.31 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.9 (s, C=O); 149.1 (C=O); 141.6 (s, H*C*=C); 134.7 (s, HC=N); 124.4 (s, HC=*C*); 62.5 (d, *J* = 6.6 Hz, POC); 44.5; 34.6; 27.2 (d, *J* = 140.9 Hz, PC); 16.4 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 27.15 ppm. Anal. Calcd. for $C_{12}H_{19}N_6O_5P$: C, 40.23; H, 5.35; N, 23.46. Found: C, 40.06; H, 5.21; N, 23.55.

^{1}H NMR



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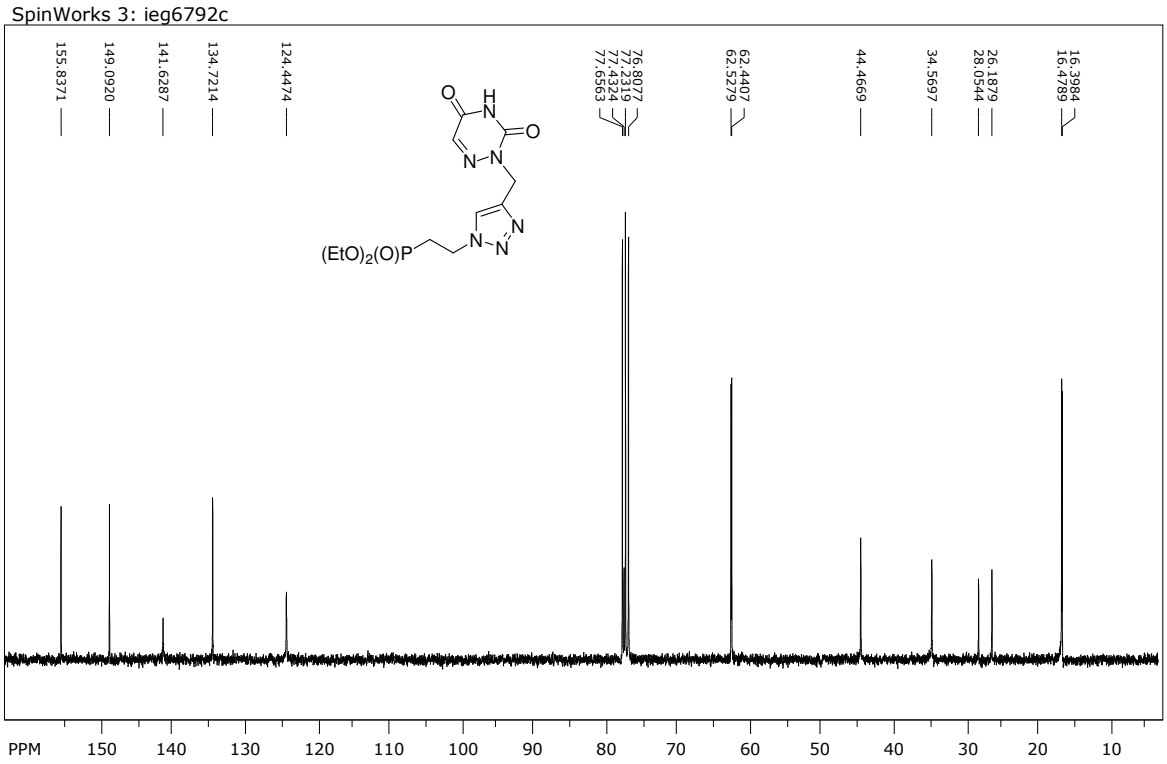
number of scans: 16

freq. of 0 ppm: 300.060195 MHz
processed size: 65536 complex points
LB: 0.000 GF: 0.0000
Hz/cm: 156.414 ppm/cm: 0.52127

^{13}C NMR



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number of scans: 608

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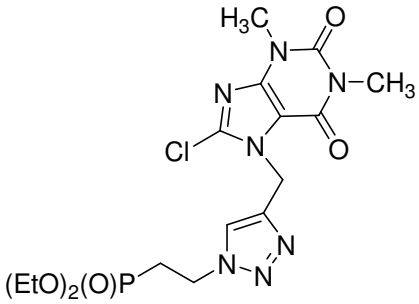
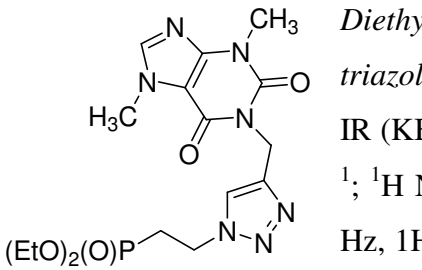
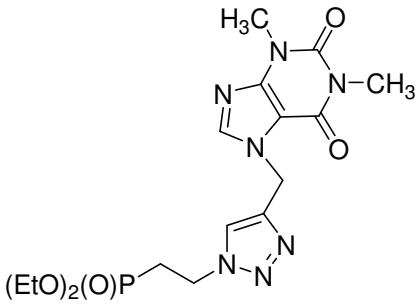


Diethyl 2-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21g**. White solid; m.p.: 101–103°C; IR (KBr): ν = 3426, 3139, 2953, 2903, 1703, 1661, 1250, 1043 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (s, 1H, *H*C5′); 5.65 (s, 2H, CH_2); 4.63–4.56 (m, 2H, PC*H*$_2$); 4.13–4.05 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.56 (s, 3H, CH_3); 3.43 (s, 3H, CH_3); 2.45–2.39 (m, 2H, PCC*H*$_2$); 1.32 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.4 (s, C=O); 151.2 (s, C=O); 147.4; 141.8; 139.0; 123.9; 107.3; 62.2 (d, *J* = 6.0 Hz, POC); 44.7; 40.9; 29.8; 28.0; 27.2 (d, *J* = 141.9 Hz, PC); 16.3 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 25.20 ppm. Anal. Calcd. for $C_{16}H_{23}ClN_7O_5P$: C, 41.79; H, 5.04; N, 21.32. Found: C, 41.85; H, 4.94; N, 21.43.

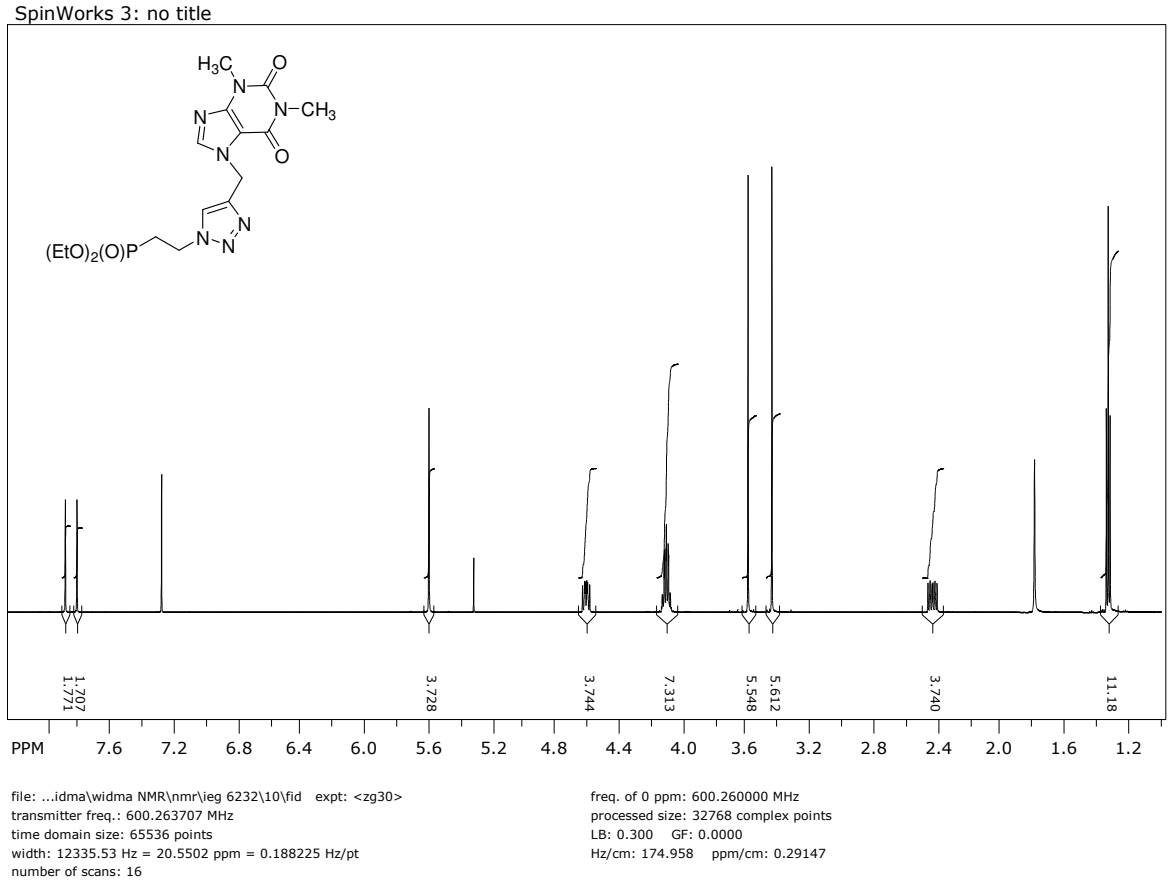


Diethyl 2-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21h**. White solid; m.p.: 100–102°C; IR (KBr): ν = 3133, 3087, 2989, 2830, 1701, 1665, 1233, 1023 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.67 (s, 1H); 7.52 (d, *J* = 0.6 Hz, 1H, *H*C5′); 5.32 (s, 2H, CH_2); 4.62–4.52 (m, 2H, PC*H*$_2$); 4.14–4.00 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.99 (d, *J* = 0.6 Hz, 3H, CH_3); 3.57 (s, 3H, CH_3); 2.46–2.34 (m, 2H, PCC*H*$_2$); 1.29 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.7 (s, C=O); 151.2 (s, C=O); 148.9; 143.6; 141.7; 123.5; 107.6; 62.2 (d, *J* = 6.3 Hz, POC); 52.4; 44.6; 36.1; 31.9 (d, *J* = 293.7 Hz, PC); 28.3; 26.5; 16.5 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 26.59 ppm. Anal. Calcd. for $C_{16}H_{24}N_7O_5P$: C, 45.18; H, 5.69; N, 23.05. Found: C, 45.00; H, 5.56; N, 22.96.



Diethyl 2-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21i**. Colourless oil; IR (film): ν = 3033, 2987, 2889, 2830, 1703, 1666, 1230, 1023 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.89 (s, 1H); 7.82 (s, 1H, *H*C5′); 5.60 (s, 2H, CH_2); 4.63–4.55 (m, 2H, PC*H*$_2$); 4.13–4.08 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.59 (s, 3H, CH_3); 3.43 (s, 3H, CH_3); 2.45–2.39 (m, 2H, PCC*H*$_2$); 1.31 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.4 (s, C=O); 151.6 (s, C=O); 149.0; 142.2; 141.4; 123.9; 106.5; 62.2 (d, *J* = 5.8 Hz, POC); 44.7; 41.4; 29.7; 28.0; 27.2 (d, *J* = 141.9 Hz, PC); 16.3 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 25.15 ppm. Anal. Calcd. for $C_{16}H_{24}N_7O_5P$: C, 45.18; H, 5.69; N, 23.05. Found: C, 45.30; H, 5.77; N, 23.17.

^1H NMR



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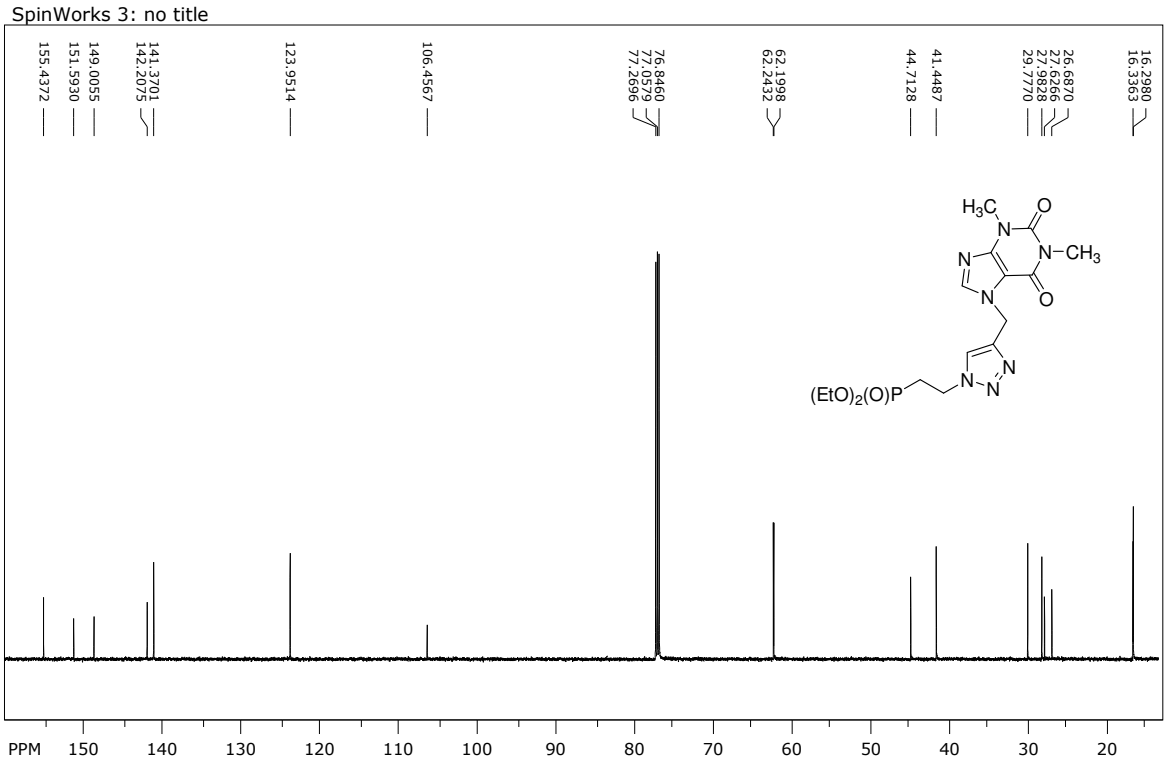
^{13}C NMR



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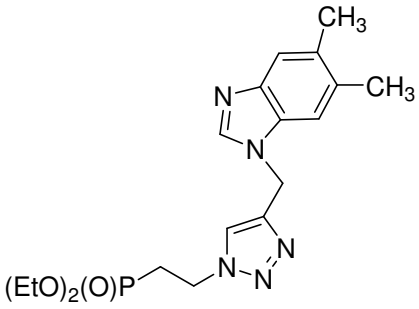
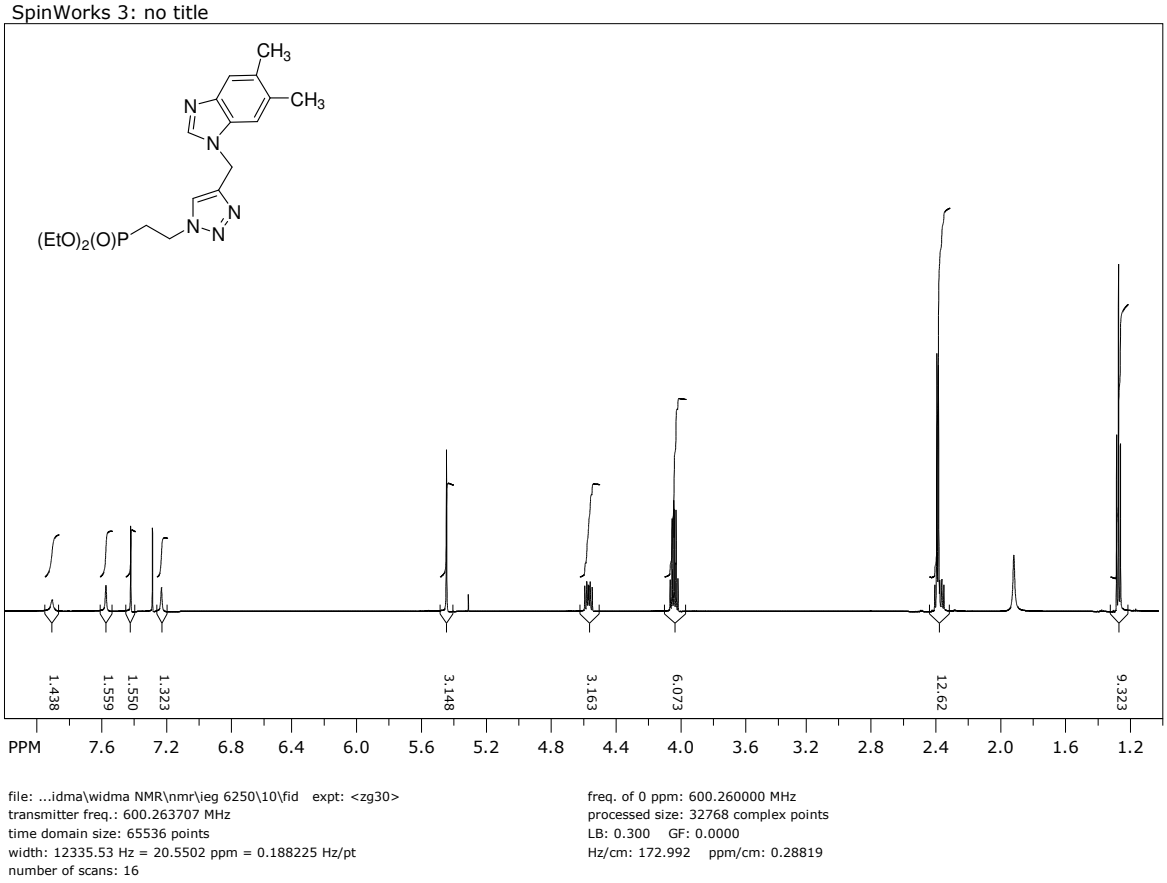


Diethyl 2-{4-[(5,6-dimethylbenzimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21j**. Colourless oil; IR (film): ν = 3014, 2950, 2895, 1045, 856, 759 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.93 (s, 1H); 7.58 (s, 1H); 7.43 (s, 1H); 7.23 (s, 1H); 5.45 (s, 2H, CH_2); 4.54 (dt, *J* = 12.7 Hz, *J* = 7.7 Hz, 2H, PC*H*$_2$); 4.06–4.00 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.38 (dt, *J* = 18.5 Hz, *J* = 7.7 Hz, 2H, PCC*H*$_2$); 2.39 (s, 3H, CH_3); 2.38 (s, 3H, CH_3);1.26 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 143.3; 142.4; 142.0; 132.5; 132.0; 131.4; 122.5; 120.3; 109.9; 62.2 (d, *J* = 6.5 Hz, POC); 44.7 (d, *J* = 1.7 Hz, C-2); 40.4; 27.0 (d, *J* = 142.0 Hz, PC); 20.5; 20.2; 16.2 (d, *J* = 6.4 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 25.27 ppm. Anal. Calcd. for $C_{18}H_{26}N_5O_3P$: C, 55.24; H, 6.70; N, 17.89. Found: C, 55.08; H, 6.84; N, 17.72.

^{1}H NMR



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number of scans: 16

freq. of 0 ppm: 600.260000 MHz
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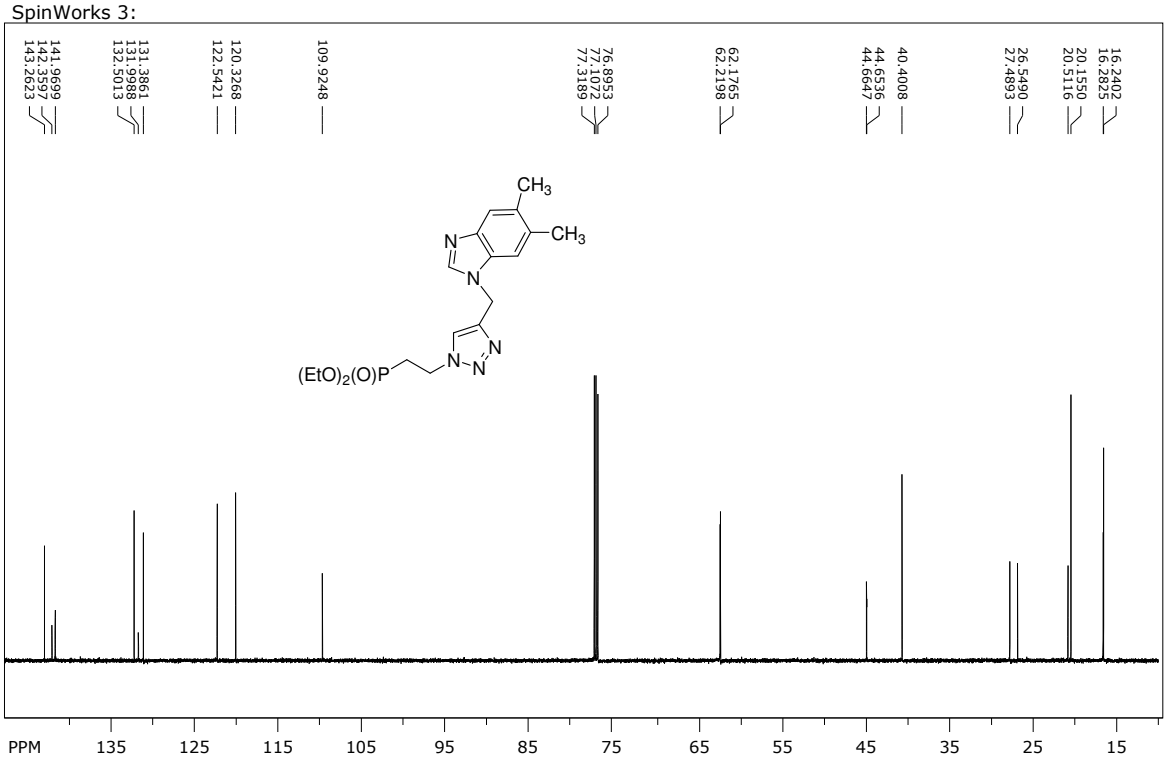
Hz/cm: 172.992 ppm/cm: 0.28819

^{13}C NMR

SpinWorks 3:



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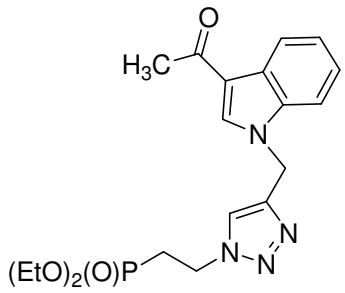
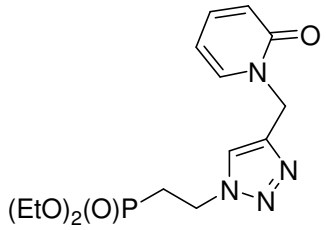
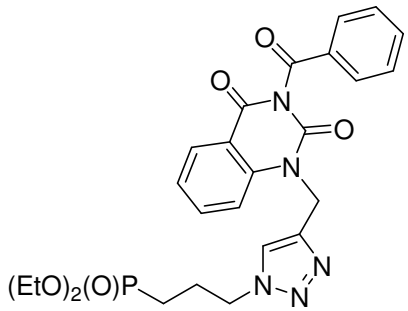


Diethyl 2-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21k**. White solid; m.p.: 83–84°C; IR (KBr): ν = 3430, 3110, 2989, 1642, 1528, 1390, 1026, 753 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.44–8.32 (m, 1H); 7.87 (s, 1H, *H*C5′); 7.47 (s, 1H); 7.45–7.42 (m, 1H); 7.32–7.29 (m, 2H); 5.47 (s, 2H, CH_2); 4.61–4.52 (m, 2H, PC*H*$_2$); 4.05–3.94 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.55 (s, 3H, CH_3); 2.42–2.31 (m, 2H, PCC*H*$_2$); 1.22 (t, *J* = 6.8 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 192.9 (s, C=O); 142.8; 136.4; 134.8; 126.3; 123.5; 122.7; 122.7; 122.6; 117.4; 109.8; 62.2 (d, *J* = 6.6 Hz, POC); 44.7 (d, *J* = 2.0 Hz, PC*C*); 42.3; 27.7 (s, CH_3); 27.1 (d, *J* = 141.4 Hz, PC); 16.4 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 26.39 ppm. Anal. Calcd. for $C_{19}H_{25}N_4O_4P$: C, 56.43; H, 6.23; N, 13.85. Found: C, 56.54; H, 6.14; N, 13.72.

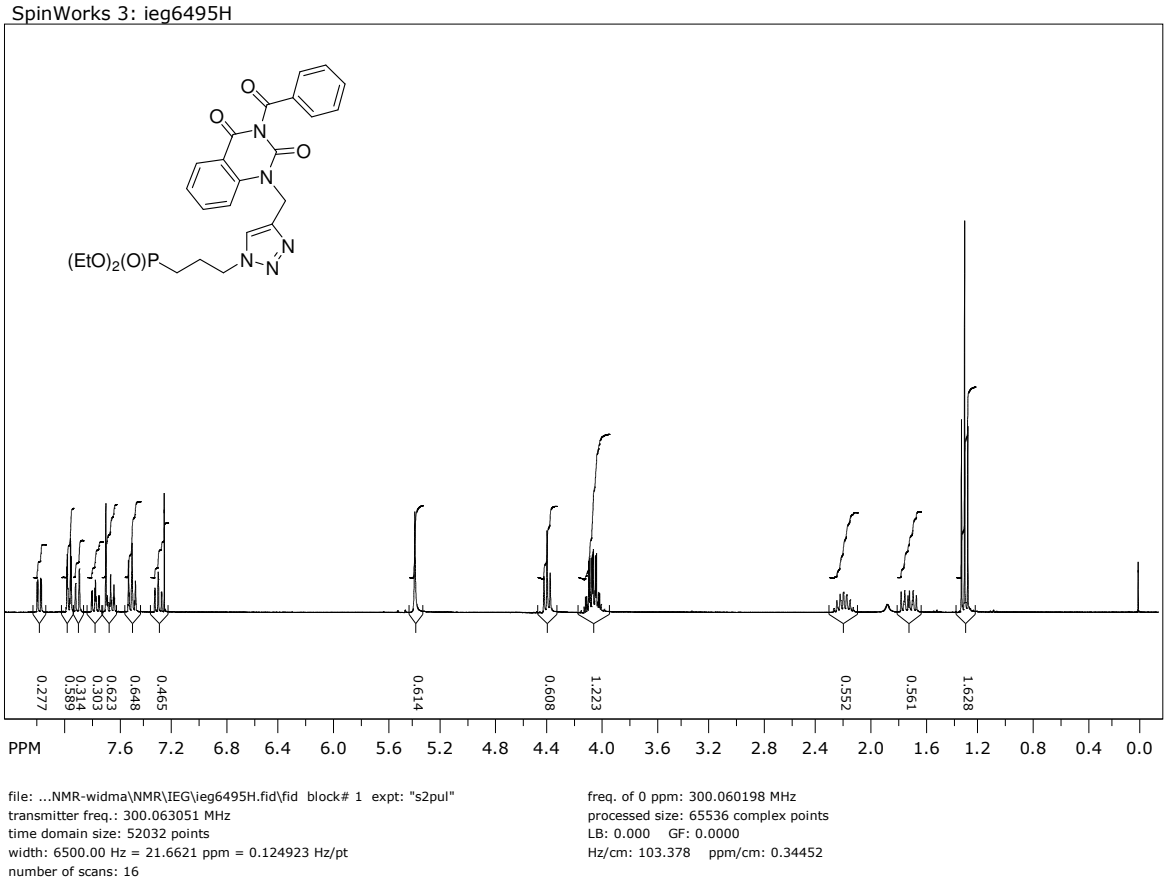


Diethyl 2-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **21l**. Brown oil; IR (film): ν = 3110, 2976, 2875, 1668, 1035, 988 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.84 (s, 1H); 7.59 (dd, *J* = 6.8 Hz, *J* = 1.6 Hz, 1H); 7.33 (ddd, *J* = 9.2 Hz, *J* = 6.8 Hz, *J* = 2.0 Hz, 1H); 6.55 (dd, *J* = 9.2 Hz, *J* = 0.5 Hz, 1H); 6.19 (dt, *J* = 6.8 Hz, *J* = 1.6 Hz, 1H); 5.18 (s, 2H, CH_2); 4.62–4.52 (m, 2H, PC*H*$_2$); 4.13–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.46–2.35 (m, 2H, PCC*H*$_2$); 1.29 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); 1.28 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.2 (s, C=O); 142.5 (s, H*C*=C); 140.0; 137.7; 124.3 (s, HC=*C*); 120.6; 106.5; 62.2 (d, *J* = 6.3 Hz, POC); 44.6 (d, *J* = 2.8 Hz, PC*C*); 27.1 (d, *J* = 141.2 Hz, PC); 16.4 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 26.37 ppm. Anal. Calcd. for $C_{14}H_{21}N_4O_4P$: C, 49.41; H, 6.22; N, 16.46. Found: C, 49.24; H, 6.09; N, 16.28.



Diethyl 3-{4-[(3-benzoyl-2,4-dioxoquinazolin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22e**. Colourless oil; IR (film): ν = 3141, 3064, 2939, 1799, 1606, 1481; 1220, 1025 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.20 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 8.00–7.95 (m, 2H, 2×*o*-CH); 7.91 (d, *J* = 8.5 Hz, 1H); 7.78 (ddd, *J* = 8.5 Hz, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 7.71 (s, 1H, *H*C5′); 7.70–7.62 (m, 1H, *p*-CH); 7.54–7.48 (m, 2H, 2×*m*-CH); 7.32 (dt, *J* = 7.9 Hz, *J* = 0.8 Hz, 1H); 5.40 (s, 2H, CH_2); 4.41 (t, *J* = 7.0 Hz, 2H, PCCCH_2); 4.16–3.99 (m, 4H, 2×POC$H_2$$CH_3$); 2.20 (dqv, *J* = 14.5 Hz, *J* = 7.0 Hz, 2H, PCCH_2); 1.71 (dt, *J* = 18.7 Hz, *J* = 7.0 Hz, 2H, PCH_2); 1.30 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.6 (s, C=O); 161.0 (s, C=O); 149.5 (s, C=O); 142.4 (s, H*C*=C); 140.2; 136.2; 135.2; 131.5; 130.5; 129.2; 128.9; 123.9 (s, HC=*C*); 123.8; 115.5; 115.3; 61.8 (d, *J* = 6.7 Hz, POC); 50.3 (d, *J* = 15.7 Hz, PCC*C*); 38.9; 23.7 (d, *J* = 4.9 Hz, PC*C*); 22.8 (d, *J* = 142.9 Hz, PC); 16.6 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121 MHz, $CDCl_3$): δ = 30.82 ppm. Anal. Calcd. for $C_{25}H_{28}N_5O_6P$: C, 57.14; H, 5.37; N, 13.33. Found: C, 57.27; H, 5.49; N, 13.4.

^1H NMR



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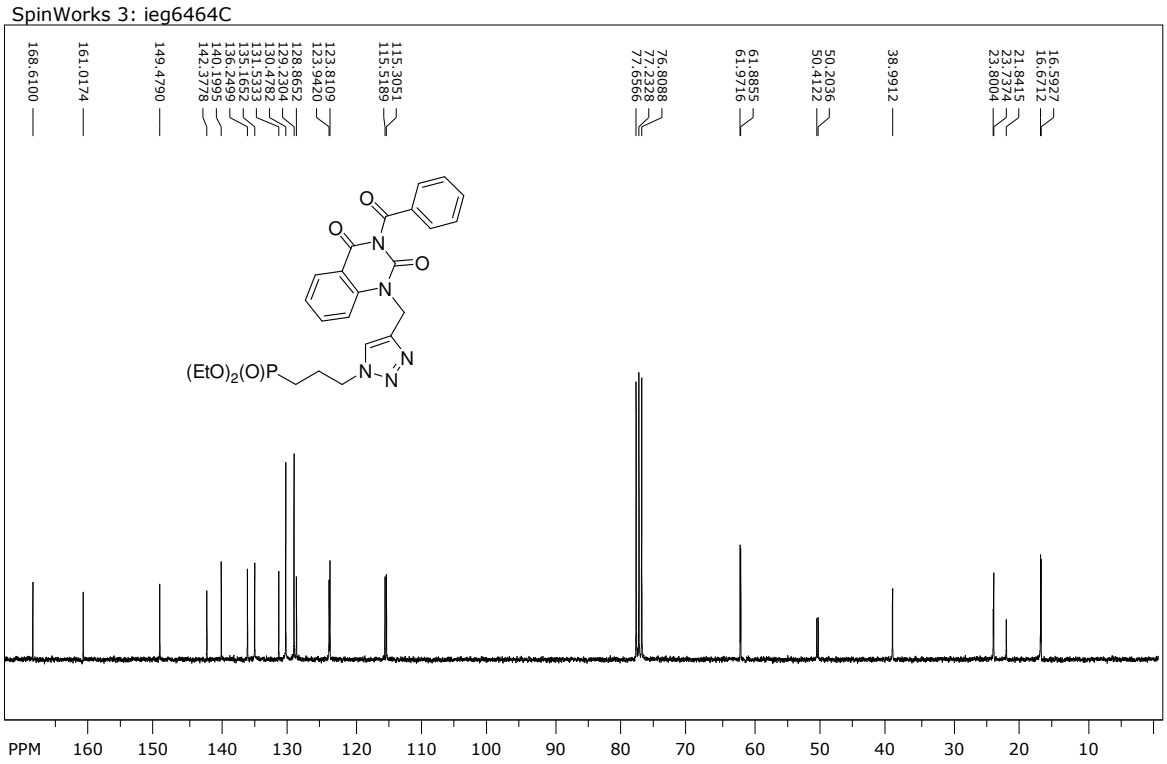
^{13}C NMR



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number of scans: 1024

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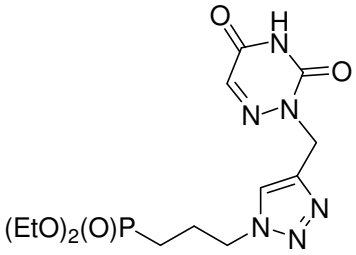
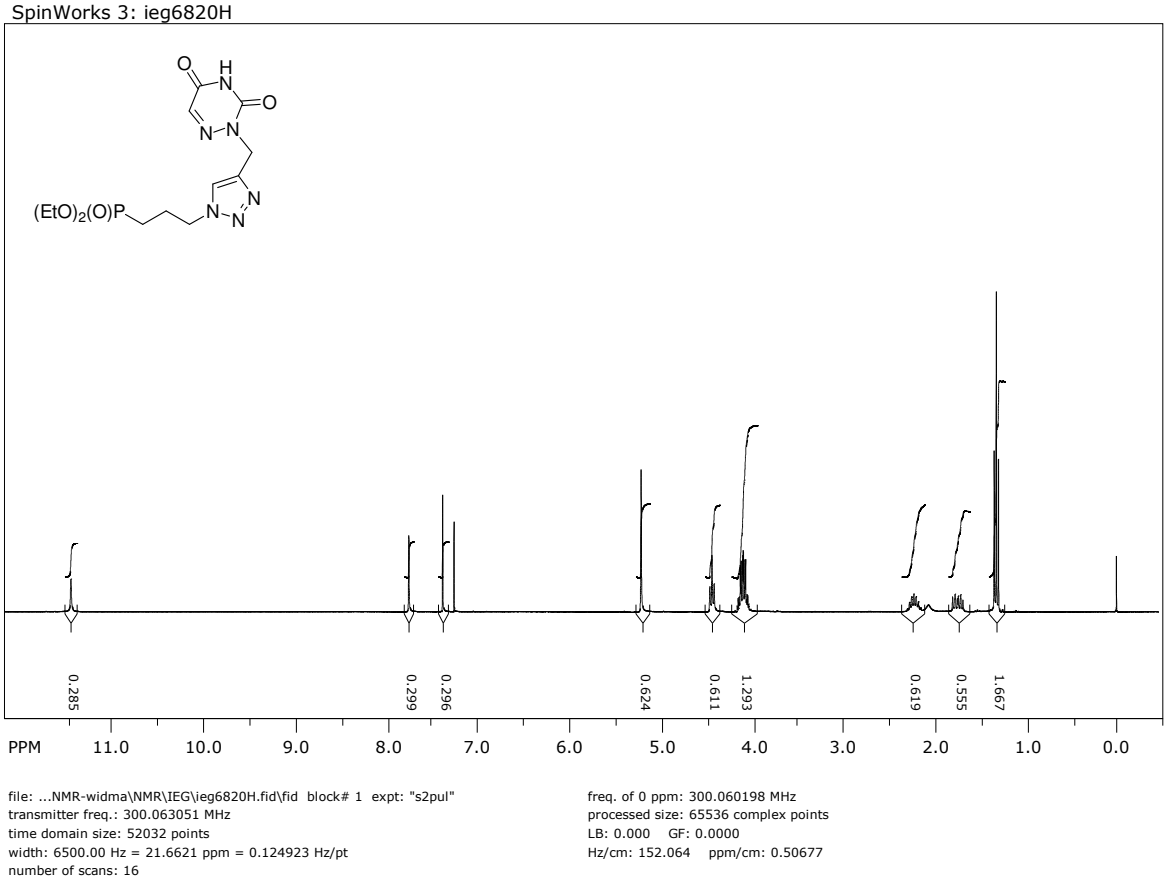
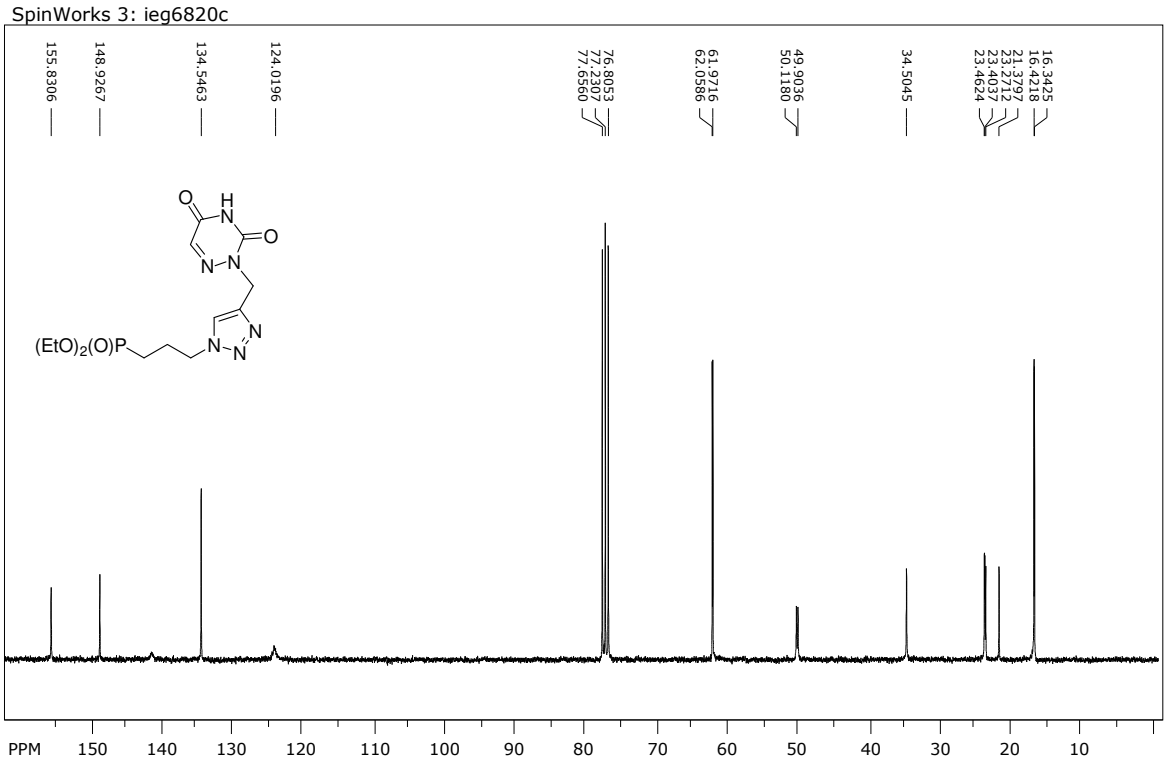


Diethyl 3-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22f**. White solid; m.p.: 96–97°C; IR (KBr): ν = 3384, 3232, 3138, 2984, 2908, 1730, 1677, 1217, 1025 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 11.51 (s, 1H, NH); 7.77 (s, 1H, *H*C5′); 7.40 (s, 1H); 5.22 (s, 2H, CH_2); 4.44 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.16–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.21 (dqv, *J* = 14.9 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.75 (dt, *J* = 19.0 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.32 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.8 (s, C=O); 148.9 (C=O); 141.3 (s, H*C*=C); 134.5 (s, HC=N); 124.2 (s, HC=*C*); 62.0 (d, *J* = 6.4 Hz, POC); 50.0 (d, *J* = 15.1 Hz, PCC*C*); 34.5; 23.4 (d, *J* = 4.3 Hz, PC*C*); 22.2 (d, *J* = 143.0 Hz, PC); 16.4 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 31.41 ppm. Anal. Calcd. for $C_{13}H_{21}N_6O_5P$: C, 41.94; H, 5.69; N, 22.57. Found: C, 42.08; H, 5.74; N, 22.67.

^1H NMR



^{13}C NMR



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number of scans: 1456

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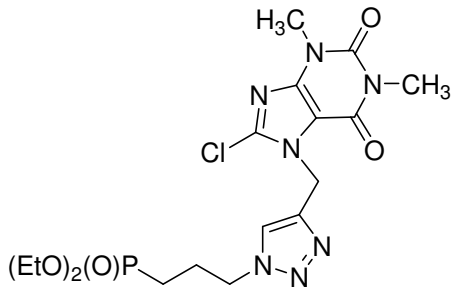
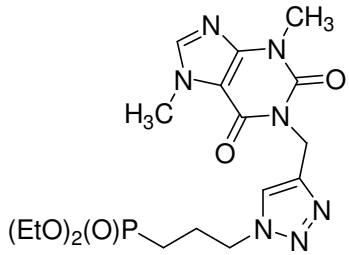
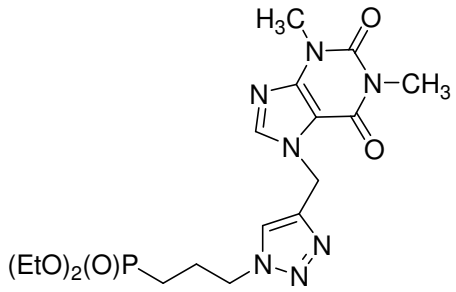


Diethyl 3-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22g**. White solid; m.p.: 127–128°C; IR (KBr): ν = 3362, 3101, 2981, 2935, 1707, 1679, 1224, 1020, 956 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.83 (s, 1H, *H*C5′); 5.66 (s, 2H, CH_2); 4.46 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.15–4.05 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.57 (s, 3H, CH_3); 3.44 (s, 3H, CH_3); 2.23 (dqv, *J* = 14.7 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.74 (dt, *J* = 18.7 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.34 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 154.5 (s, C=O); 151.2 (s, C=O); 147.4; 141.8; 139.0; 123.7; 107.4; 61.8 (d, *J* = 6.4 Hz, POC); 50.1 (d, *J* = 15.2 Hz, PCC*C*); 41.0; 29.8; 27.9; 23.6 (d, *J* = 4.8 Hz, PC*C*); 22.6 (d, *J* = 142.3 Hz, PC); 16.4 (d, *J* = 6.1 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 29.80 ppm. Anal. Calcd. for $C_{17}H_{25}ClN_7O_5P$: C, 43.09; H, 5.32; N, 20.69. Found: C, 42.88; H, 5.44; N, 20.71.

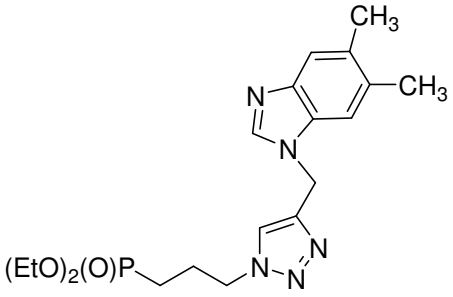


Diethyl 3-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22h**. White powder; m.p.: 175–176°C; IR (KBr): ν = 3444, 3001, 2984, 1704, 1668, 1221, 1020 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.76 (s, 1H); 7.53 (s, 1H, *H*C5′); 5.35 (s, 2H, CH_2); 4.42 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.15–4.05 (m, 4H, 2×POC*H*$_2$CH$_3$); 4.02 (s, 3H, CH_3); 3.60 (s, 3H, CH_3); 2.22 (dqv, *J* = 14.2 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.74 (dt, *J* = 18.7 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.34 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 154.8 (s, C=O); 151.4 (s, C=O); 148.9; 143.7; 141.6; 123.4; 107.7; 61.7 (d, *J* = 6.5 Hz, POC); 50.0 (d, *J* = 16.1 Hz, PCC*C*); 36.0; 33.6; 29.7; 23.6 (d, *J* = 4.5 Hz, PC*C*); 22.7 (d, *J* = 143.1 Hz, PC); 16.4 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.03 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_5P$: C, 46.47; H, 5.96; N, 22.31. Found: C, 46.33; H, 6.06; N, 22.51.

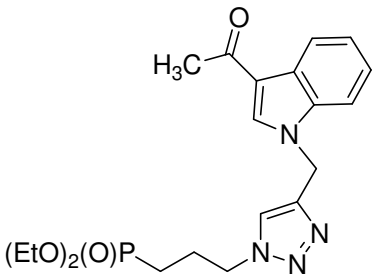


Diethyl 3-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22i**. White solid; m.p.: 187–190°C; IR (KBr): ν = 3440, 2996, 2984, 1704, 1668, 1225, 1018 cm^{-1}; ^{1}H NMR (600

MHz, $CDCl_3$): δ = 7.87 (s, 1H); 7.83 (s, 1H, *H*C5′); 5.61 (s, 2H, CH_2); 4.46 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.16–4.05 (m, 4H, 2×POC*H*$_2$$CH_3$); 3.60 (s, 3H, CH_3); 3.44 (s, 3H, CH_3); 2.24 (dqv, *J* = 14.6 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.74 (dt, *J* = 18.7 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.34 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.4 (s, C=O); 151.5 (s, C=O); 149.0; 142.2; 141.4; 123.8; 106.4; 61.8 (d, *J* = 6.5 Hz, POC); 50.1 (d, *J* = 15.3 Hz, PCC*C*); 41.4; 29.7; 27.9; 23.6 (d, *J* = 4.8 Hz, PC*C*); 22.6 (d, *J* = 142.4 Hz, PC); 16.4 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 29.75 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_5P$: C, 46.47; H, 5.96; N, 22.31. Found: C, 46.59; H, 6.11; N, 22.45.

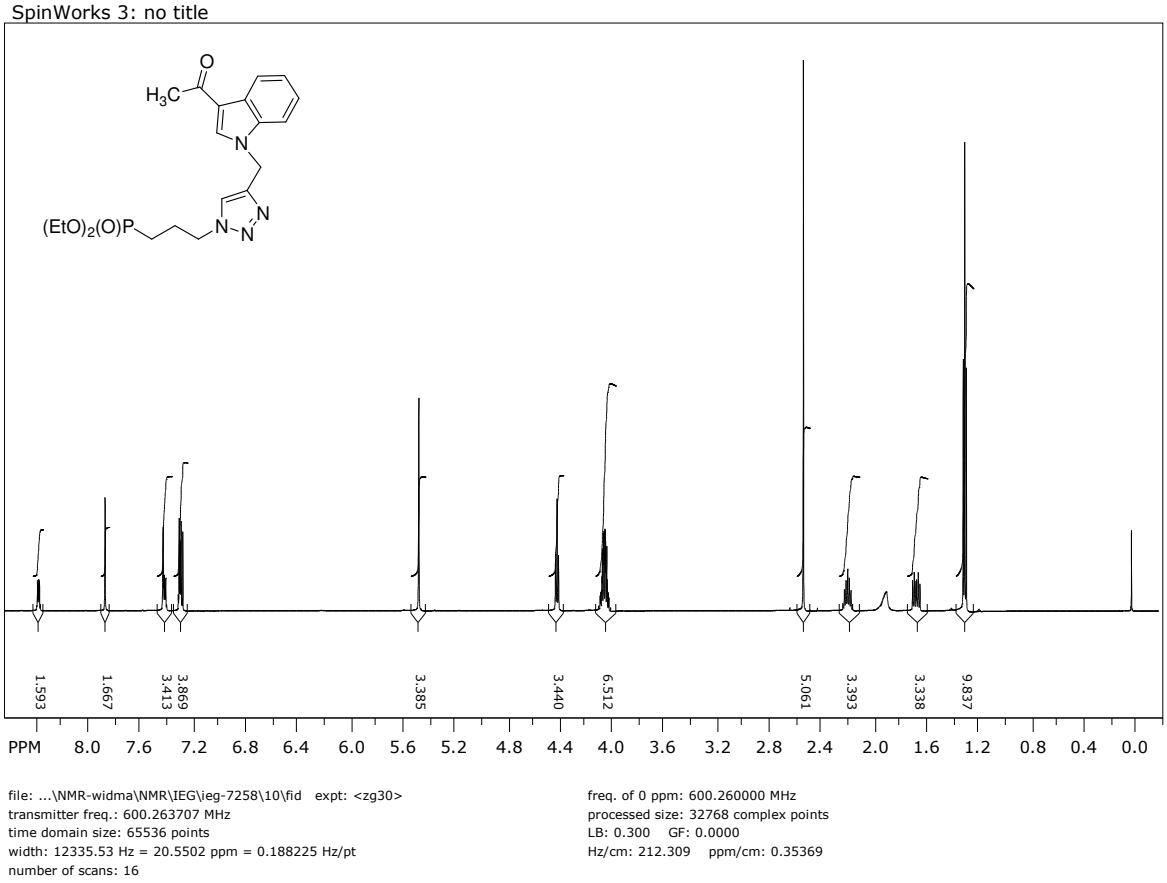


Diethyl 3-{4-[(5,6-dimethylbenzimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22j**. Colourless oil; IR (film): ν = 3446, 2990, 2938, 1498, 1444, 1224, 1050, 965 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.33 (s, 1H); 7.61 (s, 1H,); 7.54 (s, 1H,); 7.32 (s, 1H,); 5.55 (s, 2H, CH_2); 4.43 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.15–4.05 (m, 4H, 2×POC*H*$_2$$CH_3$); 2.41 (s, 3H, CH_3); 2.40 (s, 3H, CH_3); 2.21 (dqv, *J* = 14.6 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.70 (dt, *J* = 19.2 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.34 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 143.4; 142.3; 142.0; 132.4; 131.4; 122.4; 120.3; 109.9; 61.8 (d, *J* = 6.5 Hz, POC); 50.0 (d, *J* = 14.5 Hz, PCC*C*); 40.5; 23.5 (d, *J* = 4.5 Hz, PC*C*); 22.4 (d, *J* = 142.3 Hz, PC); 20.5; 20.1; 16.4 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 29.68 ppm. Anal. Calcd. for $C_{19}H_{28}N_5O_3P$: C, 56.29; H, 6.96; N, 17.27. Found: C, 56.07; H, 7.14; N, 17.10.



Diethyl 3-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22k**. Colourless oil; IR (film): ν = 3394, 3110, 2941, 2825, 1648, 1229, 1029 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.43–8.38 (m, 1H); 7.88 (s, 1H, *H*C5′); 7.43–7.38 (m, 2H); 7.36–7.27 (m, 2H); 5.48 (s, 2H, CH_2); 4.44 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 4.10–4.01 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.53 (s. 3H, CH_3); 2.20 (dqv, *J* = 14.7 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.65 (dt, *J* = 18.4 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); 1.29 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 192.9 (s, C=O); 142.9; 136.4; 134.7; 126.3; 123.5; 122.7; 122.6; 122.5; 117.5; 109.9; 61.9 (d, *J* = 6.3 Hz, POC); 50.0 (d, *J* = 14.9 Hz, PCC*C*); 42.4; 27.8; 23.6 (d, *J* = 4.9 Hz, PC*C*); 22.1 (d, *J* = 142.8 Hz, PC); 16.4 (d, *J* = 6.1 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 30.85 ppm. Anal. Calcd. for $C_{20}H_{27}N_4O_4P$: C, 57.41; H, 6.50; N, 13.39. Found: C, 57.60; H, 6.73; N, 13.50.

^{1}H NMR



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number of scans: 16

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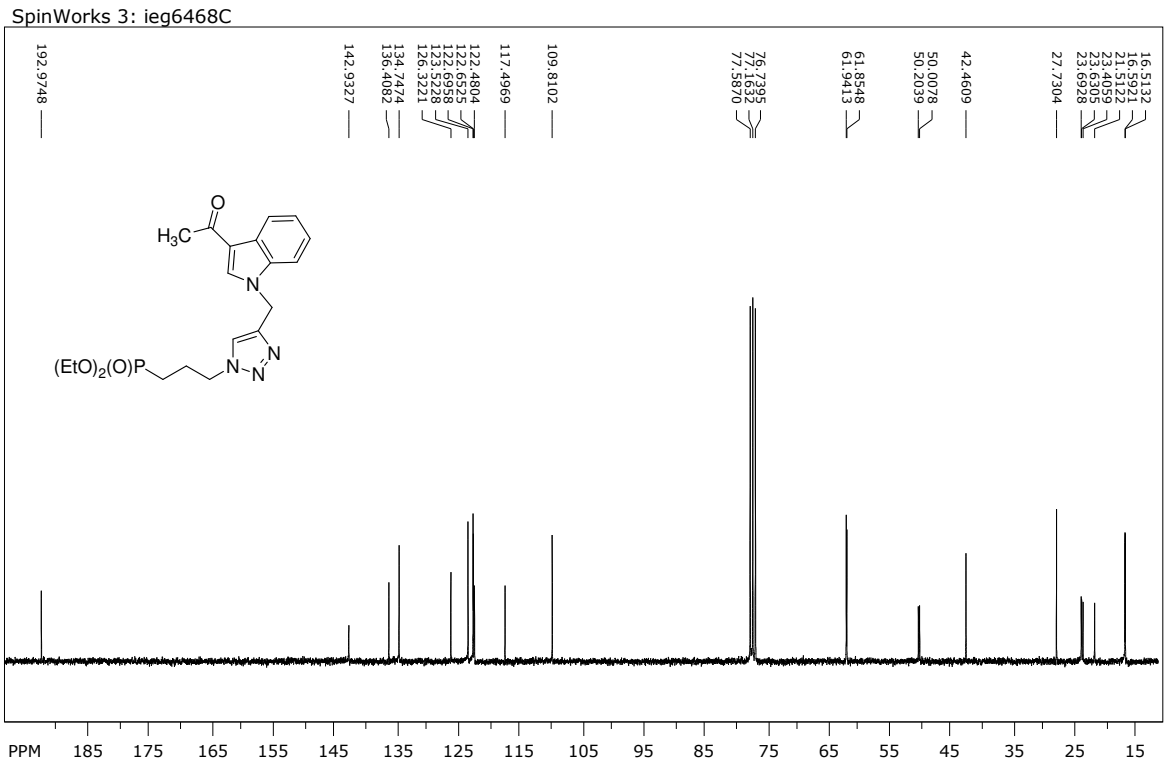
^{13}C NMR



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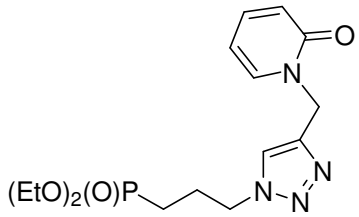
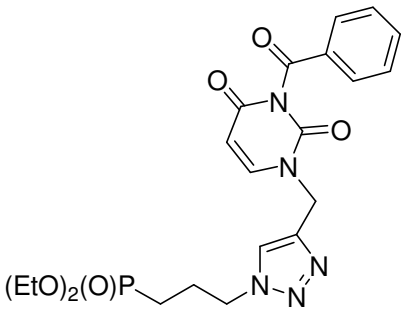


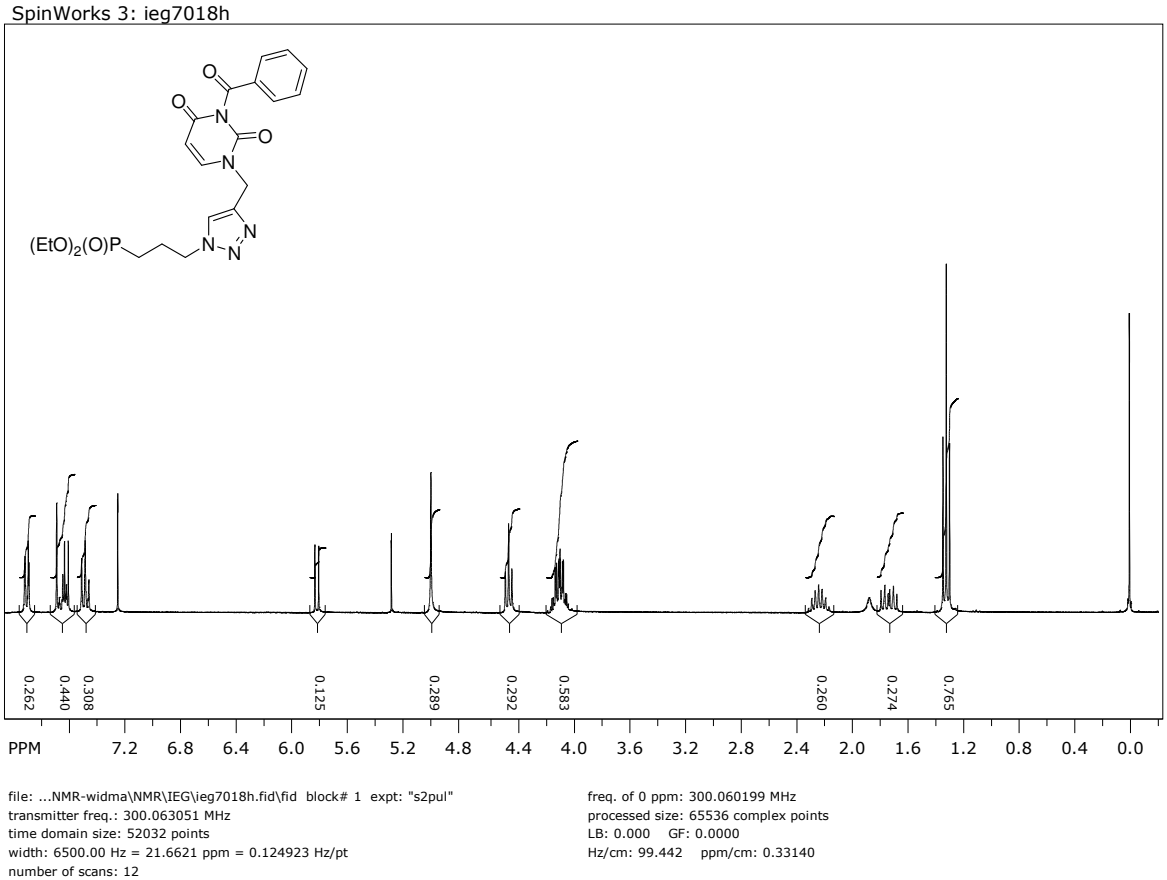
Diethyl 3-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **22l**. Brown oil after; IR (film): ν = 3426, 3144, 2986, 1657, 1226; 1026, 968 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.81(s, 1H, *H*C5′); 7.60 (ddd, *J* = 6.8 Hz, *J* = 2.1 Hz, *J* = 0.7 Hz, 1H); 7.32 (ddd, *J* = 9.2 Hz, *J* = 6.6 Hz, *J* = 2.1 Hz, 1H); 6.56 (ddd, *J* = 9.2 Hz, *J* = 1.3 Hz, *J* = 0.7 Hz, 1H); 6.20 (dt, *J* = 6.8 Hz, *J* = 1.3 Hz, 1H); 5.19 (s, 2H, CH_2); 4.41 (t, *J* = 7.1 Hz, 2H, PCCC*H*$_2$); 4.15–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.22 (dqv, *J* = 14.9 Hz, *J* = 7.1 Hz, 2H, PCC*H*$_2$); 1.66 (dt, *J* = 18.2 Hz, *J* = 7.1 Hz, 2H, PC*H*$_2$); 1.34 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.1 (s, C=O); 142.5 (s, H*C*=C); 139.9; 137.6; 124.0 (s, HC=*C*); 120.4; 106.4; 61.8 (d, *J* = 6.4 Hz, POC); 50.0 (d, *J* = 16.1 Hz, PCC*C*); 44.5; 23.5 (d, *J* = 4.4 Hz, PC*C*); 22.1 (d, *J* = 147.1 Hz, PC); 16.4 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 31.05 ppm. Anal. Calcd. for $C_{15}H_{23}N_4O_4P$: C, 50.84; H, 6.54; N, 15.81. Found: C, 50.61; H, 6.39; N, 15.64.



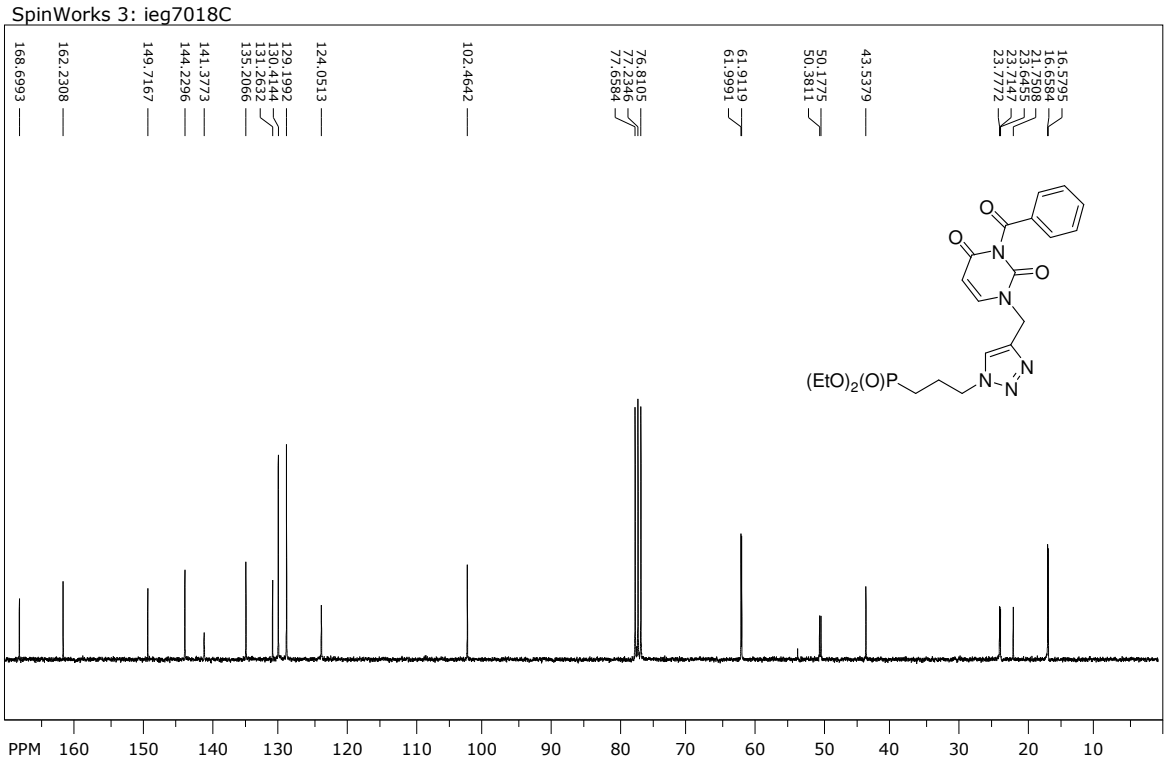
Diethyl 3-(4-{[3-benzoyl--2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)propylphosphonate **22m**.

Colourless oil; IR (film): ν = 3020, 3005, 2963, 2899, 1669, 1664, 1220, 1020, 772, 689 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.94–7.90 (m, 2H, 2×*o*-CH); 7.71 (s, 1H, *HC*5′); 7.69–7.63 (m, 1H, *p*-CH); 7.64 (d, *J* = 8.0 Hz, 1H, *H*C=CH); 7.53–7.47 (m, 2H, 2×*m*-CH); 5.84 (d, *J* = 8.0 Hz, 1H, HC=C*H*); 5.02 (s, 2H, CH_2); 4.46 (t, *J* = 7.3 Hz, 2H, PCCCH_2); 4.18–4.01 (m, 4H, 2×POC$H_2$$CH_3$); 2.23 (dqv, *J* = 14.7 Hz, *J* = 7.3 Hz, 2H, PCCH_2); 1.73 (dt, *J* = 18.7 Hz, *J* = 7.3 Hz, 2H, PCH_2); 1.31 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.7 (s, C=O); 162.2 (s, C=O); 149.7; 144.2 (s, C=O); 141.3 (s, H*C*=C); 135.2; 131.3; 130.4; 129.2; 124.1 (s, HC=*C*); 102.5; 61.9 (d, *J* = 6.6 Hz, POC); 50.2 (d, *J* = 15.4 Hz, PCC*C*); 43.5; 23.7 (d, *J* = 4.7 Hz, PC*C*); 22.7 (d, *J* = 143.0 Hz, PC); 16.6 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121 MHz, $CDCl_3$): δ = 30.12 ppm. Anal. Calcd. for $C_{21}H_{26}N_5O_6P$: C, 53.05; H, 5.51; N, 14.73. Found: C, 52.89; H, 5.33; N, 14.58.

^1H NMR



^{13}C NMR



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number of scans: 1168

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processed size: 131072 complex points
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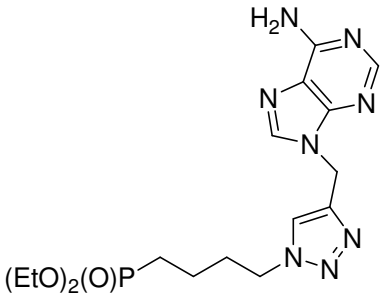
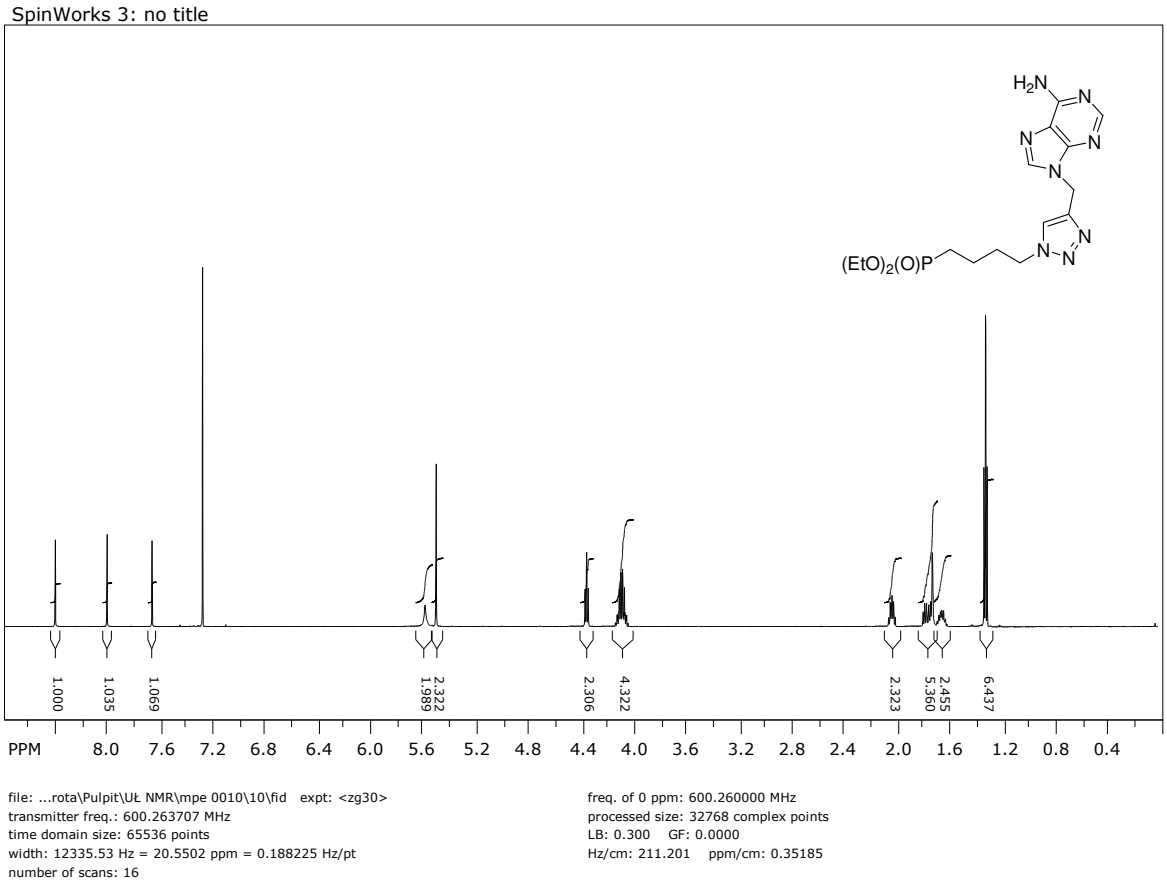


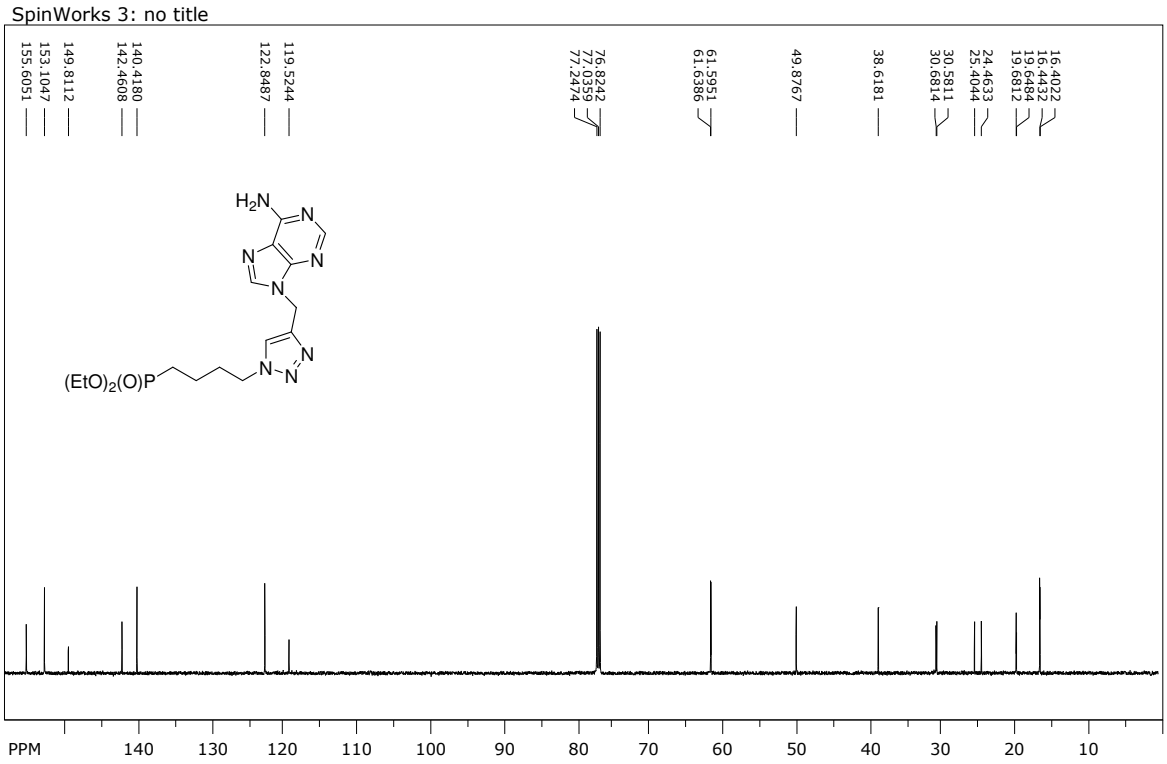
Diethyl 4-(4-{[6-aminopurin-9-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonate **23a**.

White powder; m.p.: 119–120°C; IR (KBr): ν = 3462, 3306, 3140, 2984, 2912, 2870, 1662, 1597, 1244, 1033 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.41 (s, 1H); 8.02 (s, 1H); 7.68 (s, 1H); 5.59 (brs, 2H, NH_2); 5.51 (s, 2H, CH_2); 4.36 (t, *J* = 7.1 Hz, 2H, PCCCC*H*$_2$); 4.14–4.04 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.03 (qv, *J* = 7.1 Hz, 2H, PCCC*H*$_2$); 1.80–1.73 (m, 2H, PC*H*$_2$); 1.65 (dqv, *J* = 14.1 Hz, *J* = 7.1 Hz, 2H, PCC*H*$_2$); 1.32 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.6; 153.1; 149.8; 142.4; 140.4; 122.8; 119.5; 61.6 (d, *J* = 6.6 Hz, POC); 49.9; 38.6; 30.6 (d, *J* = 15.1 Hz, PCC*C*); 24.9 (d, *J* = 142.1 Hz, PC); 19.6 (d, *J* = 5.0 Hz, PC*C*); 16.4 (d, *J* = 6.2 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.73 ppm. Anal. Calcd. for $C_{16}H_{25}N_8O_3P$: C, 47.06; H, 6.17; N, 27.44. Found: C, 46.88; H, 6.02; N, 27.29.

^{1}H NMR



^{13}C NMR



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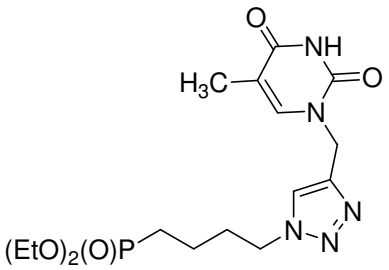
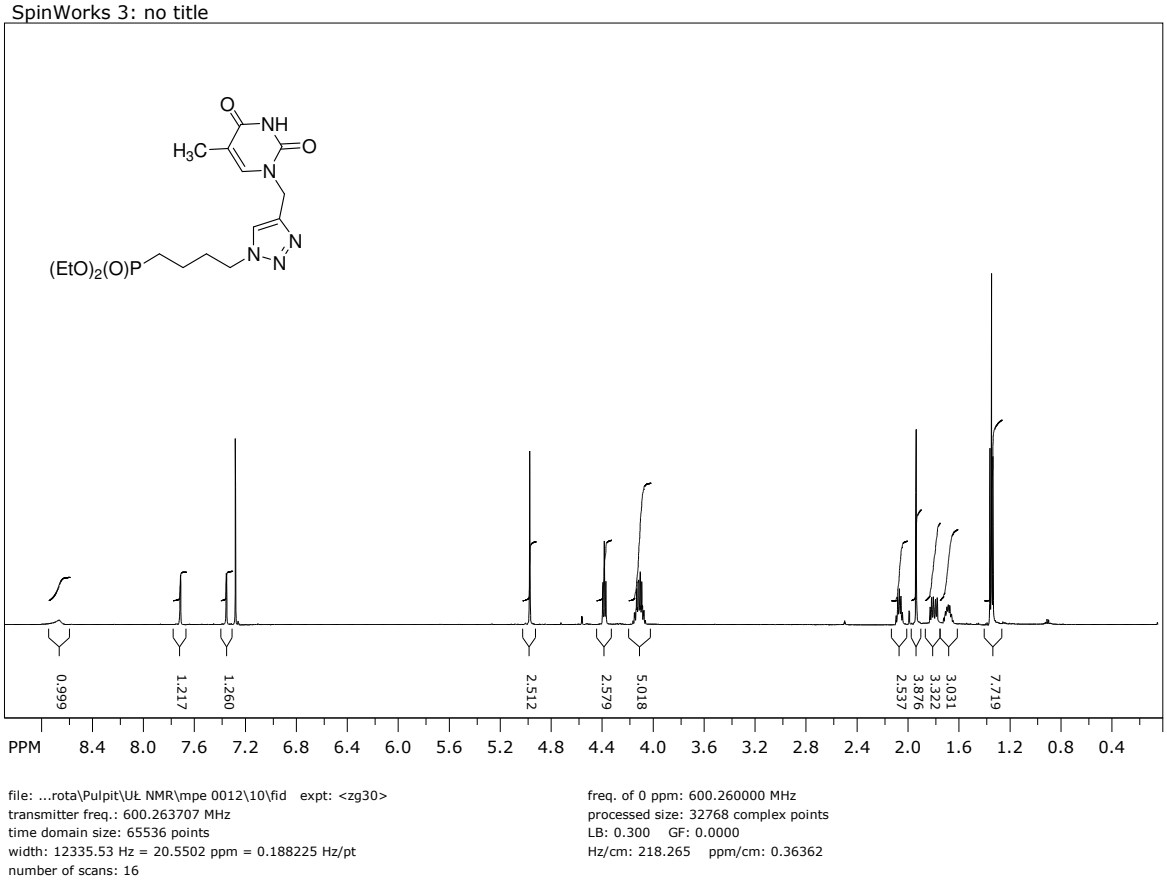
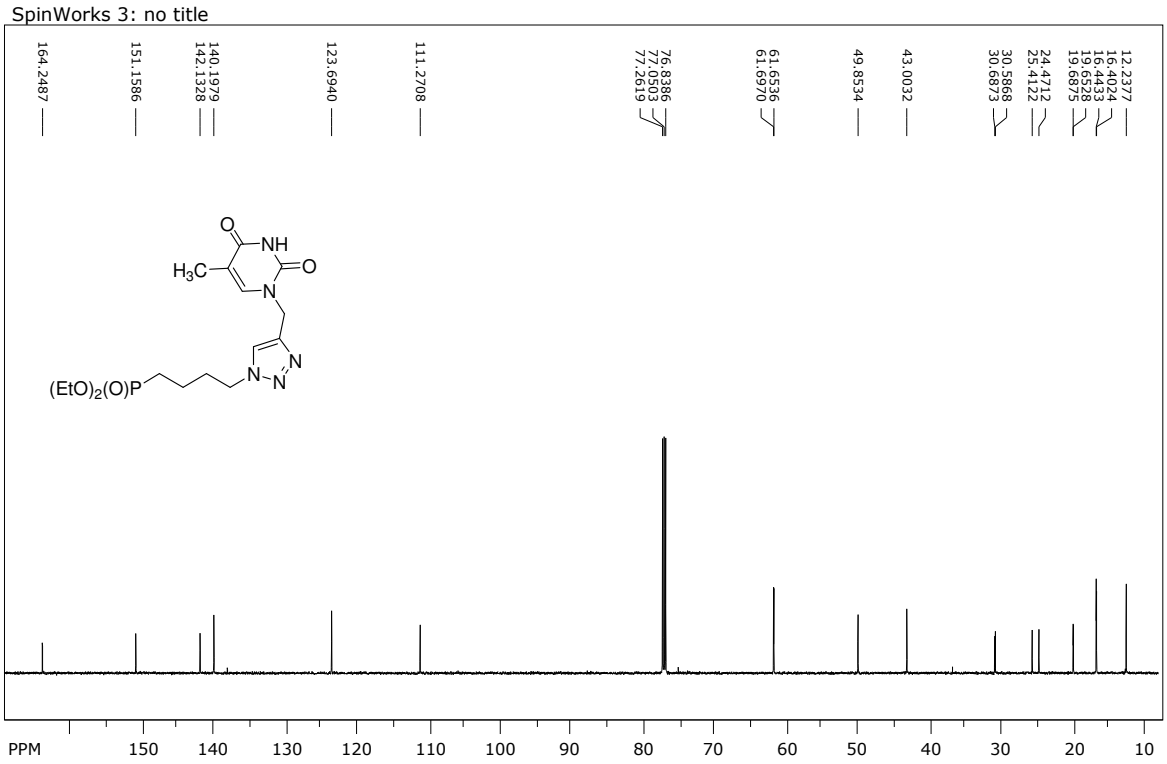


Diethyl 4-(4-{[5-methyl-2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonate **23b**. White powder; m.p.: 63–65°C; IR (KBr): ν = 3425, 3132, 2986, 2912, 2827, 1688, 1219, 1027 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.69 (brs, 1H, NH); 7.72 (s, 1H, *H*C5′); 7.36 (d, *J* = 1.0 Hz, 1H, *H*C=CCH$_3$); 4.97 (s, 2H, CH$_2$); 4.38 (t, *J* = 7.1 Hz, 2H, PCCCC*H*$_2$); 4.16–4.06 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.06 (qv, *J* = 7.1 Hz, 2H, PCCC*H*$_2$); 1.93 (d, *J* = 1.0 Hz, 3H, HC=CC*H*$_3$); 1.78 (dt, *J* = 15.7 Hz, *J* = 7.1 Hz, 2H, PC*H*$_2$); 1.69–1.64 (m, 2H, PCC*H*$_2$); 1.33 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 164.2 (s, C=O); 151.2 (s, C=O); 142.1; 140.2; 123.7; 111.3; 61.6 (d, *J* = 6.6 Hz, POC); 49.9; 43.0; 30.6 (d, *J* = 15.2 Hz, PCC*C*); 24.9 (d, *J* = 142.0 Hz, PC); 19.7 (d, *J* = 5.2 Hz, PC*C*); 16.4 (d, *J* = 6.2 Hz, POC*C*); 12.2 (s, CH$_3$); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.84 ppm. Anal. Calcd. for $C_{16}H_{26}N_5O_5P$: C, 48.12; H, 6.56; N, 17.54. Found: C, 47.90; H, 6.33; N, 17.41.

^1H NMR



^{13}C NMR



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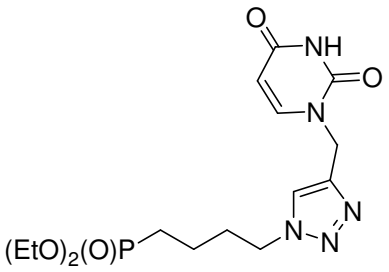
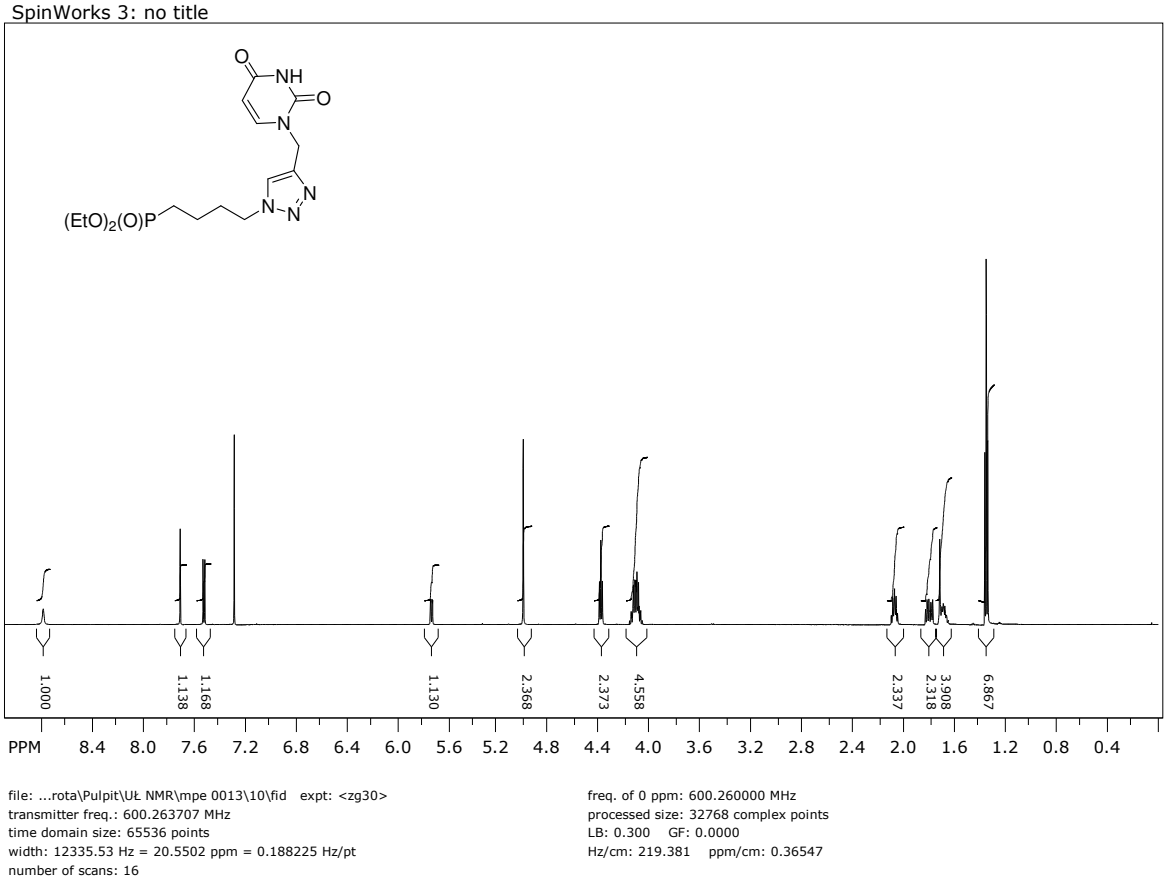


Diethyl 4-(4-{[2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonate **23c**. White powder; m.p.: 124–125°C; IR (KBr): ν = 3435, 3142, 2994, 2952, 2867, 1648, 1229, 1023 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.80 (brs, 1H, NH); 7.72 (s, 1H, *H*C5′); 7.53 (d, *J* = 8.0 Hz, 1H, *H*C=CH); 5.73 (d, *J* = 8.0 Hz, 1H, HC=C*H*); 5.00 (s, 2H, CH_2); 4.39 (t, *J* = 7.1 Hz, 2H, PCCCCH_2); 4.16–4.06 (m, 4H, 2×POC$H_2$$CH_3$); 2.06 (qv, *J* = 7.1 Hz, 2H, PCCCH_2); 1.82–1.76 (m, 2H, PCCH_2); 1.71–1.64 (dqv, *J* = 14.3 Hz, *J* = 7.1 Hz, 2H, PCH_2); 1.34 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$CH_3); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 163.7 (s, C=O); 151.1 (s, C=O); 144.3; 141.9; 123.7; 102.7; 61.6 (d, *J* = 6.6 Hz, POC); 49.9; 43.2; 30.6 (d, *J* = 15.2 Hz, PCC*C*); 25.0 (d, *J* = 142.0 Hz, PC); 19.7 (d, *J* = 5.3 Hz, PC*C*); 16.5 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.77 ppm. Anal. Calcd. for $C_{15}H_{24}N_5O_5P$: C, 46.75; H, 6.28; N, 18.17. Found: C, 46.84; H, 6.36; N, 18.00.

^1H NMR



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number of scans: 16

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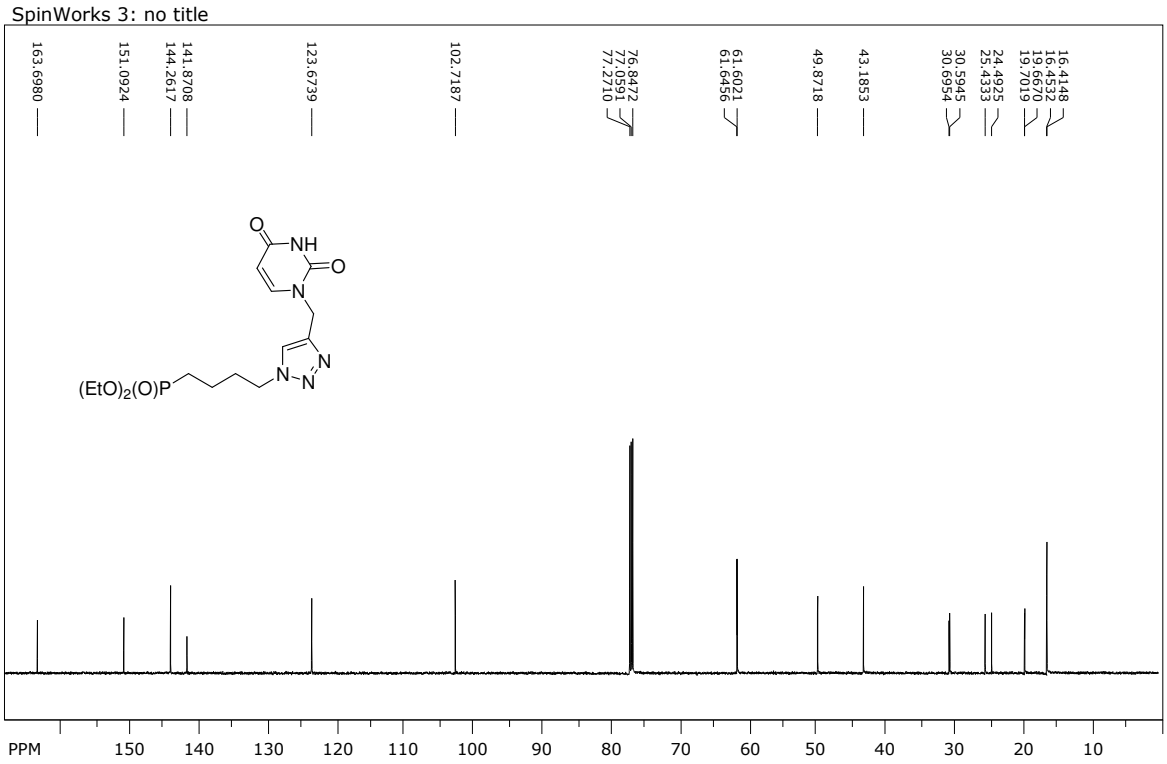
^{13}C NMR



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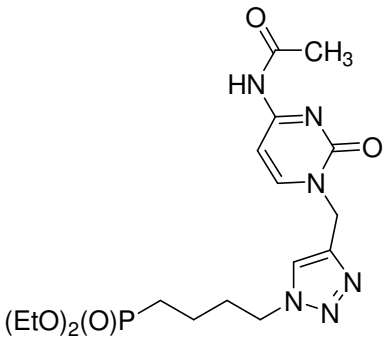
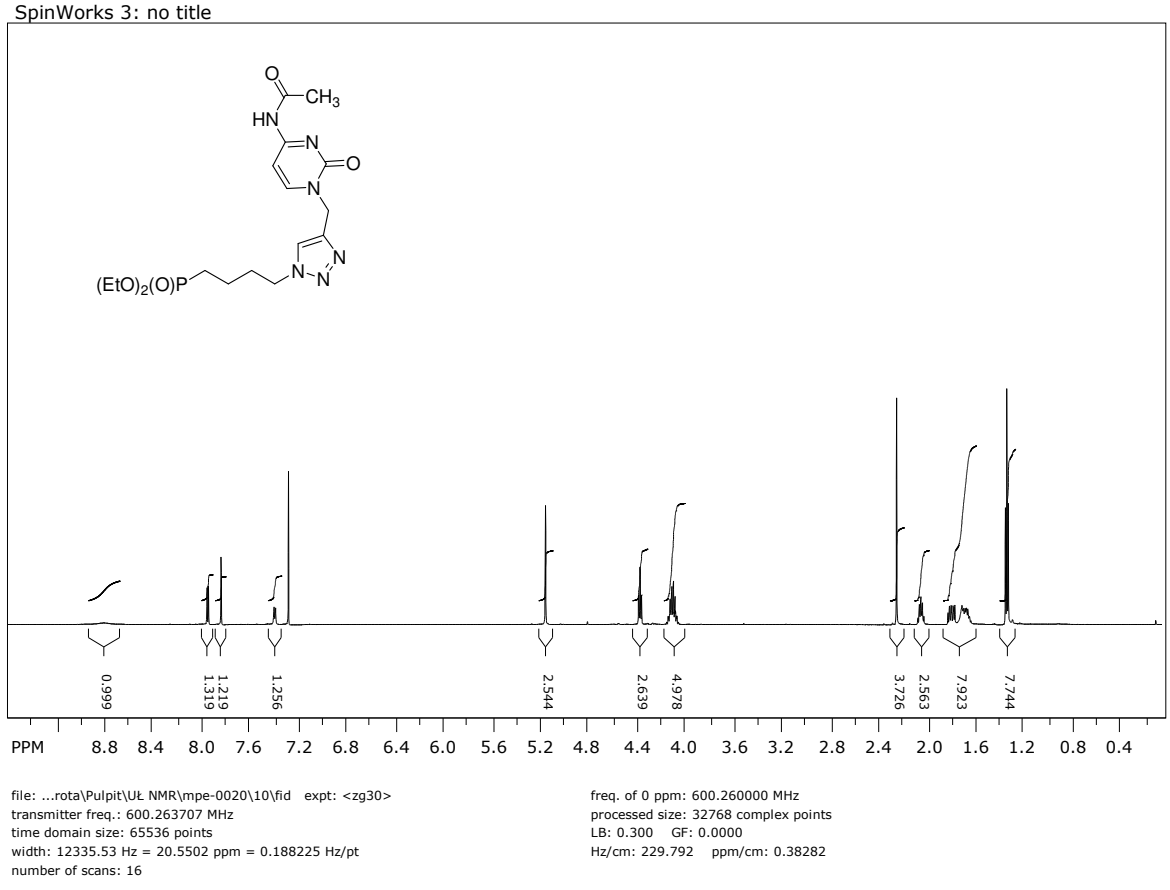


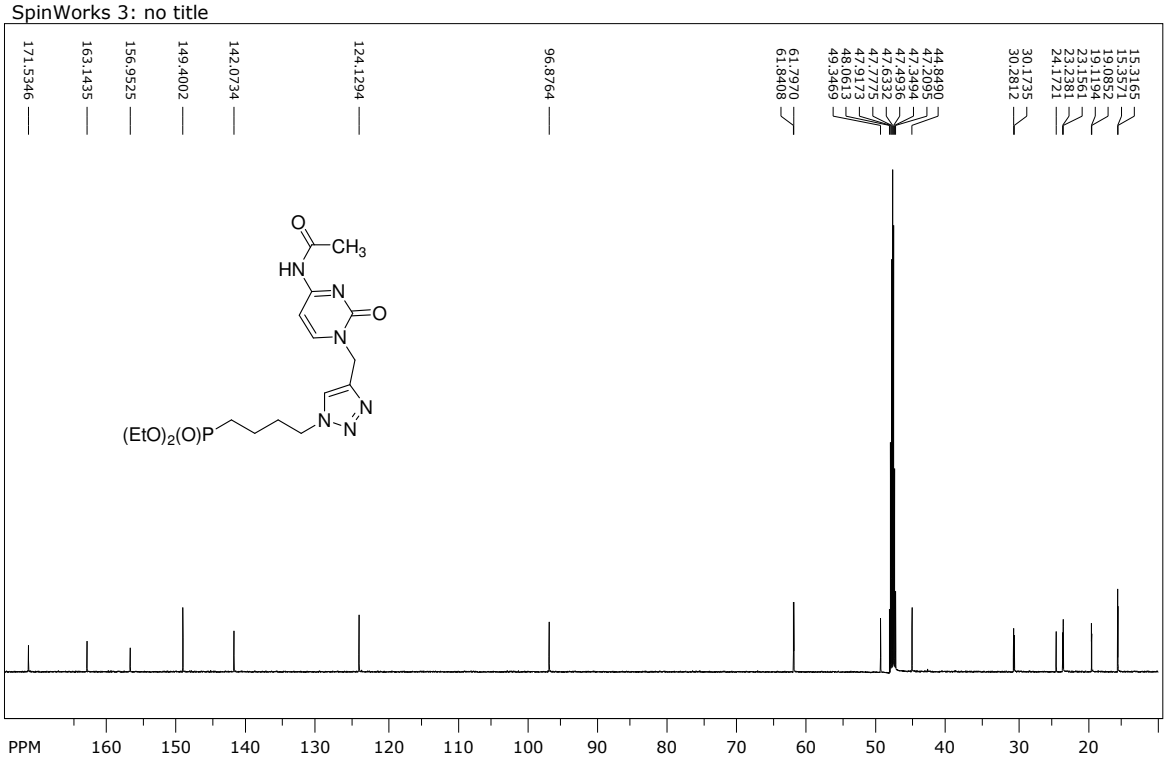
Diethyl 4-(4-{[N^4-acetylamino-2-oxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonate **23d**. White powder; m.p.: 159–161°C; IR (KBr): ν = 3217, 3133, 3084, 2982, 1707, 1650, 1217, 1025 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.83 (brs, 1H, NH); 7.96 (d, *J* = 7.3 Hz, 1H, *H*C=CH); 7.84 (s, 1H, *H*C5′); 7.40 (d, *J* = 7.3 Hz, 1H, HC=C*H*); 5.16 (s, 2H, CH_2); 4.37 (t, *J* = 7.1 Hz, 2H, PCCCCH_2); 4.16–4.04 (m, 4H, 2×POC$H_2$$CH_3$); 2.25 (s, 3H, CH_3); 2.05 (qv, *J* = 7.1 Hz, 2H, PCCCH_2); 1.79 (dt, *J* = 15.5 Hz, *J* = 7.1 Hz, 2H, PCH_2); 1.71–1.63 (m, 2H, PCCH_2); 1.33 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$CH_3); ^{13}C NMR (151 MHz, CD_3OD): δ = 171.5; 163.1; 157.0; 149.4; 142.1; 124.1; 96.9; 61.8 (d, *J* = 6.6 Hz, POC); 49.3; 44.9; 30.2 (d, *J* = 16.2 Hz, PCC*C*); 23.7 (d, *J* = 140.4 Hz, PC); 23.2; 19.1 (d, *J* = 5.2 Hz, POC*C*); 15.4; ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.90 ppm. Anal. Calcd. for $C_{17}H_{27}N_6O_5P$: C, 47.88; H, 6.38; N, 19.71. Found: C, 48.03; H, 6.22; N, 19.75.

^1H NMR



^{13}C NMR

SpinWorks 3: no title



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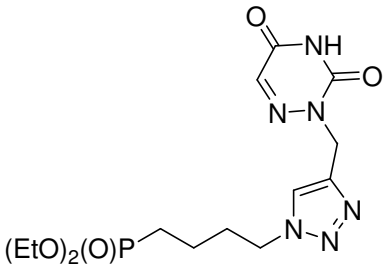
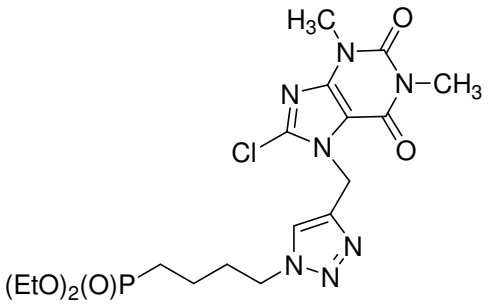
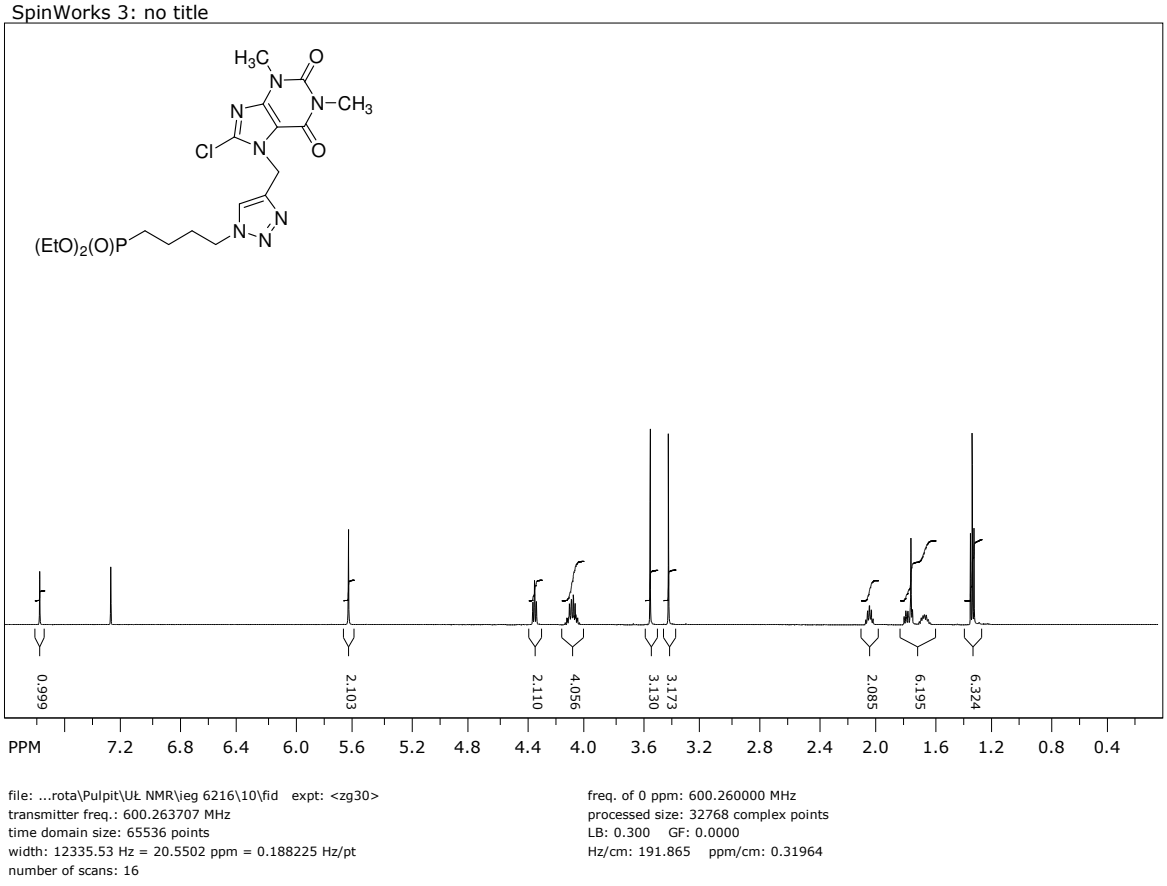


Diethyl 4-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23f**. Colourless oil; IR (film): ν = 3439, 3231, 3141, 3012, 2909, 1730, 1676, 1216, 1027, 754 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 11.58 (brs, 1H, NH); 7.70 (s, 1H, *H*C5′); 7.39 (s, 1H, *H*C=N); 5.20 (s, 2H, CH_2); 4.33 (t, *J* = 7.2 Hz, 2H, PCCCC*H*$_2$); 4.15–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.01 (qv, *J* = 7.1 Hz, 2H, PCCC*H*$_2$); 1.83–1.56 (m, 4H, PC*H*$_2$C*H*$_2$); 1.31 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.9 (s, C=O); 148.9 (s, C=O); 141.5; 134.6; 123.8; 61.8 (d, *J* = 6.6 Hz, POC); 49.7; 34.5; 30.6 (d, *J* = 15.5 Hz, PCC*C*); 24.7 (d, *J* = 141.4 Hz, PC); 19.5 (d, *J* = 4.9 Hz, PC*C*); 16.4 (d, *J* = 6.1 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 32.44 ppm. Anal. Calcd. for $C_{14}H_{23}N_6O_5P$: C, 43.52; H, 6.00; N, 21.75. Found: C, 43.65; H, 5.87; N, 21.69.

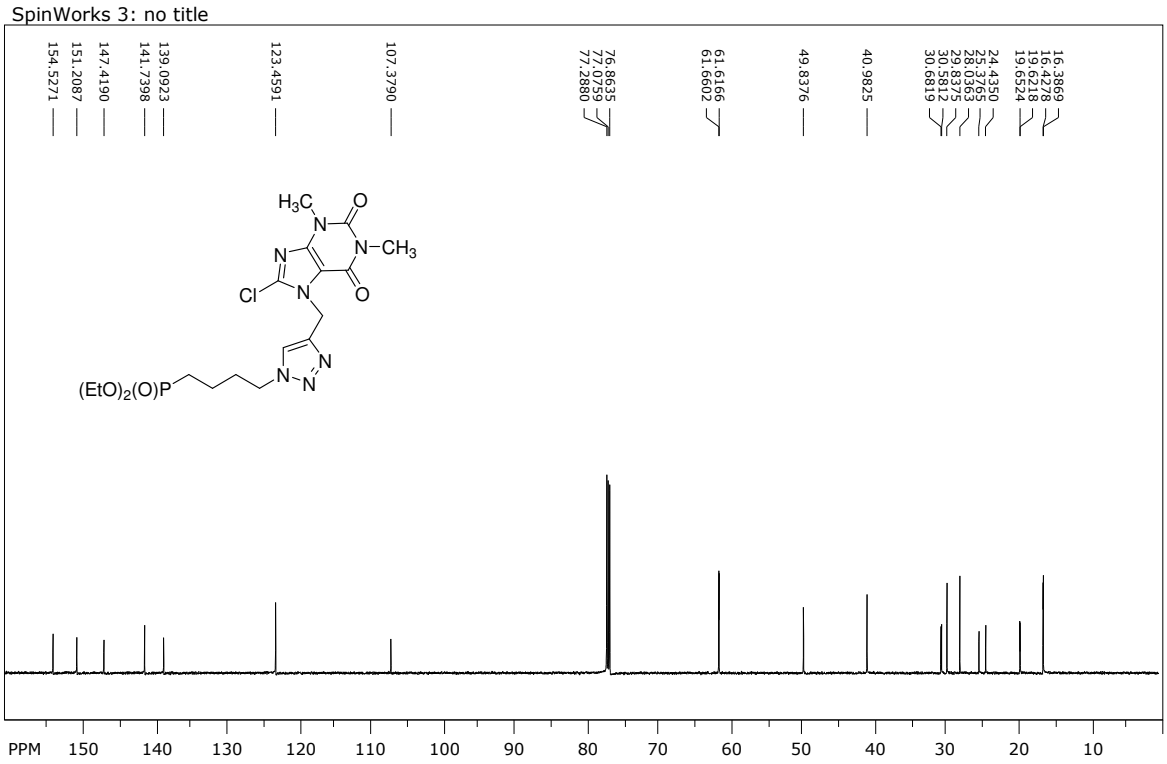


Diethyl 4-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23g**. White solid; m.p.: 69–70°C; IR (KBr): ν = 3013, 2988, 2962, 1707, 1668, 1225, 1015 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.79 (s, 1H, *H*C5′); 5.62 (s, 2H, CH_2); 4.35 (t, *J* = 7.3 Hz, 2H, PCCCC*H*$_2$); 4.14–4.04 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.55 (s, 3H, CH_3); 3.42 (s, 3H, CH_3); 2.04 (qv, *J* = 7.3 Hz, 2H, PCCC*H*$_2$); 1.77 (dt, *J* = 14.8 Hz, *J* = 7.3 Hz, 2H, PC*H*$_2$); 1.69–1.61 (m, 2H, PCC*H*$_2$); 1.32 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 154.5 (s, C=O); 151.2 (s, C=O); 147.4; 141.7; 139.1; 123.5; 107.3; 61.6 (d, *J* = 6.5 Hz, POC); 49.8; 41.0; 30.6 (d, *J* = 15.1 Hz, PCC*C*); 29.8; 28.0; 24.9 (d, *J* = 142.1 Hz, PC); 19.6 (d, *J* = 4.8 Hz, PC*C*); 16.4 (d, *J* = 5.9 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.49 ppm. Anal. Calcd. for $C_{18}H_{27}ClN_7O_5P$: C, 44.31; H, 5.58; N, 20.10. Found: C, 44.50; H, 5.61; N, 20.22.

^{1}H NMR



^{13}C NMR



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number of scans: 512

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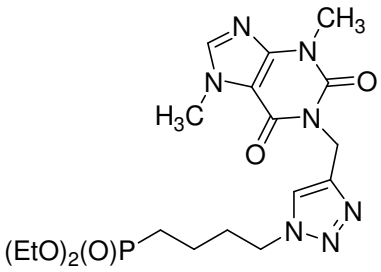
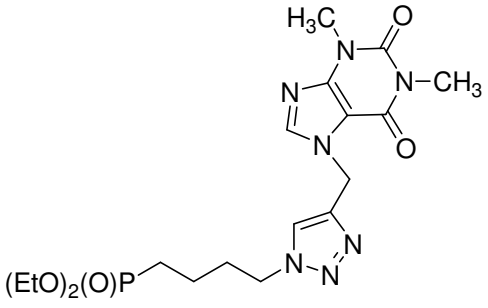
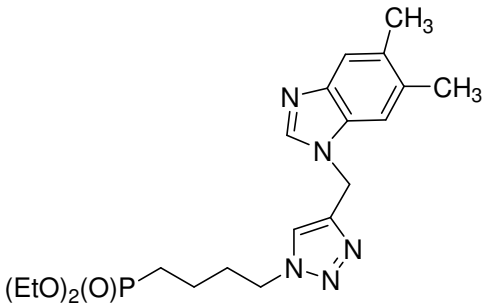


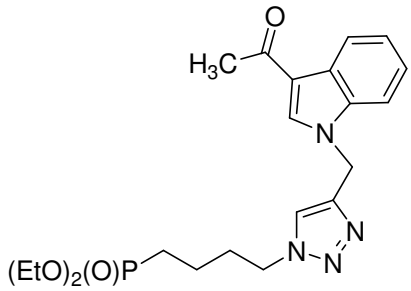
Diethyl 4-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23h**. White solid; m.p.: 59–61°C; IR (KBr): ν = 3432, 3115, 2983, 2952, 1708, 1662, 1235, 1025 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.62 (s, 1H); 7.51 (s, 1H); 5.33 (s, 2H, CH_2); 4.33 (t, *J* = 7.3 Hz, 2H, PCCCC*H*$_2$); 4.13–4.05 (m, 4H, 2×POC*H*$_2$CH$_3$); 4.01 (s, 3H, CH_3); 3.59 (s, 3H, CH_3); 2.02 (qv, *J* = 7.3 Hz, 2H, PCCC*H*$_2$); 1.73 (dt, *J* = 18.0 Hz, *J* = 7.3 Hz, 2H, PC*H*$_2$); 1.63 (dqv, *J* = 14.0 Hz, *J* = 7.3 Hz, 2H, PCC*H*$_2$); 1.32 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 154.8 (s, C=O); 151.3 (s, C=O); 148.9; 143.6; 141.7; 123.1; 107.6; 61.6 (d, *J* = 6.5 Hz, POC); 49.6; 36.0; 33.5; 30.7 (d, *J* = 15.3 Hz, PCC*C*); 29.7; 25.0 (d, *J* = 144.9 Hz, PC); 19.6 (d, *J* = 4.7 Hz, PC*C*); 16.4 (d, *J* = 6.1 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.91 ppm. Anal. Calcd. for $C_{18}H_{28}N_7O_5P$: C, 47.68; H, 6.22; N, 21.62. Found: C, 47.74; H, 6.03; N, 21.71.



Diethyl 4-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23i**. White solid; m.p.: 58–59°C; IR (KBr): ν = 3432, 3115, 2983, 2952, 1708, 1662, 1235, 1025 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.84 (s, 1H); 7.83 (s, 1H); 5.60 (s, 2H, CH_2); 4.37 (t, *J* = 7.1 Hz, 2H, PCCCC*H*$_2$); 4.15–4.05 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.60 (s, 3H, CH_3); 3.44 (s, 3H, CH_3); 2.06 (qv, *J* = 7.1 Hz, 2H, PCCC*H*$_2$); 1.80–1.74 (m, 2H, PC*H*$_2$); 1.69–1.62 (m, 2H, PCC*H*$_2$); 1.33 (t, *J* = 7.4 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.4 (s, C=O); 151.6 (s, C=O); 149.0; 142.2; 141.4; 123.5; 106.5; 61.6 (d, *J* = 6.4 Hz, POC); 49.9; 41.5; 30.6 (d, *J* = 14.7 Hz, PCC*C*); 29.8; 25.0 (d, *J* = 142.2 Hz, PC); 19.6 (d, *J* = 4.5 Hz, PC*C*); 16.4 (d, *J* = 6.4 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.79 ppm. Anal. Calcd. for $C_{18}H_{28}N_7O_5P$: C, 47.68; H, 6.22; N, 21.62. Found: C, 47.80; H, 6.00; N, 21.74.

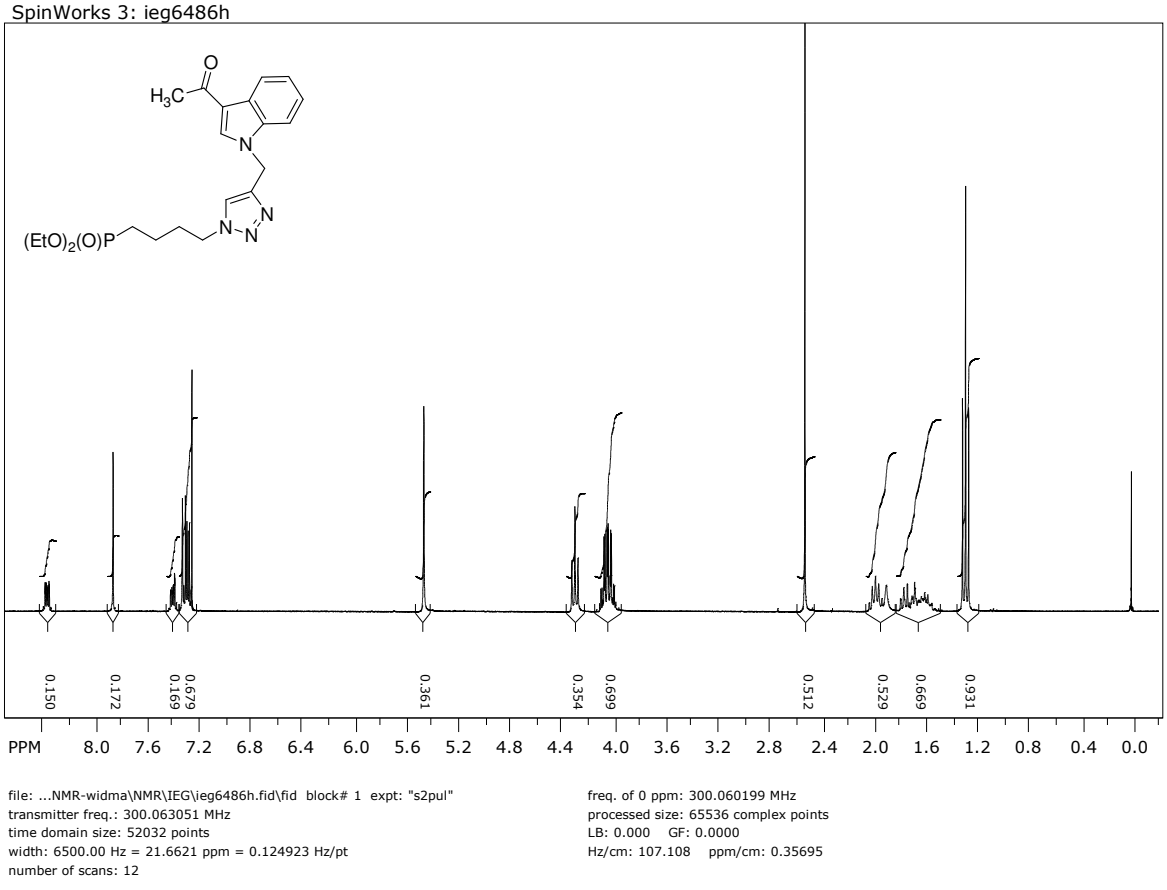


Diethyl 4-{4-[(5,6-dimethylbenzimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23j**. Yellow oil; IR (film): ν = 3303, 3102, 2982, 1219, 1027 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.30 (s, 1H); 7.60 (s, 1H,); 7.30 (s, 1H,); 7.32 (s, 1H,); 5.48 (s, 2H, CH_2); 4.38 (t, *J* = 7.4 Hz, 2H, PCCCC*H*$_2$); 4.16–4.04 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.40 (s, 3H, CH_3); 2.39 (s, 3H, CH_3); 1.99 (qv, *J* = 7.4 Hz, 2H, PCCC*H*$_2$); 1.75 (dt, *J* = 18.2 Hz, *J* = 7.4 Hz, 2H, PC*H*$_2$); 1.63 (dq, *J* = 15.4 Hz, *J* = 7.4 Hz, 2H, PCC*H*$_2$); 1.31 (t, *J* = 7.1 Hz, 6H, 2×POCH$_2$C*H*$_3$);^{13}C NMR (151 MHz, $CDCl_3$): δ = 143.0; 132.7; 130.8; 122.1; 120.3; 61.6 (d, *J* = 6.6 Hz, POC); 49.8; 30.5 (d, *J* = 15.1 Hz, PCC*C*); 24.9 (d, *J* = 142.1 Hz, PC); 20.4; 20.2; 19.5 (d, *J* = 4.7 Hz, PC*C*); 16.4 (d, *J* = 5.8 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 30.84 ppm. Anal. Calcd. for $C_{20}H_{30}N_5O_3P$: C, 57.27; H, 7.21; N, 16.70. Found: C, 57.10; H, 7.08; N, 16.79.

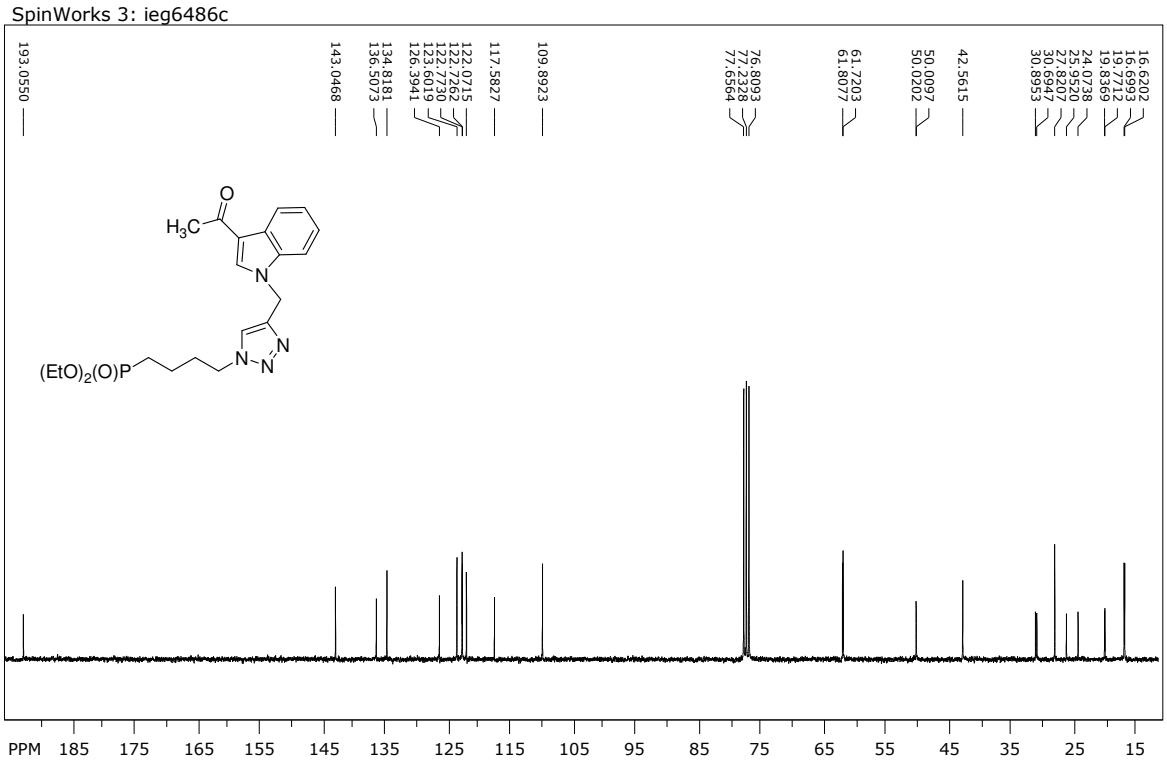


Diethyl 4-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23k**. Colourless oil; IR (film): ν = 3283, 3110, 2983, 2872, 1797, 1231, 1045, 750 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.45–8.38 (m, 1H); 7.76 (s, 1H, *H*C5′); 7.43–7.39 (m, 1H); 7.36–7.27 (m, 3H); 5.42 (s, 2H, CH_2); 4.37 (t, *J* = 7.0 Hz, 2H, PCCCC*H*$_2$); 4.10–4.00 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.53 (s, 3H, CH_3); 1.98 (qv, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 1.85–1.50 (m, 4H, PC*H*$_2$C*H*$_2$); 1.28 (t, *J* = 7.0 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 193.0 (s, C=O); 143.0; 136.5; 134.8; 123.6; 122.8; 122.7; 122.1; 117.5; 109.9; 61.7 (d, *J* = 6.4 Hz, POC); 50.0; 42.5; 30.8 (d, *J* = 15.2 Hz, PCC*C*); 27.8; 24.9 (d, *J* = 141.7 Hz, PC); 19.7 (d, *J* = 4.9 Hz, PC*C*); 16.6 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 31.92 ppm. Anal. Calcd. for $C_{21}H_{29}N_4O_4P$: C, 58.32; H, 6.76; N, 12.96. Found: C, 58.48; H, 6.81; N, 13.10.

^1H NMR



^{13}C NMR



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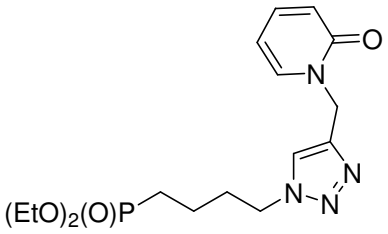
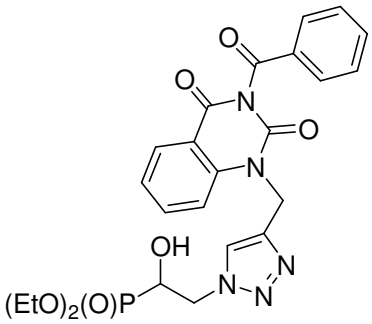
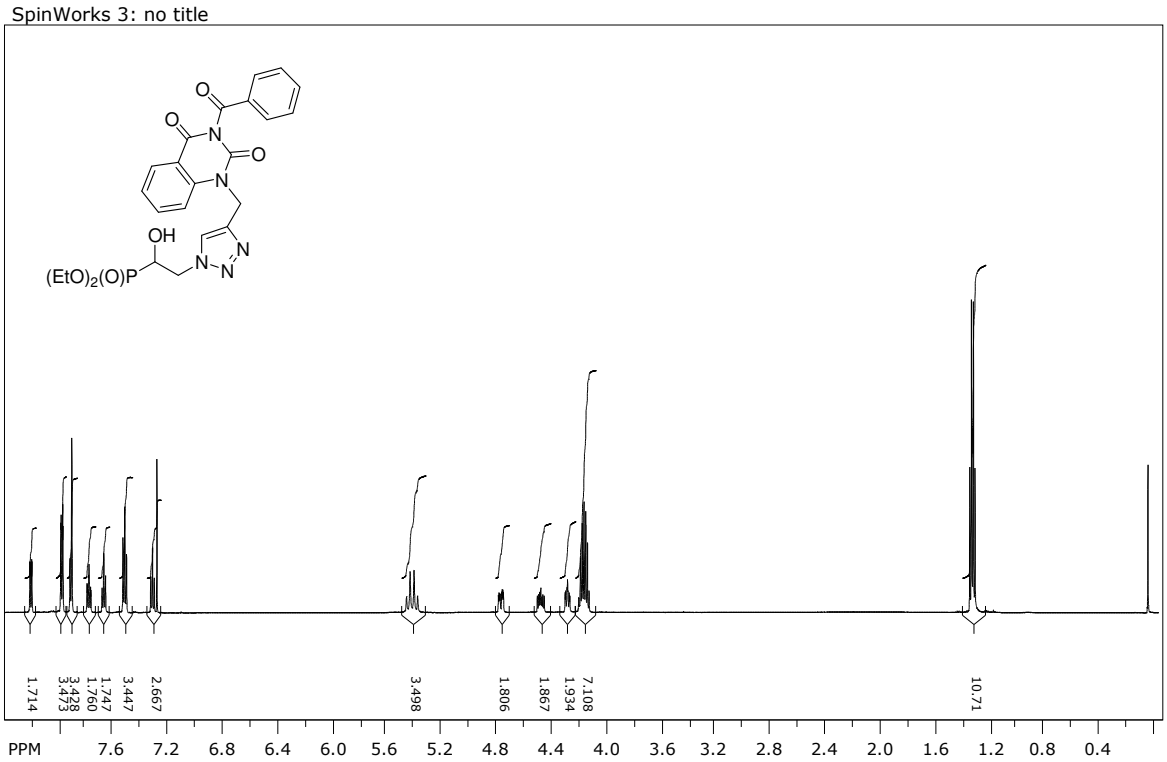


Diethyl 4-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}butylphosphonate **23l**. Brown oil; IR (film): ν = 3134, 2996, 2935, 1659, 1222; 1020, 968 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.78 (s, 1H, *H*C5′); 7.60 (dd, *J* = 6.7 Hz, *J* = 2.2 Hz, 1H); 7.38 (ddd, *J* = 9.1 Hz, *J* = 6.7 Hz, *J* = 2.2 Hz, 1H); 6.54 (d, *J* = 9.1 Hz, 1H); 6.19 (dt, *J* = 6.7 Hz, *J* = 1.5 Hz, 1H); 5.18 (s, 2H, CH_2); 4.33 (t, *J* = 7.2 Hz, 2H, PCCCC*H*$_2$); 4.17–4.00 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.22–1.96 (m, 2H, PCCC*H*$_2$); 1.82–1.60 (m, 4H, PC*H*$_2$C*H*$_2$); 1.31 (t, *J* = 6.9 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.3 (s, C=O); 142.7 (s, H*C*=C); 140.0; 137.8; 123.9 (s, HC=*C*); 120.8; 106.6; 61.7 (d, *J* = 6.5 Hz, POC); 49.9; 44.7; 30.8 (d, *J* = 15.5 Hz, PCC*C*); 25.1 (d, *J* = 141.7 Hz, PC); 19.8 (d, *J* = 5.2 Hz, PC*C*); 16.6 (d, *J* = 6.0 Hz, POC*C*); 12.2 (s, CH_3); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 32.08 ppm. Anal. Calcd. for $C_{16}H_{25}N_4O_4P$: C, 52.17; H, 6.84; N, 15.21. Found: C, 51.90; H, 6.78; N, 15.11.



Diethyl 2-(4-{[3-benzoyl--2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)-1-hydroxyethylphosphonate **24e**. Colourless oil; IR (film): ν = 3356, 2982, 2831, 1750, 1702, 1668, 1234, 1027, 785, 688 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.16 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H); 7.97–7.94 (m, 2H, 2×*o*-CH); 7.92 (s, 1H, *H*C5′); 7.88 (brd, *J* = 8.3 Hz, 1H); 7.75 (ddd, *J* = 8.3 Hz, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H); 7.68–7.62 (m, 1H, *p*-CH); 7.52–7.46 (m, 2H, 2×*m*-CH); 7.31 (dt, *J* = 7.9 Hz, *J* = 0.6 Hz, 1H); 5.44 (AB, *J* = 15.8 Hz, 1H, CH_aH_b); 5.42 (AB, *J* = 15.8 Hz, 1H, CH_aH_b); 4.77 (ddd, *J* = 14.3 Hz, *J* = 5.3 Hz, *J* = 2.8 Hz, 1H, $PCCH_aH_b$); 4.48 (ddd, *J* = 14.3 Hz, *J* = 10.0 Hz, *J* = 5.8 Hz, 1H, $PCCH_aH_b$); 4.23 (ddd, *J* = 10.3 Hz, *J* = 7.9 Hz, *J* = 2.8 Hz, 1H, PC*H*(OH)); 4.16–4.04 (m, 4H, 2×$POCH_2CH_3$); 1.27 (t, *J* = 7.0 Hz, 3H, $POCH_2CH_3$); 1.26 (t, *J* = 7.0 Hz, 3H, $POCH_2CH_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.6 (s, C=O); 161.0 (s, C=O); 149.4 (s, C=O); 142.0 (s, H*C*=C); 140.2; 136.2; 135.2; 131.6; 130.5; 129.3; 128.8; 125.6 (s, HC=*C*); 123.8; 115.5; 115.4; 67.0 (d, *J* = 163.2 Hz, PC); 63.8 (d, *J* = 7.5 Hz, POC); 63.6 (d, *J* = 7.5 Hz, POC); 51.6 (d, *J* = 10.0 Hz, PC*C*); 39.0; 16.6 (d, *J* = 5.3 Hz, POC*C*); 16.5 (d, *J* = 5.3 Hz, POC*C*);^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 21.21 ppm. Anal. Calcd. for $C_{24}H_{26}N_5O_7P$: C, 54.65; H, 4.97; N, 13.28. Found: C, 54.47; H, 5.11; N, 13.12.

^{1}H NMR



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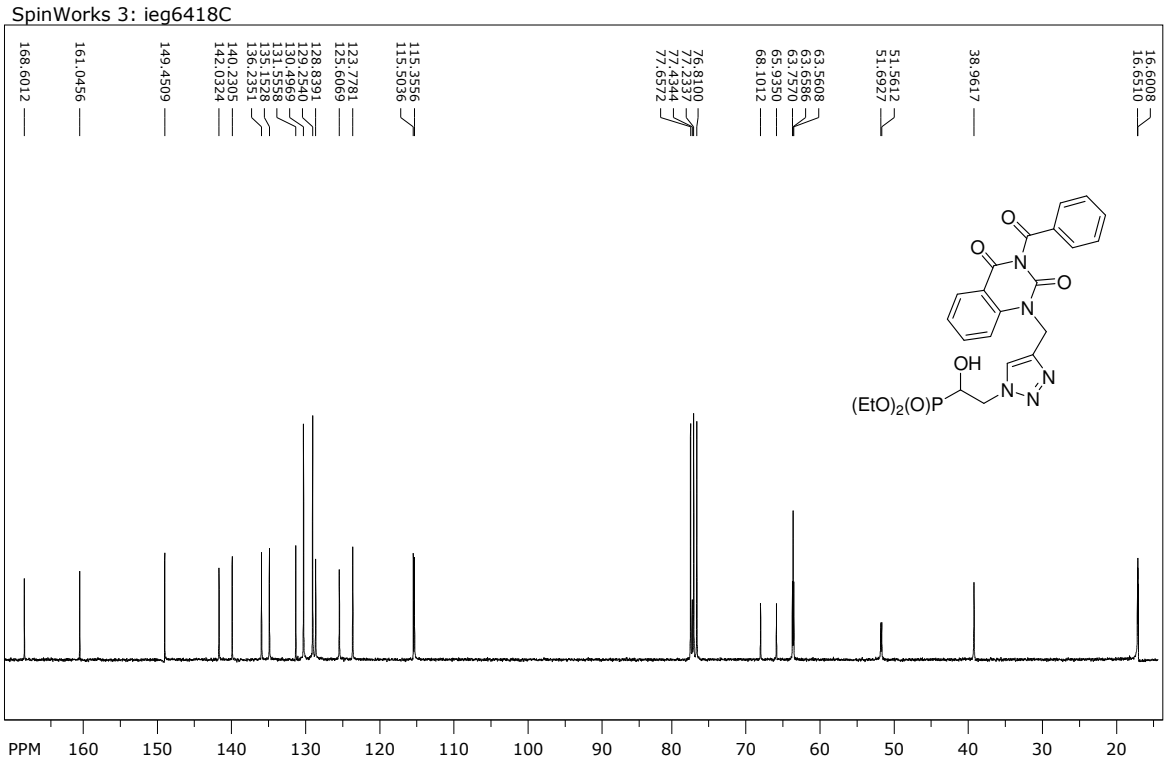
^{13}C NMR



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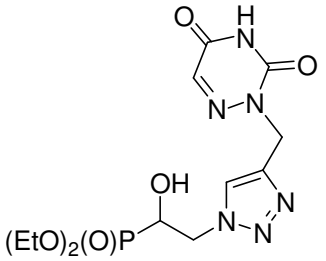
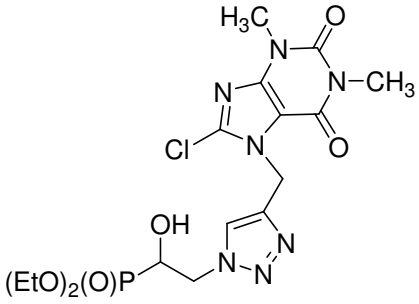
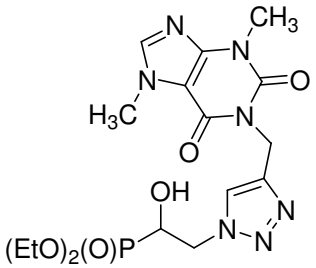


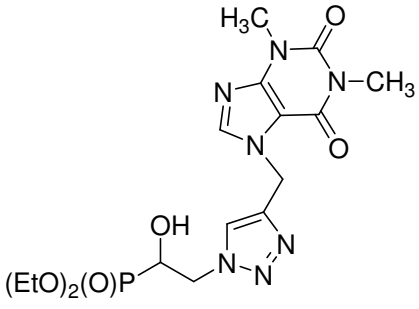
Diethyl 2-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24f**. White solid; m.p.: 145–147°C; IR (KBr): ν = 3300, 2913, 2837, 1729,1674, 1023 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 12.07 (s, 1H, NH); 7.92 (s, 1H); 7.41 (s, 1H); 5.30 (brs, 1H, OH); 5.15 (s, 2H, CH_2); 4.82 (ddd, *J* = 14.0 Hz, *J* = 4.6 Hz, *J* = 2.2 Hz, 1H, PCCH_aH$_b$); 4.52–4.34 (m, 2H, PC*H*(OH), PCCH$_a$$H_b$); 4.15–4.02 (m, 4H, 2×POCH_2CH$_3$); 1.36 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); 1.34 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.9 (s, C=O); 149.5 (C=O); 141.2 (s, H*C*=C); 135.1 (s, HC=N); 125.7 (s, HC=*C*); 66.8 (d, *J* = 144.0 Hz, PC); 63.8 (d, *J* = 6.6 Hz, POC); 63.7 (d, *J* = 6.6 Hz, POC); 51.7 (d, *J* = 10.6 Hz); 34.7; 16.6 (d, *J* = 5.5 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 21.60 ppm. Anal. Calcd. for $C_{12}H_{19}N_6O_6P$: C, 38.51; H, 5.12; N, 22.45. Found: C, 38.27; H, 5.02; N, 22.55.



Diethyl 2-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24g**. White solid; m.p.: 183–184°C; IR (KBr): ν = 3281, 3057, 2986, 1707, 1665, 1216, 1047 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.95 (s, 1H, *H*C5′); 5.61 (s, 2H, CH_2); 5.08 (t, *J* = 5.7 Hz, 1H, OH); 4.75 (ddd, *J* = 14.2 Hz, *J* = 5.1 Hz, *J* = 2.6 Hz, 1H, PCCH_aH$_b$); 4.44 (ddd, *J* = 14.2 Hz, *J* = 10.0 Hz, *J* = 5.6 Hz, 1H, PCCH$_a$$H_b$); 4.28 (dddd, *J* = 10.0 Hz, *J* = 8.0 Hz, *J* = 5.7 Hz, *J* = 5.1 Hz, 1H, PC*H*(OH)); 4.21–4.10 (m, 4H, 2×POCH_2CH$_3$); 3.51 (s, 3H, CH_3); 3.37 (s, 3H, CH_3); 1.33 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.32 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.4 (s, C=O); 151.1 (s, C=O); 147.3; 139.0; 125.2; 107.4; 67.0 (d, *J* = 163.8 Hz, PC); 63.7 (d, *J* = 7.2 Hz, POC); 63.5 (d, *J* = 7.2 Hz, POC); 51.7 (d, *J* = 9.7 Hz, PC*C*); 41.1; 30.0; 28.2; 16.6 (d, *J* = 5.5 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 20.42 ppm. Anal. Calcd. for $C_{16}H_{23}ClN_7O_6P$: C, 40.39; H, 4.87; N, 20.61. Found: C, 40.22; H, 5.00; N, 20.56.

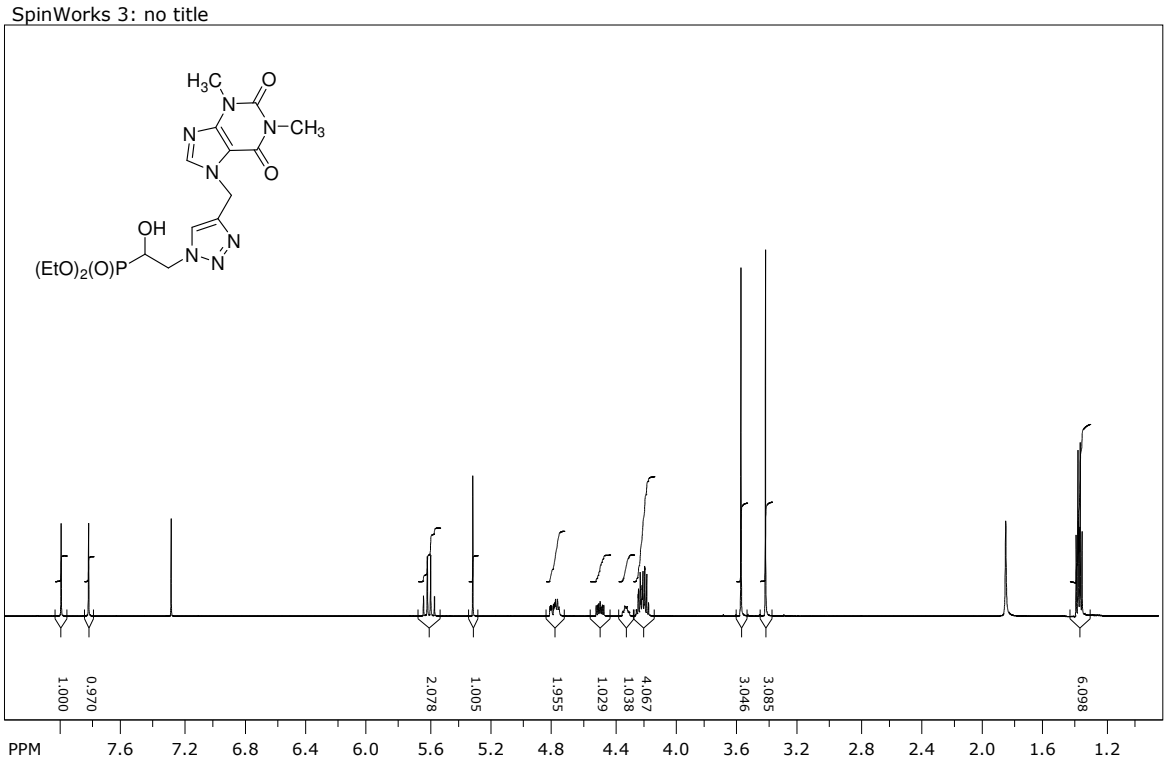


Diethyl 2-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24h**. White powder; m.p.: 166–168°C; IR (KBr): ν = 3237, 2989, 1708, 1663, 1235, 1023 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.80 (s, 1H); 7.53 (s, 1H, *H*C5′); 5.35 (AB, *J* = 14.6 Hz, 1H, CH_aH$_b$); 5.30 (AB, *J* = 14.6 Hz, 1H, CH$_a$$H_b$); 4.79 (ddd, *J* = 14.2 Hz, *J* = 6.0 Hz, *J* = 2.5 Hz, 1H, PCCH_aH$_b$); 4.47 (ddd, *J* = 14.2 Hz, *J* = 9.7 Hz, *J* = 5.2 Hz, 1H, PCCH$_a$$H_b$); 4.40–4.34 (m, 1H, PC*H*(OH)); 4.27–4.15 (m, 4H, 2×POCH_2CH$_3$); 4.06 (dd, *J* = 9.4 Hz, *J* = 5.8 Hz, 1H); 4.01 (s, 3H, CH_3); 3.60 (s, 3H, CH_3); 1.38 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.36 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (151.5 MHz, $CDCl_3$): δ = 154.7 (s, C=O); 151.2 (s, C=O); 148.8; 143.2; 141.9; 124.9; 107.6; 67.0 (d, *J* = 165.1 Hz, PC); 64.4 (d, *J* = 6.9 Hz, POC); 63.2 (d, *J* = 6.9 Hz, POC); 51.7 (d, *J* = 9.6 Hz, PC*C*); 36.0; 33.6; 29.7; 16.4 (d, *J* = 5.3 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 19.86 ppm. Anal. Calcd. for $C_{16}H_{24}N_7O_6P$: C, 43.54; H, 5.48; N, 22.21. Found: C, 43.67; H, 5.28; N, 22.30.



Diethyl 2-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24i**. White powder; m.p.: 164–165°C; IR (KBr): ν = 3264, 3152, 2990, 1705, 1660, 1224, 1025 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.00 (s, 1H); 7.84 (s, 1H, *H*C5′); 5.62 (AB, *J* = 15.0 Hz, 1H, CH_aH$_b$); 5.58 (AB, *J* = 15.0 Hz, 1H, CH$_a$$H_b$); 4.80 (ddd, *J* = 14.3 Hz, *J* = 5.2 Hz, *J* = 2.7 Hz, 1H, PCCH_aH$_b$); 4.78 (dd, *J* = 13.3 Hz, *J* = 5.9 Hz, 1H); 4.49 (ddd, *J* = 14.3 Hz, *J* = 10.0 Hz, *J* = 5.6 Hz, 1H, PCCH$_a$$H_b$); 4.36–4.28 (m, 1H, PC*H*(OH)); 4.27–4.16 (m, 4H, 2×POCH_2CH$_3$); 3.57 (s, 3H, CH_3); 3.41 (s, 3H, CH_3); 1.37 (t, *J* = 7.1 Hz, 3H, POCH$_2$CH_3); 1.36 (t, *J* = 7.1 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 155.4 (s, C=O); 151.6 (s, C=O); 148.9; 141.8; 141.5; 125.4; 106.5; 67.0 (d, *J* = 164.6 Hz, PC); 63.6 (d, *J* = 7.4 Hz, POC); 63.4 (d, *J* = 7.4 Hz, POC); 51.7 (d, *J* = 9.6 Hz, PC*C*); 41.4; 29.8; 27.9; 16.4 (d, *J* = 5.9 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 19.90 ppm. Anal. Calcd. for $C_{16}H_{24}N_7O_6P$: C, 43.54; H, 5.48; N, 22.21. Found: C, 43.38; H, 5.55; N, 22.30.

^{1}H NMR



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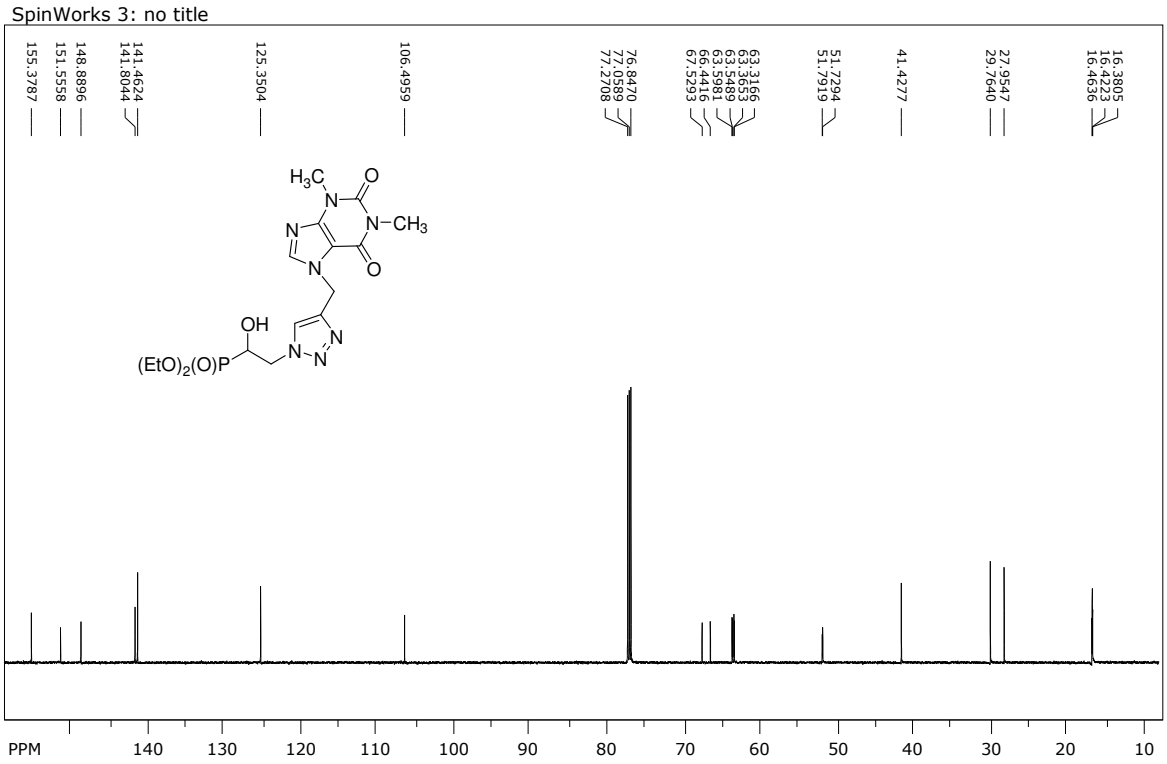
^{13}C NMR



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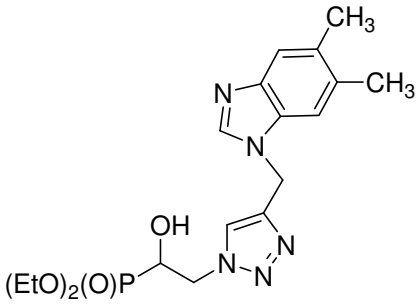
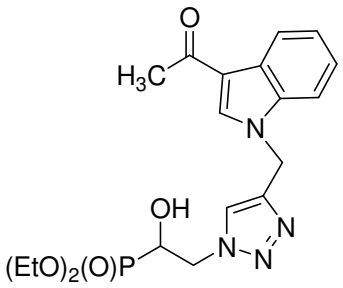
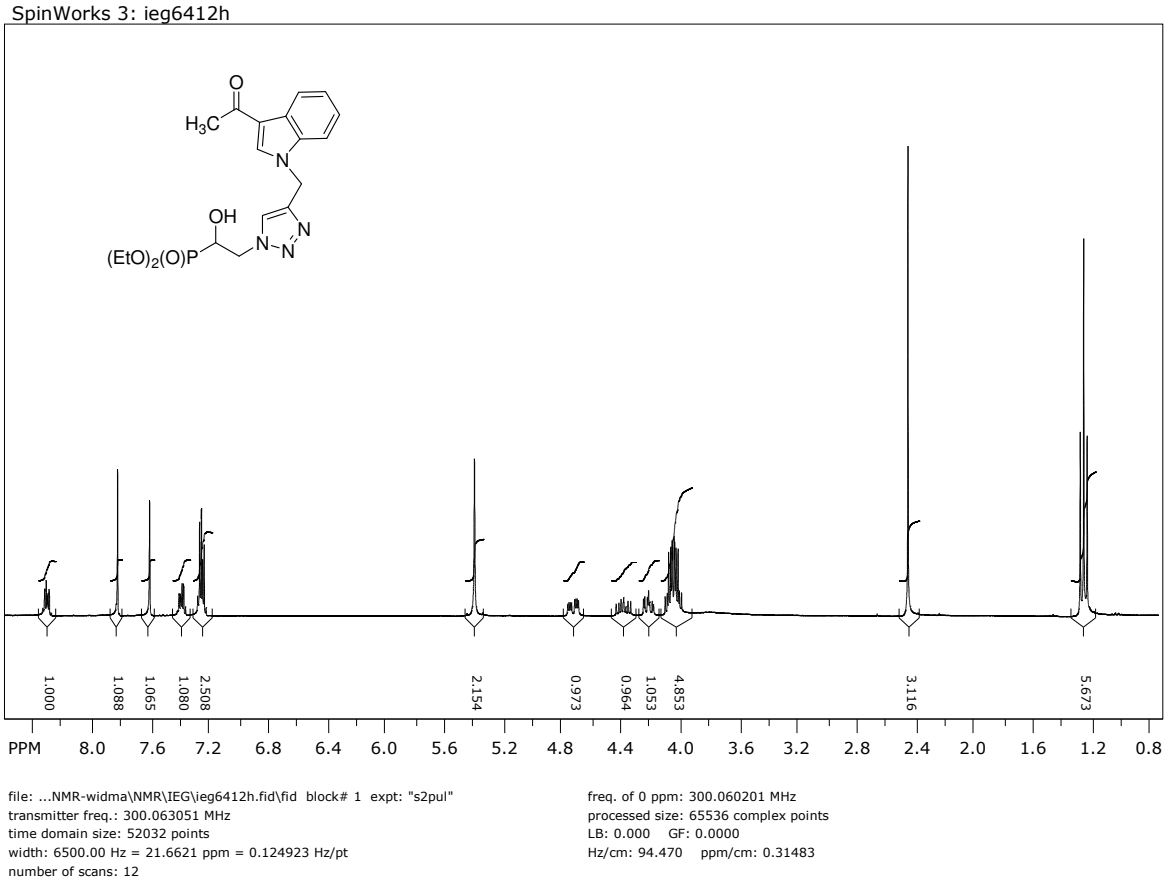


Diethyl 2-{4-[(5,6-dimethylbenzoimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24j**. Yellow oil; IR (film): ν = 3131, 2990, 2945, 1217, 1048, 757 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.91 (s, 1H); 7.76 (s, 1H); 7.43 (s, 1H); 7.23 (s, 1H); 5.38 (AB, *J* = 15.7 Hz, 1H, CH_aH$_b$); 5.34 (AB, *J* = 15.7 Hz, 1H, CH$_a$$H_b$); 4.82 (ddd, *J* = 14.2 Hz, *J* = 4.9 Hz, *J* = 2.5 Hz, 1H, PCCH_aH$_b$); 4.46 (ddd, *J* = 14.2 Hz, *J* = 9.9 Hz, *J* = 5.3 Hz, 1H, PCCH$_a$$H_b$); 4.31 (dt, *J* = 9.9 Hz, *J* = 5.2 Hz, 1H, PC*H*(OH)); 4.12–4.06 (m, 4H, 2×POCH_2CH$_3$); 2.34 (s, 3H, CH$_3$); 2.33 (s, 3H, CH$_3$); 1.32 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.30 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (151 MHz, $CDCl_3$): δ = 142.1; 141.5; 141.2; 132.7; 131.7; 131.6; 124.5; 119.6; 110.1; 66.6 (d, *J* = 166.1 Hz, PC); 63.4 (d, *J* = 7.1 Hz, POC); 63.2 (d, *J* = 7.1 Hz, POC); 51.7 (d, *J* = 9.6 Hz, PC*C*); 40.2; 20.7; 20.4; 16.7 (d, *J* = 5.4 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 21.28 ppm. Anal. Calcd. for $C_{18}H_{26}N_5O_4P$: C, 53.07; H, 6.43; N, 17.19. Found: C, 52.88; H, 6.17; N, 17.05.



Diethyl 2-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethylphosphonate **24k**. Colourless oil; IR (film): ν = 3266, 2959, 2911, 1642, 1528, 1390, 1217, 1024, 754 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.36–8.26 (m, 1H); 7.84 (s, 1H, *H*C5′); 7.62 (s, 1H); 7.43–7.35 (m, 1H); 7.30–7.23 (m, 2H); 5.46 (AB, J = 15.4 Hz, 1H, C*H*$_a$H$_b$); 5.44 (AB, J = 15.4 Hz, 1H, CH$_a$*H*$_b$); 4.77 (ddd, *J* = 14.3 Hz, *J* = 6.0 Hz, *J* = 2.6 Hz, 1H, PCC*H*$_a$H$_b$); 4.44 (ddd, *J* = 14.3 Hz, *J* = 10.0 Hz, *J* = 5.6 Hz, 1H, PCCH$_a$*H*$_b$); 4.21 (ddd, *J* = 10.0 Hz, *J* = 7.9 Hz, *J* = 2.6 Hz, 1H, PC*H*(OH)); 4.14–4.06 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.85 (brs, 1H, OH); 2.51 (s, 3H, CH_3); 1.29 (t, *J* = 6.8 Hz, 6H, 2×POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 193.2 (s, C=O); 142.6; 136.6; 135.0; 126.4; 124.2; 123.6; 122.8; 122.7; 117.5; 110.0; 66.2 (d, *J* = 159.3 Hz, PC); 63.4 (d, *J* = 7.0 Hz, POC); 63.3 (d, *J* = 7.0 Hz, POC); 51.9 (d, *J* = 9.7 Hz, PC*C*); 42.4; 27.7 (s, CH_3); 16.6 (d, *J* = 5.4 Hz, POC*C*); 16.5 (d, *J* = 5.4 Hz, POC*C*);^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 21.03 ppm. Anal. Calcd. for $C_{19}H_{25}N_4O_5P$: C, 54.28; H, 5.99; N, 13.33. Found: C, 54.10; H, 6.12; N, 13.20.

^1H NMR



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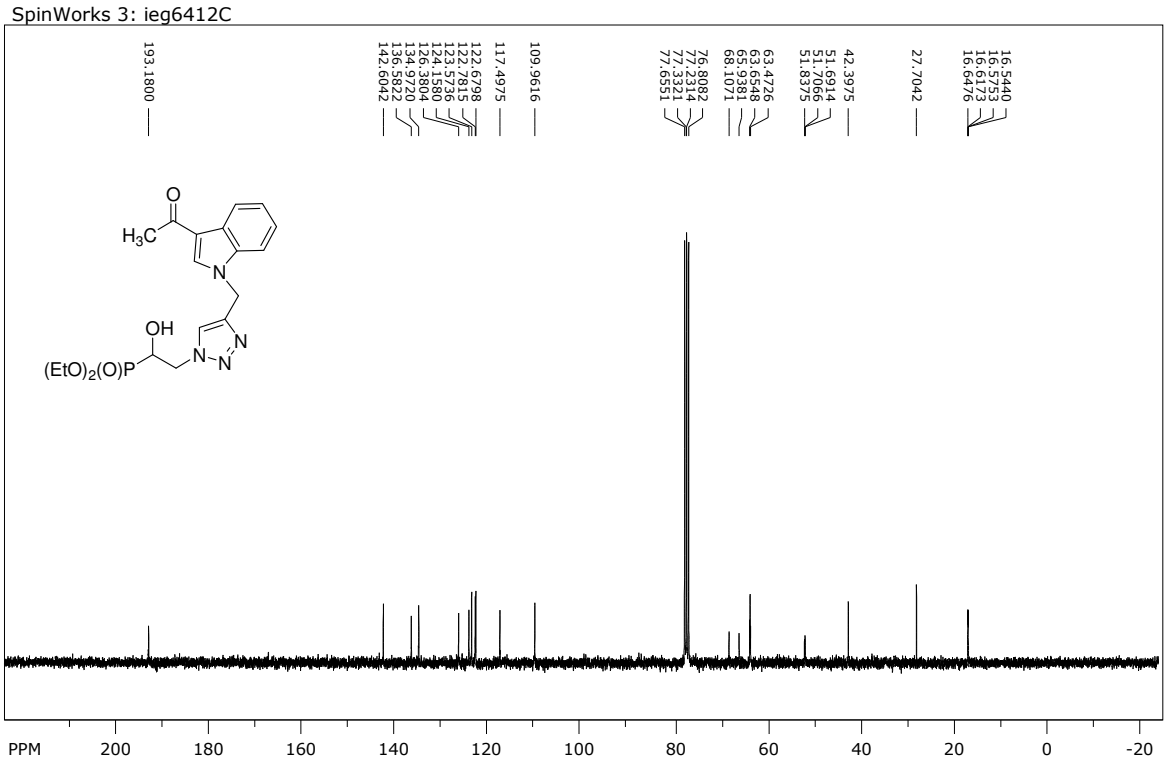
^{13}C NMR



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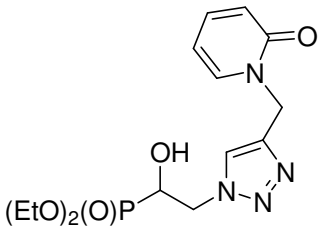
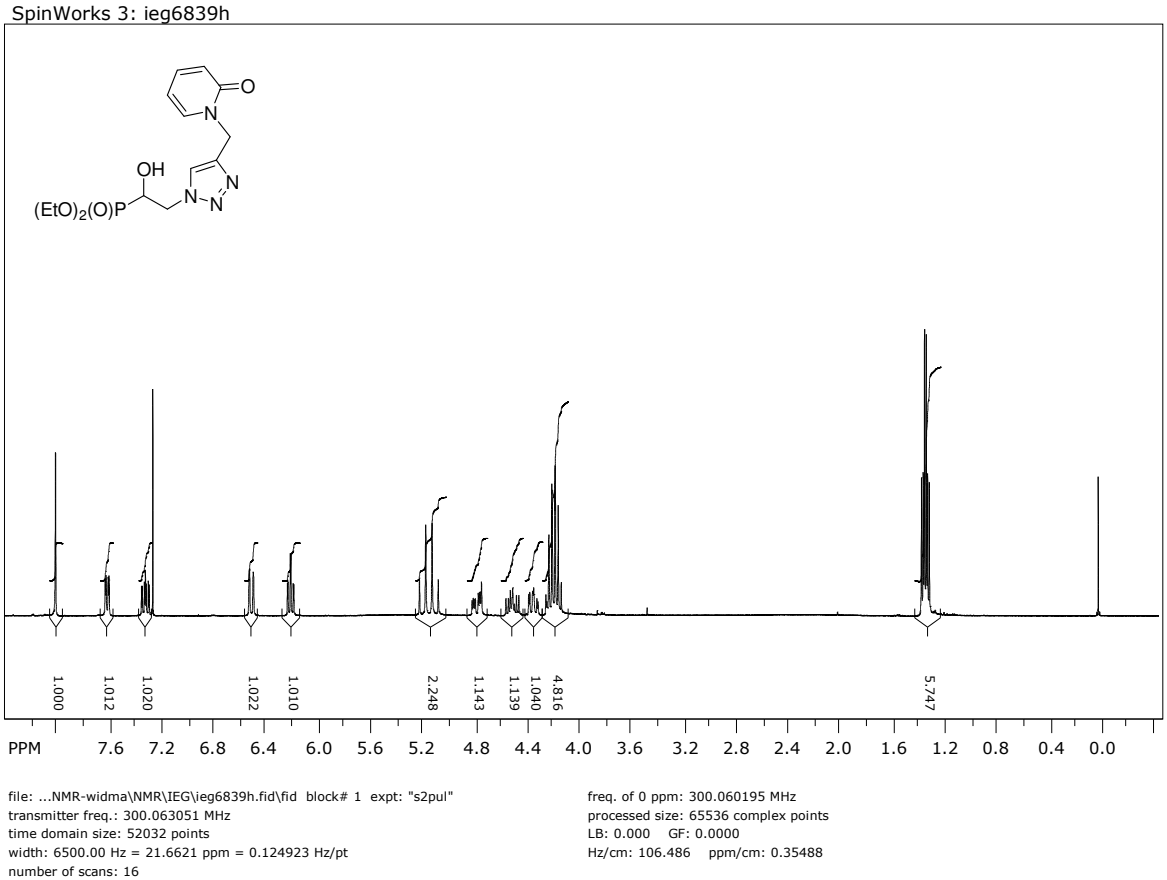


Diethyl 1-hydroxy-2-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}ethylphosphonate **24l**. Brown oil; IR (film): ν = 3274, 2984, 2831, 1673, 1027 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.03 (s, 1H); 7.64 (ddd, *J* = 6.7 Hz, *J* = 2.0 Hz, *J* = 0.6 Hz, 1H); 7.36 (ddd, *J* = 9.2 Hz, *J* = 6.7 Hz, *J* = 2.0 Hz, 1H); 6.52 (dd, *J* = 9.2 Hz, *J* = 0.6 Hz, 1H); 6.22 (dt, *J* = 6.7 Hz, *J* = 1.3 Hz, 1H); 5.20 (AB, *J* = 14.3 Hz, 1H, CH_aH$_b$); 5.12 (AB, *J* = 14.3 Hz, 1H, CH$_a$$H_b$); 4.79 (ddd, *J* = 14.2 Hz, *J* = 5.0 Hz, *J* = 2.6 Hz, 1H, PCCH_aH$_b$); 4.51 (ddd, *J* = 14.2 Hz, *J* = 10.0 Hz, *J* = 5.0 Hz, 1H, PCCH$_a$$H_b$); 4.36 (ddd, *J* = 10.0 Hz, *J* = 8.9 Hz, *J* = 2.6 Hz, 1H, PC*H*(OH)); 4.26–4.14 (m, 4H, 2×POCH_2CH$_3$); 2.56 (brs, 1H, OH); 1.35 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.3 (s, C=O); 141.9 (s, H*C*=C); 140.2; 137.8; 125.6 (s, HC=*C*); 120.2; 106.9; 66.7 (d, *J* = 164.9 Hz, PC); 63.3 (d, *J* = 7.1 Hz, POC); 63.2 (d, *J* = 7.1 Hz, POC); 51.8 (d, *J* = 10.4 Hz, PC*C*); 44.5; 16.5 (d, *J* = 5.2 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 21.29 ppm. Anal. Calcd. for $C_{14}H_{21}N_4O_5P$: C, 47.19; H, 5.94; N, 15.72. Found: C, 47.01; H, 6.10; N, 15.80.

^1H NMR



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number of scans: 16

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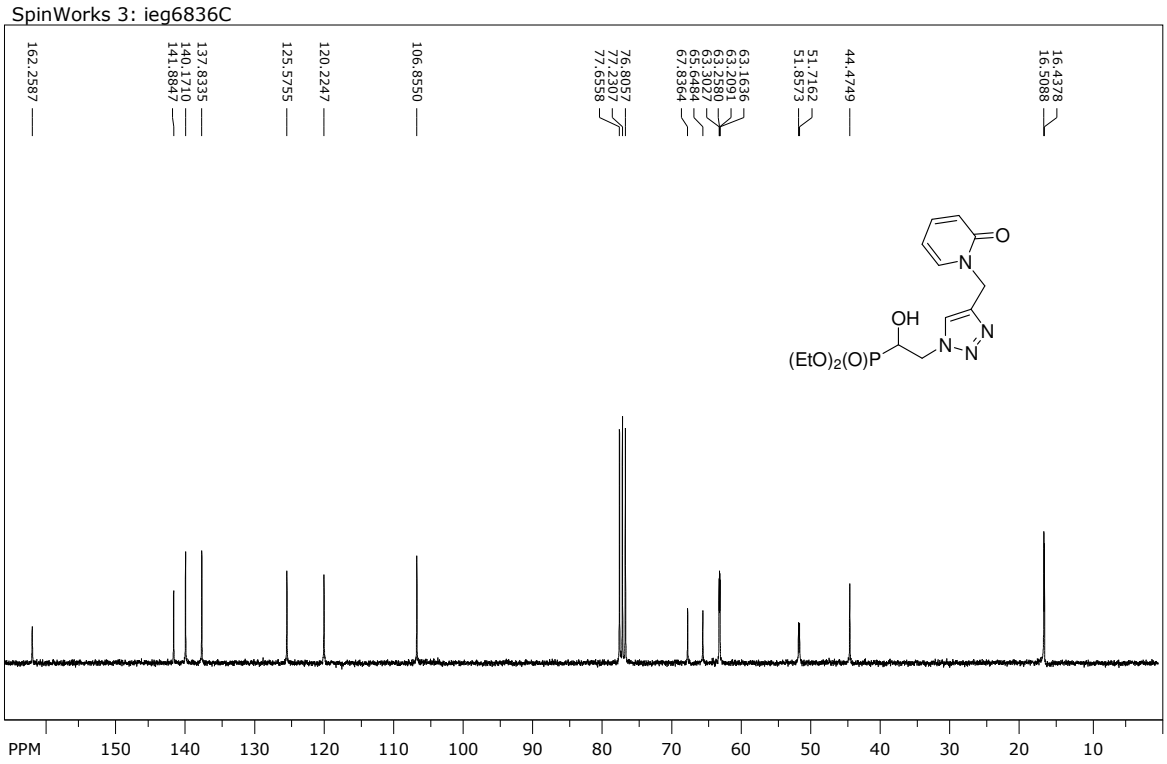
Hz/cm: 106.486 ppm/cm: 0.35488

^{13}C NMR



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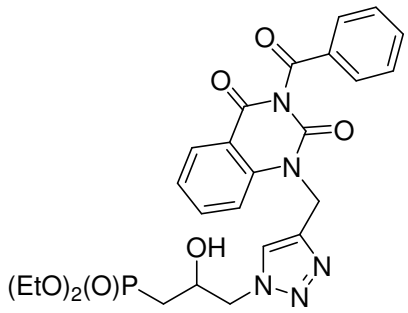
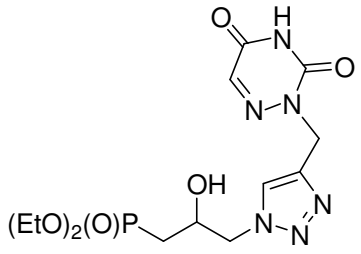
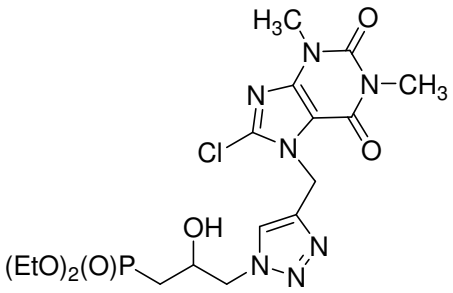


Diethyl 3-(4-{[3-benzoyl-2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)-2-hydroxyethylphosphonate **25e**. White solid; m.p.: 75–77°C; IR (KBr): ν = 3386, 3054, 2988, 2851, 1754, 1709, 1658, 1224, 1025, 795, 694 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.17 (dd, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H); 7.97–7.93 (m, 2H, 2×*o*-CH); 7.87 (brd, *J* = 8.4 Hz, 1H); 7.85 (s, 1H, *H*C5′); 7.75 (ddd, *J* = 8.4 Hz, *J* = 7.9 Hz, *J* = 1.5 Hz, 1H); 7.67–7.61 (m, 1H, *p*-CH); 7.51–7.45 (m, 2H, 2×*m*-CH); 7.29 (dt, *J* = 7.9 Hz, *J* = 0.5 Hz, 1H); 5.44 (AB, *J* = 14.2 Hz, 1H, CH_aH$_b$); 5.36 (AB, *J* = 14.2 Hz, 1H, CH$_a$$H_b$); 4.45 (dd, *J* = 15.4 Hz, *J* = 6.5 Hz, 1H, PCCCH_aH$_b$); 4.44–4.32 (m, 2H, PCC*H*CH$_a$$H_b$); 4.14–4.01 (m, 4H, 2×POCH_2CH$_3$); 3.40 (brs, 1H, OH); 1.96 (ddd, *J* = 19.2 Hz, *J* = 15.1 Hz, *J* = 3.3 Hz, 1H, PCH_aH$_b$); 1.73 (ddd, *J* = 16.4 Hz, *J* = 15.1 Hz, *J* = 9.1 Hz, 1H, PCH$_a$$H_b$); 1.30 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.27 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.6 (s, C=O); 161.0 (s, C=O); 149.5 (s, C=O); 142.3 (s, H*C*=C); 140.3; 136.3; 135.2; 131.6; 130.6; 129.3; 128.9; 125.4 (s, HC=*C*); 123.8; 115.6; 115.4; 65.5 (d, *J* = 4.0 Hz, PC*C*); 62.5 (d, *J* = 5.8 Hz, POC); 62.4 (d, *J* = 5.8 Hz, POC); 52.4 (d, *J* = 14.1 Hz, PCC*C*); 39.0; 30.0 (d, *J* = 140.4 Hz, PC); 16.6 (d, *J* = 5.2 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 29.27 ppm. Anal. Calcd. for $C_{25}H_{28}N_5O_7P$: C, 55.45; H, 5.21; N, 12.93. Found: C, 55.28; H, 5.15; N, 13.11.



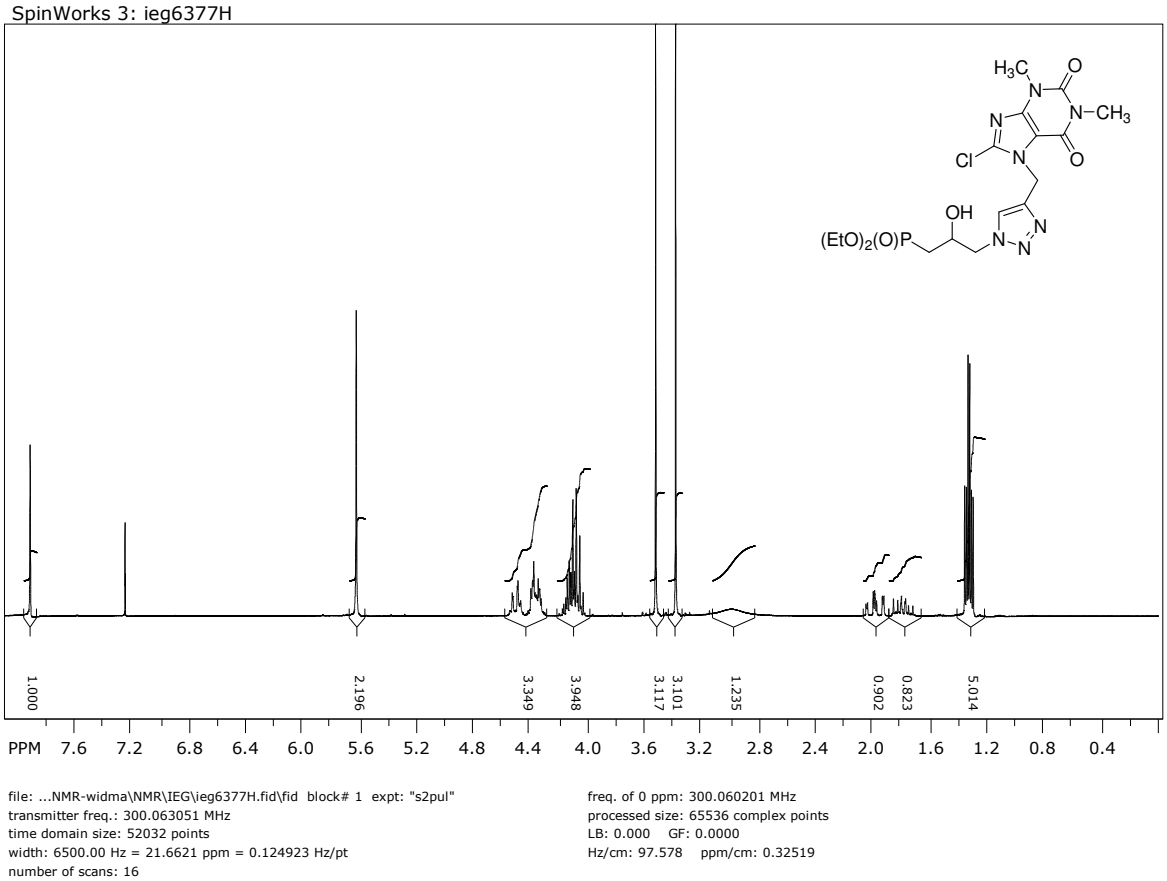
Diethyl 3-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25f**. Colourless oil; IR (film): ν = 3302, 2986, 2913, 2833, 1730, 1673, 1028, 970 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 11.80 (s, 1H, NH); 7.89 (s, 1H); 7.46 (s, 1H); 5.25 (AB, *J* = 15.6 Hz, 1H, CH_aH$_b$); 5.19 (AB, *J* = 15.6 Hz, 1H, CH$_a$$H_b$); 4.55 (dd, *J* = 13.7 Hz, *J* = 3.0 Hz, 1H, PCCCH_aH$_b$); 4.43 (ddddd, *J* = 8.6 Hz, *J* = 7.0 Hz, *J* = 3.9 Hz, *J* = 3.0 Hz, 1H, PCC*H*(OH)); 4.38 (dd, *J* = 13.7 Hz, *J* = 7.0 Hz, 1H, PCCCH$_a$$H_b$); 4.19–4.02 (m, 4H, 2×POCH_2CH$_3$); 2.05 (ddd, 2H, *J* = 19.2 Hz, *J* = 15.2 Hz, *J* = 3.9 Hz,PCH_aH$_b$); 1.97 (ddd, 2H, *J* = 17.6 Hz, *J* = 15.2 Hz, *J* = 8.6 Hz,PCH$_a$$H_b$);1.31 (t, *J* = 7.2 Hz, 3H, POCH$_2$CH_3); 1.30 (t, *J* = 7.2 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 156.0 (s, C=O); 149.4 (C=O); 141.4 (s, H*C*=C); 135.1 (s, HC=N); 125.7 (s, HC=*C*); 65.6 (s, PC*C*); 62.7 (d, *J* = 6.3 Hz, POC); 62.4 (d, *J* = 6.3 Hz, POC); 56.2 (d, *J* = 16.6 Hz, PCC*C*); 34.8; 31.0 (d, *J* = 140.9 Hz, PC); 16.6 (d, *J* = 6.0 Hz,

POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 29.38 ppm. Anal. Calcd. for $C_{13}H_{21}N_6O_6P$: C, 40.21; H, 5.45; N, 21.64. Found: C, 40.08; H, 5.59; N, 21.72.

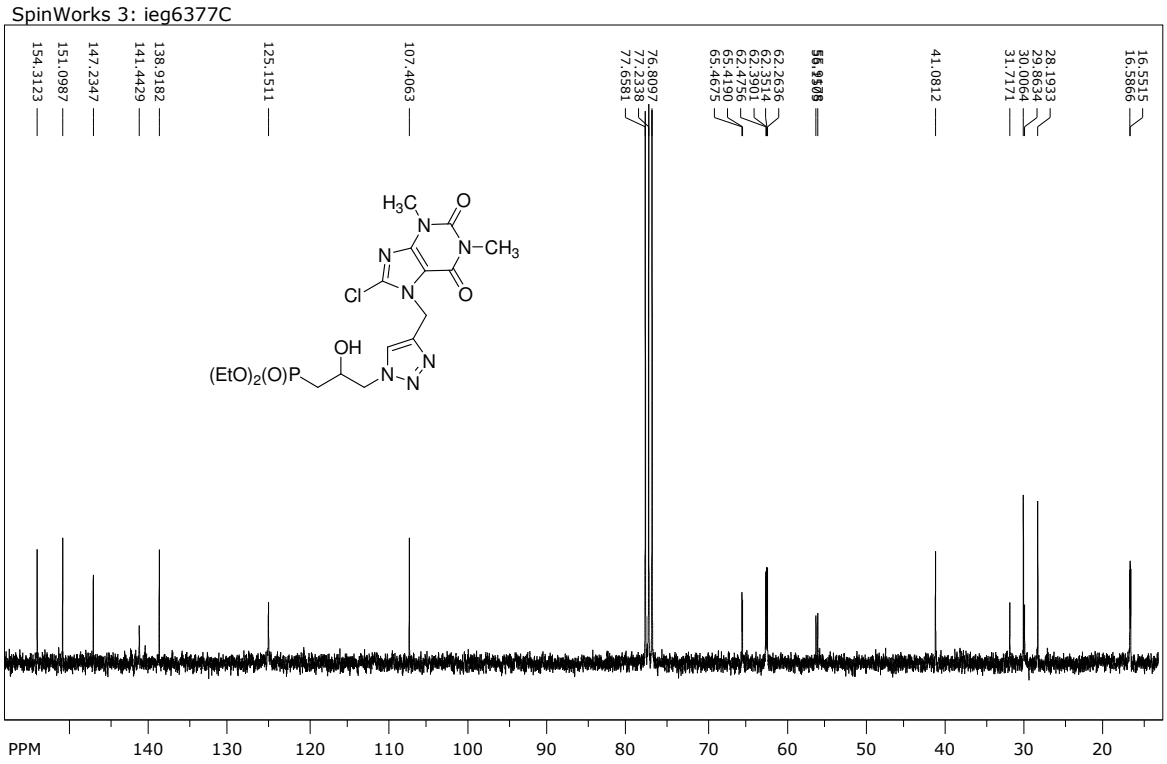


Diethyl 3-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25g**. White solid; m.p.: 137–139°C; IR (KBr): ν = 3354, 3151, 2983, 2928, 1702, 1675, 1221, 1027 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.93 (s, 1H, *H*C5′); 5.63 (s, 2H, CH_2); 4.53–4.33 (m, 3H, PCC*H*C*H*$_2$); 4.17–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.52 (s, 3H, CH_3); 3.38 (s, 3H, CH_3); 1.98 (ddd, *J* = 19.0 Hz, *J* = 15.3 Hz, *J* = 3.1 Hz, 1H, PC*H*$_a$H$_b$); 1.77 (ddd, *J* = 16.8 Hz, *J* = 15.3 Hz, *J* = 9.2 Hz, 1H, PCH$_a$*H*$_b$); 1.32 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); 1.31 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.3 (s, C=O); 151.1 (s, C=O); 147.2; 141.4; 138.9; 125.2; 107.4; 65.4 (d, *J* = 3.7 Hz, PC*C*); 62.4 (d, *J* = 6.5 Hz, POC); 62.3 (d, *J* = 6.5 Hz, POC); 56.0 (d, *J* = 18.4 Hz, PCC*C*); 41.1; 30.8 (d, *J* = 135.9 Hz, PC); 30.0; 28.2; 16.6 (d, *J* = 5.7 Hz, POC*C*); 16.5 (d, *J* = 5.7 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 28.72 ppm. Anal. Calcd. for $C_{17}H_{25}ClN_7O_6P$: C, 41.68; H, 5.14; N, 20.02. Found: C, 41.67; H, 5.08; N, 19.90.

^1H NMR



^{13}C NMR



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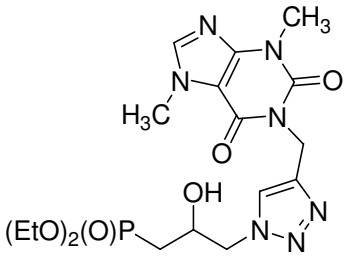
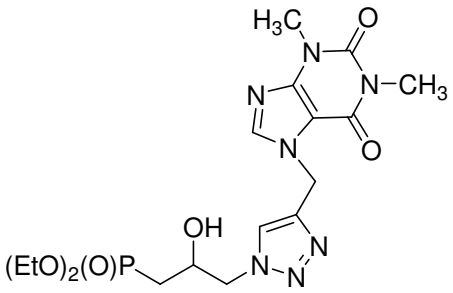
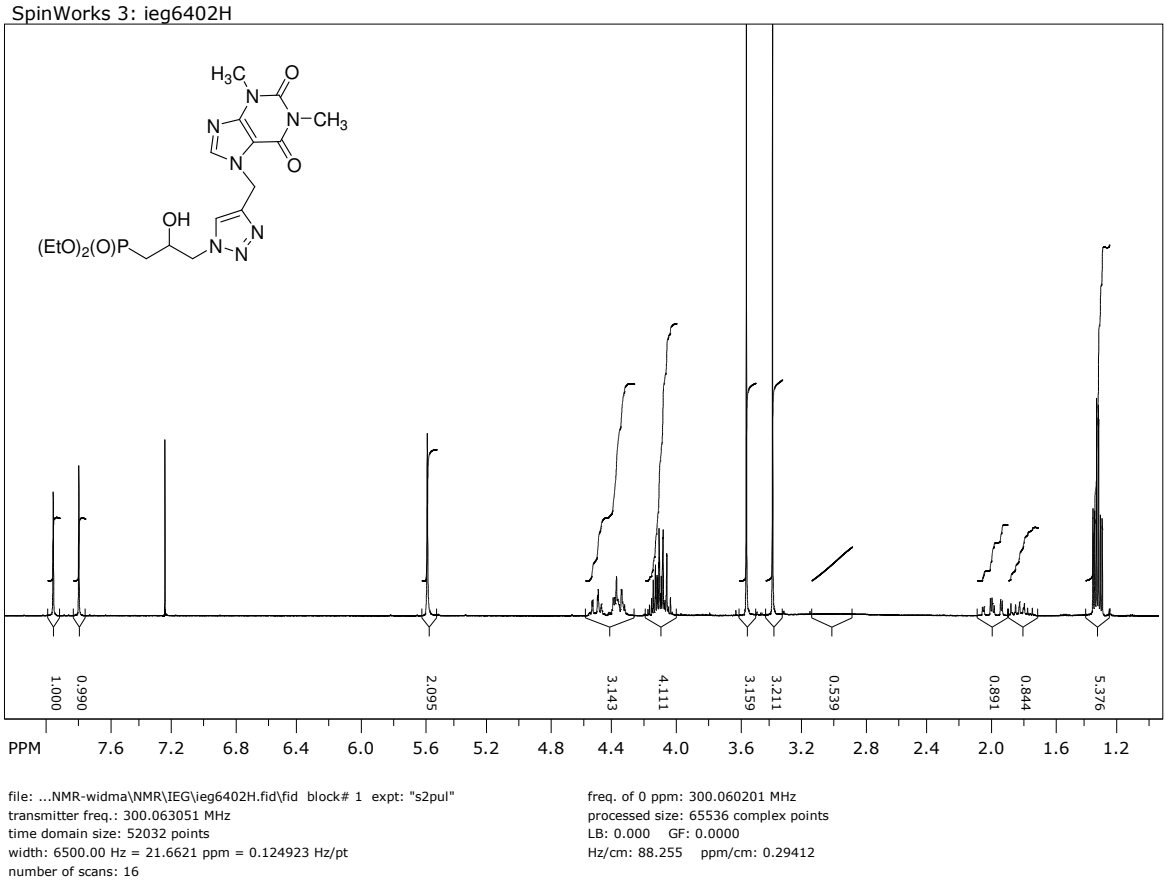


Diethyl 3-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25h**. White powder; m.p.: 148–150°C; IR (KBr): ν = 3445, 2984, 2924, 1707, 1664, 1231, 1025 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.78 (s, 1H); 7.51 (d, *J* = 0.6 Hz, 1H, *H*C5′); 5.30 (s, 2H, CH_2); 4.52–4.32 (m, 3H, PCC*H*CH_2); 4.17–4.03 (m, 4H, 2×POC$H_2$$CH_3$); 3.98 (d, *J* = 0.6 Hz, 3H, CH_3); 3.55 (s, 3H, CH_3); 3.02 (brs, 1H, OH); 2.46–2.34 (m, 2H, PCH_2); 1.30 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.28 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3);^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.8 (s, C=O); 151.3 (s, C=O); 148.9; 143.5; 141.7; 124.9; 107.7; 65.6 (d, *J* = 3.8 Hz, PC*C*); 62.5 (d, *J* = 6.4 Hz, POC); 62.4 (d, *J* = 6.4 Hz, POC); 55.8 (d, *J* = 15.3 Hz, PCC*C*); 36.2; 33.9; 32.0 (d, *J* = 292.9 Hz, PC); 31.7; 30.0; 16.6 (d, *J* = 5.6 Hz, POC*C*); 16.5 (d, *J* = 5.6 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 29.53 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_6P$: C, 44.84; H, 5.75; N, 21.53. Found: C, 44.70; H, 5.59; N, 21.60.



Diethyl 3-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25i**. White solid; m.p.: 132–133°C; IR (KBr): ν = 2994, 2989, 2930, 1701, 1663, 1245, 1033 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.97 (s, 1H); 7.81 (s, 1H, *H*C5′); 5.58 (s, 2H, CH_2); 4.55–4.39 (m, 3H, PCC*H*C*H*$_2$); 4.18–4.04 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.55 (s, 3H, CH_3); 3.38 (s, 3H, CH_3); 2.46–2.34 (m, 2H, PC*H*$_2$); 1.31 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); 1.28 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.2 (s, C=O); 151.5 (s, C=O); 148.8; 141.9; 141.4; 125.3; 106.5; 65.5 (d, *J* = 3.8 Hz); 62.4 (d, *J* = 6.6 Hz, POC); 62.2 (d, *J* = 6.6 Hz, POC); 56.1 (d, *J* = 17.2 Hz, PCC*C*); 41.6; 31.8; 29.0 (d, *J* = 136.6 Hz, PC); 16.6 (d, *J* = 6.0 Hz, POC*C*); 16.5 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 29.34 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_6P$: C, 44.84; H, 5.75; N, 21.53. Found: C, 45.00; H, 5.92; N, 21.41.

^1H NMR



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number of scans: 16

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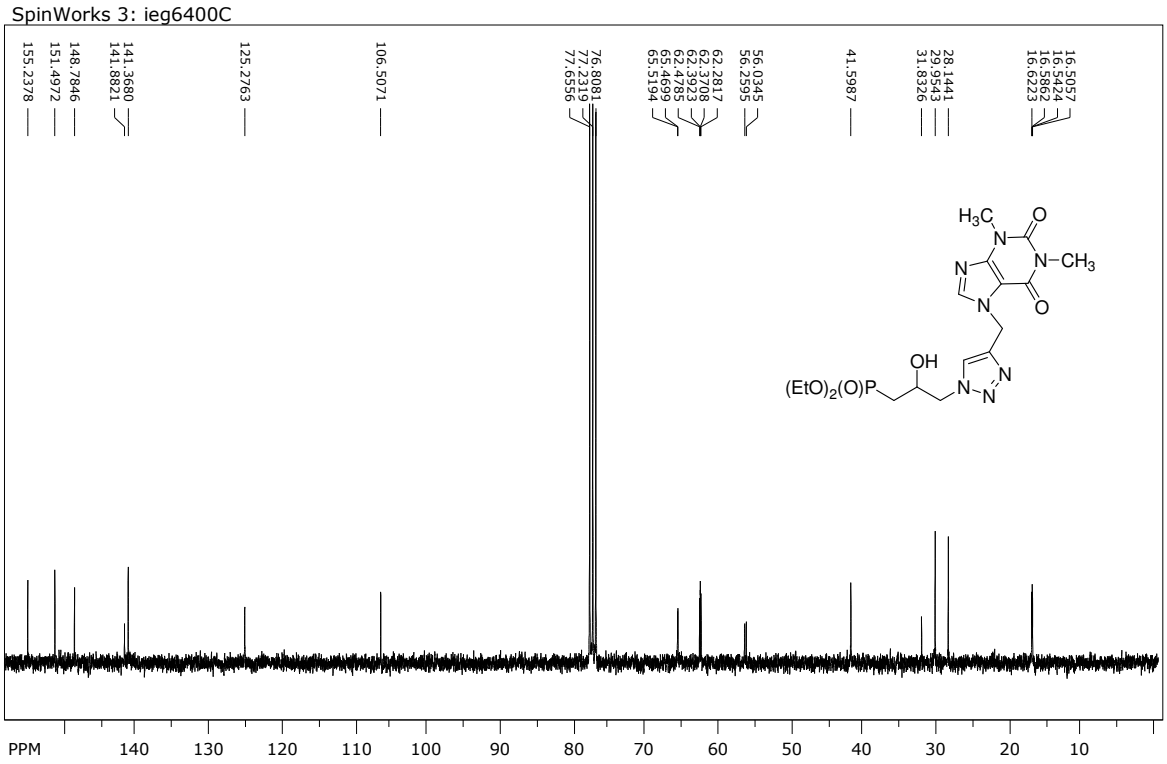
^{13}C NMR



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number of scans: 2000

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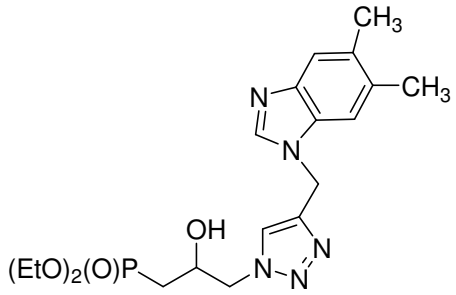
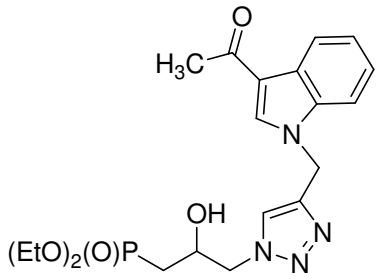
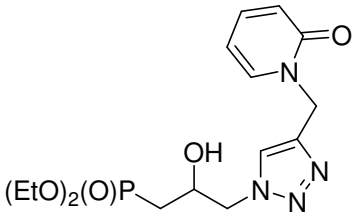


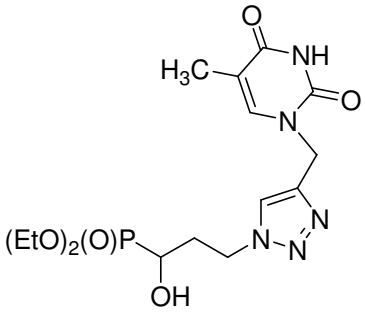
Diethyl 3-{4-[(5,6-dimethylbenzoimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25j**. Yellow oil; IR (film): ν = 3339, 3140, 2982, 2935, 1222, 1048, 965, 838 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.83 (s, 1H); 7.61 (s, 1H); 7.49 (s, 1H); 7.20 (s, 1H); 5.36 (s, 2H, CH_2); 4.53–4.47 (m, 1H, PCCCH_aH_b); 4.42–4.28 (m, 2H, PCCHCH_aH_b); 4.15–4.05 (m, 4H, 2×POCH_2CH_3); 3.63 (brs, 1H, OH); 2.34 (s, 3H, CH_3); 2.33 (s, 3H, CH_3); 2.04–1.75 (m, 2H, PCH_2); 1.30 (t, *J* = 7.0 Hz, 3H, POCH_2CH_3); 1.28 (t, *J* = 7.0 Hz, 3H, POCH_2CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 142.5; 141.9; 141.5; 132.7; 131.9; 131.6; 124.3; 119.8; 110.2; 65.3 (d, *J* = 3.4 Hz, PC*C*); 62.4 (d, *J* = 6.3 Hz, POC); 62.3 (d, *J* = 6.3 Hz, POC); 56.3 (d, *J* = 16.0 Hz, PCC*C*); 40.5; 31.1 (d, *J* = 139.8 Hz, PC); 20.7; 20.4; 16.6 (d, *J* = 6.3 Hz, POC*C*); 16.5 (d, *J* = 6.3 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 28.53 ppm. Anal. Calcd. for $C_{19}H_{28}N_5O_4P$: C, 54.15; H, 6.70; N, 16.62. Found: C, 53.98; H, 6.64; N, 16.56.



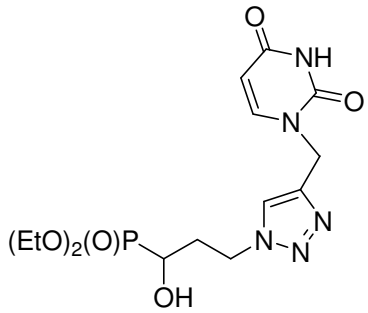
Diethyl 3-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-2-hydroxypropylphosphonate **25k**. Colourless oil; IR (film): ν = 3352, 2984, 2924, 1799, 1528, 1391, 1025 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 8.40–8.34 (m, 1H); 7.88 (s, 1H, *H*C5′); 7.65 (s, 1H); 7.47–7.41 (m, 1H); 7.33–7.28 (m, 2H); 5.46 (s, 2H, CH_2); 4.54–4.47 (m, 1H, PCCCH_aH_b); 4.40–4.32 (m, 2H, PCCHCH_aH_b); 4.17–4.01 (m, 4H, 2×POCH_2CH_3); 2.49 (s, 3H, CH_3); 1.97 (ddd, *J* = 19.3 Hz, *J* = 15.2 Hz, *J* = 3.2 Hz, 1H, PCH_aH_b); 1.77 (ddd, *J* = 16.6 Hz, *J* = 15.2 Hz, *J* = 9.0 Hz, 1H, PCH$_a$$H_b$); 1.32 (t, *J* = 6.9 Hz, 3H, POCH_2CH_3); 1.30 (t, *J* = 6.9 Hz, 3H, POCH_2CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 193.2 (s, C=O); 142.6; 136.5; 135.0; 126.3; 124.1; 123.5; 122.7; 122.6; 117.4; 109.9; 65.4 (d, *J* = 3.7 Hz, PC*C*); 62.4 (d, *J* = 6.4 Hz, POC); 62.3 (d, *J* = 6.4 Hz, POC); 56.1 (d, *J* = 17.2 Hz, PCC*C*); 42.4; 30.8 (d, *J* = 140.0 Hz, PC); 27.7 (s, CH_3); 16.6 (d, *J* = 6.0 Hz, POC*C*); 16.5 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 28.12 ppm. Anal. Calcd. for $C_{20}H_{27}N_4O_5P$: C, 55.29; H, 6.26; N, 12.90. Found: C, 55.04; H, 6.14; N, 13.06.



Diethyl 2-hydroxy-3-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **25l**. Brown oil; IR (film): ν = 3307, 2988, 2909, 1658, 1226; 1048, 776 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.95 (s, 1H); 7.60 (dd, *J* = 6.6 Hz, *J* = 3.0 Hz, 1H); 7.33 (ddd, *J* = 9.3 Hz, *J* = 6.3 Hz, *J* = 1.8 Hz, 1H); 6.53 (d, *J* = 9.0 Hz, 1H); 6.20 (dt, *J* = 6.6 Hz, *J* = 0.9 Hz, 1H); 5.18 (AB, *J* = 14.4 Hz, 1H, C*H*$_a$H$_b$); 5.16 (AB, *J* = 14.4 Hz, 1H, CH$_a$*H*$_b$); 4.53 (dd, *J* = 15.6 Hz, *J* = 6.6 Hz, 1H, PCCC*H*$_a$H$_b$); 4.56–4.34 (m, 2H, PCC*H*CH$_a$*H*$_b$); 4.18–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 2.95 (brs, 1H, OH); 2.07–1.80 (m, 2H, PCH$_2$); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.32 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.2 (s, C=O); 141.8 (s, H*C*=C); 140.1; 137.8; 125.4 (s, HC=*C*); 120.2; 106.7; 65.2 (d, *J* = 2.6 Hz, PC*C*); 62.2 (d, *J* = 6.6 Hz, POC); 61.9 (d, *J* = 6.6 Hz, POC); 55.9 (d, *J* = 14.9 Hz, PCC*C*); 44.4; 31.0 (d, *J* = 139.7 Hz, PC); 16.3 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 29.28 ppm. Anal. Calcd. for $C_{15}H_{23}N_4O_5P$: C, 48.65; H, 6.26; N, 15.13. Found: C, 48.88; H, 6.34; N, 15.00.

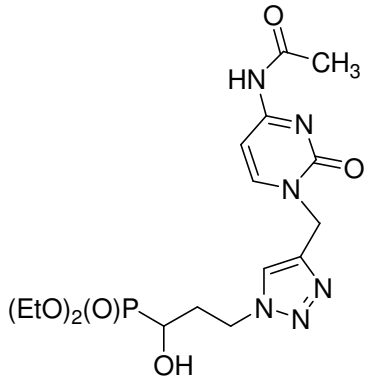


Diethyl 1-hydroxy-3-(4-{[5-methyl-2,4-dioxopyrimidin-1(2H)-yl]methyl}-1H-1,2,3-triazol-1-yl)propylphosphonate **26b**. White powder; m.p.: 169–171°C; IR (KBr): ν = 3410, 2989, 2938, 1682, 1225, 1022 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 9.89 (brs, 1H, NH); 7.87 (s, 1H, *H*C5′); 7.37 (d, *J* = 1.0 Hz, 1H, *H*C=CH); 4.95 (AB, *J* = 14.9 Hz, 1H, C*H*$_a$H$_b$); 4.92 (AB, *J* = 14.9 Hz, 1H, CH$_a$*H*$_b$); 4.63–4.55 (m, 2H, PCCC*H*$_2$); 4.23–4.09 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.80 (ddd, *J* = 10.7 Hz, *J* = 6.3 Hz, *J* = 3.3 Hz, 1H, PC*H*(OH)); 2.40–2.17 (m, 3H, PCC*H*$_2$, OH); 1.91 (d, *J* = 1.0 Hz, 3H, CH$_3$); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.30 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, CD_3OD): δ = 166.7 (s, C=O); 152.6 (s, C=O); 142.6; 125.5; 111.6; 65.1 (d, *J* = 167.8 Hz, PC); 64.4 (d, *J* = 7.5 Hz, POC); 64.2 (d, *J* = 7.5 Hz, POC); 47.7 (d, *J* = 16.1 Hz, PCC*C*); 43.9; 33.2 (d, *J* = 4.0 Hz, PC*C*); 17.0 (d, *J* = 4.9 Hz, POC*C*); 16.9 (d, *J* = 4.9 Hz, POC*C*); 12.5;^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.76 ppm. Anal. Calcd. for $C_{15}H_{24}N_5O_6P$: C, 44.89; H, 6.03; N, 17.45. Found: C, 45.10; H, 5.89; N, 17.38.

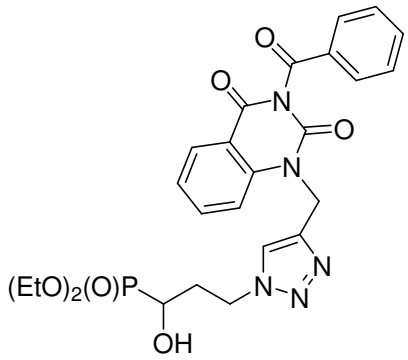


Diethyl 3-(4-{[2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)-1-hydroxypropylphosphonate **26c**. White solid; m.p.: 136–138°C; IR (KBr): ν = 3405, 2984, 2932, 1680, 1227, 1025 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 10.49 (brs, 1H, NH); 7.90 (s, 1H, *H*C5′); 7.59 (d, *J* = 7.9 Hz, 1H, *H*C=CH); 5.72 (d, *J* = 7.9 Hz, 1H, HC=C*H*); 5.01 (AB, *J* = 15.5 Hz, 1H, CH_aH$_b$); 4.97 (AB, *J* = 15.5 Hz, 1H, CH$_a$$H_b$); 4.61 (brt, *J* = 6.4 Hz, 2H, PCCCH_2); 4.23–4.10 (m, 4H, 2×POCH_2CH$_3$); 3.86–3.74 (m, 1H, PC*H*(OH)); 2.44–2.17 (m, 2H, PCCH_2); 1.32 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.30 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 164.5 (s, C=O); 151.4 (s, C=O); 144.9; 141.7; 124.9; 102.6; 64.0 (d, *J* = 166.0 Hz, PC); 63.3 (d, *J* = 7.0 Hz, POC); 63.1 (d, *J* = 7.0 Hz, POC); 46.7 (d, *J* = 17.2 Hz, PCC*C*); 43.3; 31.9; 16.6 (d, *J* = 5.4 Hz, POC*C*); 16.5 (d, *J* = 5.4 Hz, POC*C*);^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.84 ppm.

Anal. Calcd. for $C_{14}H_{22}N_5O_6P$: C, 43.41; H, 5.73; N, 18.08. Found: C, 43.57; H, 5.61; N, 17.89.

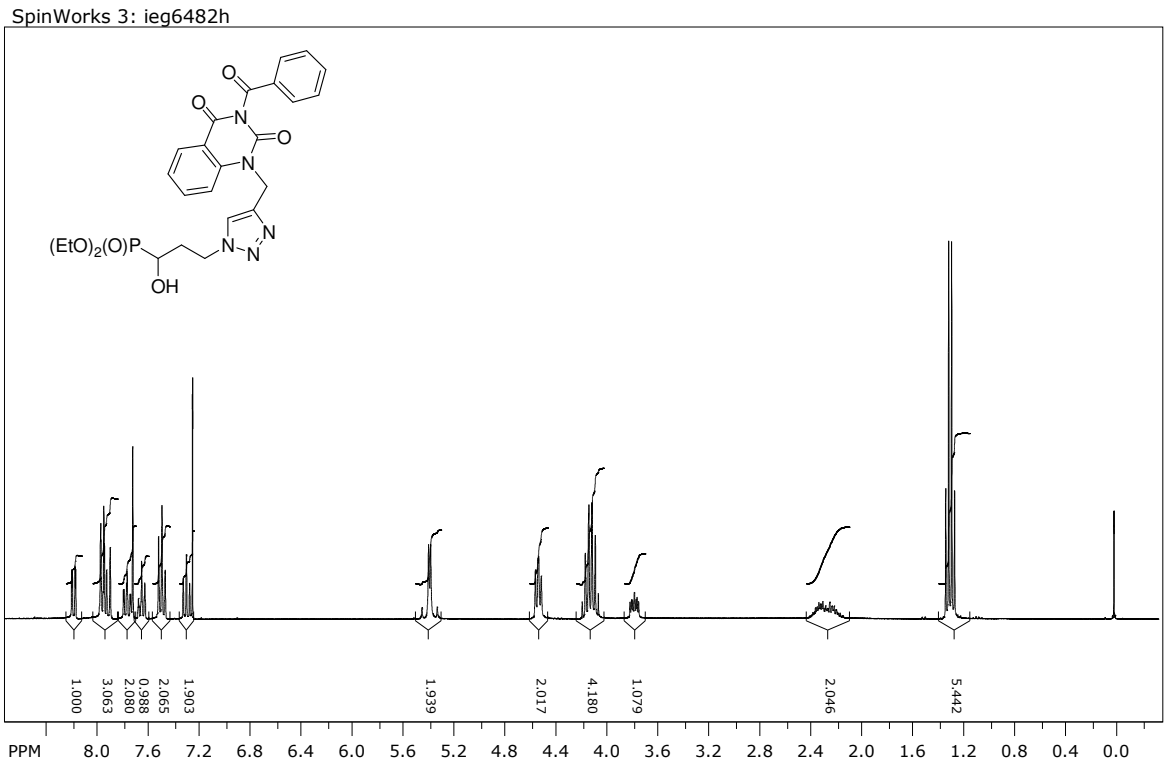


Diethyl 3-(4-{[N^4-acetylamino-2-oxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)-1-hydroxypropylphosphonate **26d**. White powder; m.p.: 175–177°C; IR (KBr): ν = 3406, 3124, 2930, 2873, 1706, 1654, 1221, 1021 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 10.96 (brs, 1H, NH); 8.71 (s, 1H, *H*C5′); 7.93 (d, *J* = 7.4 Hz, 1H, *H*C=CH); 7.44 (d, *J* = 7.4 Hz, 1H, *H*C=CH); 5.32 (d, *J* = 14.6 Hz, 1H, CH_aH$_b$); 5.05 (d, *J* = 14.6 Hz, 1H, CH$_a$$H_b$); 4.91–4.83 (m, 1H, PCCCH_aH$_b$); 4.75–4.65 (m, 1H, PCCCH$_a$$H_b$); 4.25–4.14 (m, 2H, POC$H_2CH_3$); 4.13–4.03 (m, 2H, POC$H_2CH_3$); 3.87–3.81 (m, 1H, PC*H*(OH)); 2.32–2.24 (m, 3H, PCCH_2, OH); 2.24 (s, 3H, CH$_3$); 1.35 (t, *J* = 7.1 Hz, 3H, POCH$_2$CH_3); 1.27 (t, *J* = 7.1 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, CD_3OD): δ = 172.8; 164.4; 158.2; 150.7; 143.2; 125.9; 98.4; 65.0 (d, *J* = 168.0 Hz, PC); 64.4 (d, *J* = 7.5 Hz, POC); 64.1 (d, *J* = 7.5 Hz, POC); 47.7 (d, *J* = 16.3 Hz, PCC*C*); 46.4; 33.2 (s, PC*C*); 24.7; 16.9 (d, *J* = 4.9 Hz, POC*C*);^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 25.96 ppm. Anal. Calcd. for $C_{16}H_{25}N_6O_6P$: C, 44.86; H, 5.88; N, 19.62. Found: C, 45.10; H, 6.00; N, 19.74.



Diethyl 3-(4-{[3-benzoyl-2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)-1-hydroxyethylphosphonate **26e**. White powder; m.p.: 82–84°C; IR (KBr): ν = 3299, 2988, 1746, 1702, 1664, 1233, 1027, 757, 674 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.20 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 7.99–7.95 (m, 2H, 2×*o*-CH); 7.93 (brd, *J* = 8.5 Hz, 1H); 7.78 (ddd, *J* = 8.5 Hz, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 7.74 (s, 1H, *H*C5′); 7.70–7.64 (m, 1H, *p*-CH); 7.54–7.46 (m, 2H, 2×*m*-CH); 7.29 (dt, *J* = 7.9 Hz, *J* = 0.8 Hz, 1H); 5.42 (AB, *J* = 15.7 Hz, 1H, C$H_a$$H_b$); 5.36 (AB, *J* = 15.7 Hz, 1H, C$H_a$$H_b$); 4.66–4.54 (m, 2H, PCCCH_2); 4.18–4.04 (m, 4H, 2×POC$H_2$$CH_3$); 3.78 (ddd, *J* = 10.7 Hz, *J* = 6.2 Hz, *J* = 3.4 Hz, 1H, PC*H*(OH)); 2.38–2.10 (m, 2H, PCCH_2); 1.30 (t, *J* = 7.0 Hz, 3H, $POCH_2CH_3$); 1.28 (t, *J* = 7.0 Hz, 3H, $POCH_2CH_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 168.7 (s, C=O); 161.1 (s, C=O); 149.6 (s, C=O); 142.3 (s, H*C*=C); 140.3; 136.3; 135.2; 131.6; 130.7; 129.3; 128.9; 124.4 (s, HC=*C*); 123.9; 115.6; 115.4; 64.4 (d, *J* = 166.4 Hz, PC); 63.3 (d, *J* = 6.8 Hz, POC); 63.0 (d, *J* = 6.8 Hz, POC); 48.6 (d, *J* = 16.1 Hz, PCC*C*); 39.0; 31.9 16.7 (d, *J* = 5.2 Hz, POC*C*); 16.6 (d, *J* = 5.2 Hz, POC*C*);^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.57 ppm. Anal. Calcd. for $C_{25}H_{28}N_5O_7P$: C, 55.45; H, 5.21; N, 12.93. Found: C, 55.60; H, 5.34; N, 13.09.

^{1}H NMR



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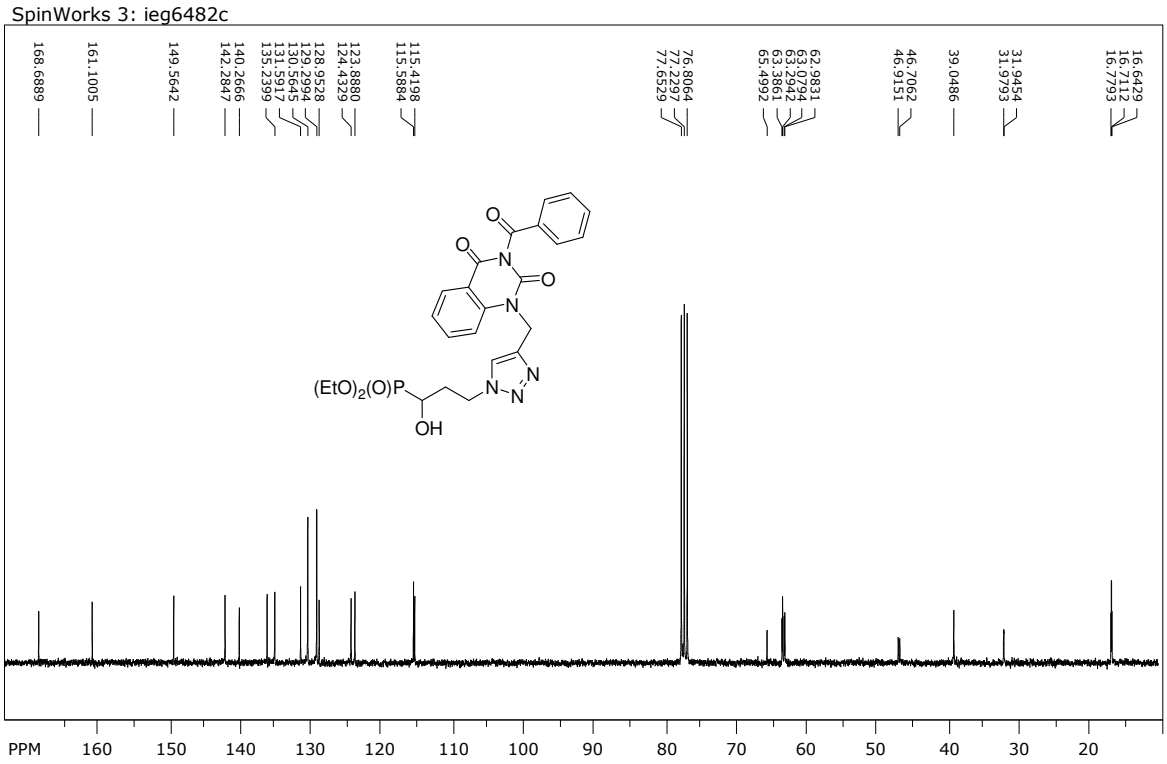
^{13}C NMR



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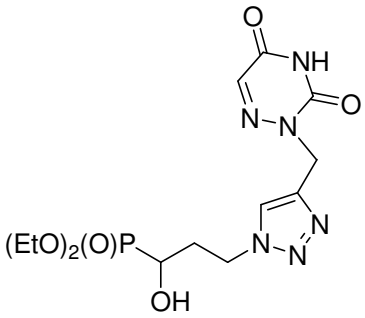
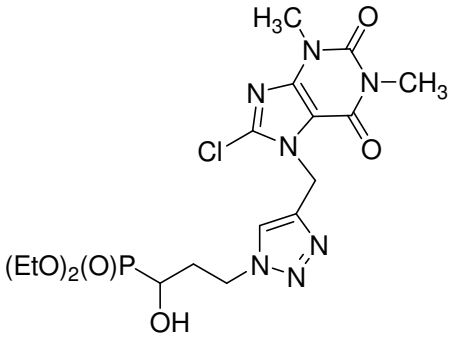
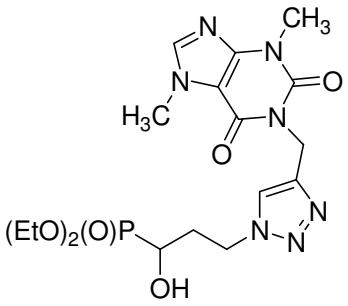


Diethyl 1-hydroxy-3-{4-[(3,5-dioxo-1,2,4-triazin-2-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26f**. Yellow solid; m.p.: 116–118°C; IR (KBr): ν = 3284, 3152, 2988, 2912, 1731, 1658, 1050 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 12.1 (s, 1H, NH); 7.85 (s, 1H); 7.40 (s, 1H); 5.17 (s, 1H, CH_2); 4.60–4.51 (m, 2H, PCCCH_2); 4.21–4.09 (m, 4H, 2×POCH_2CH$_3$); 3.87 (ddd, *J* = 10.1 Hz, *J* = 6.1 Hz, *J* = 2.9 Hz, 1H, PC*H*(OH)); 2.41–2.16 (m, 3H, PCCH_2, OH); 1.31 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.29 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.9 (s, C=O); 149.4 (C=O); 141.4 (s, H*C*=C); 135.0 (s, HC=N); 124.8 (s, HC=*C*); 64.1 (d, *J* = 166.3 Hz, PC); 63.3 (d, *J* = 7.2 Hz, POC); 63.2 (d, *J* = 7.2 Hz, POC); 46.6 (d, *J* = 17.2 Hz, PCC*C*); 34.7; 31.9; 16.6 (d, *J* = 5.6 Hz, POC*C*); 16.5 (d, *J* = 5.6 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 25.12 ppm. Anal. Calcd. for $C_{13}H_{21}N_6O_6P$: C, 40.21; H, 5.45; N, 21.64. Found: C, 40.05; H, 5.61; N, 21.77.

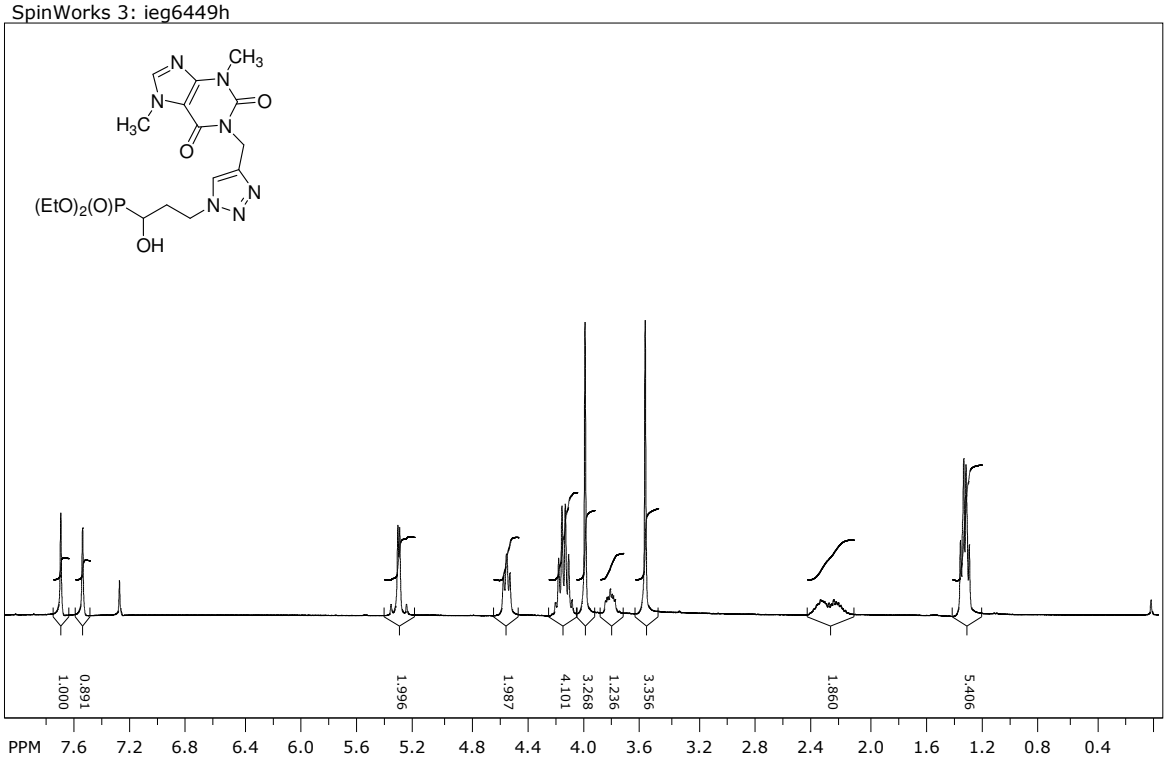


Diethyl 3-{4-[(8-chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26g**. White powder; m.p.: 164–165°C; IR (KBr): ν = 3300, 2993, 1706, 1663, 1217, 1027 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.84 (s, 1H); 5.64 (AB, *J* = 14.8 Hz, 1H, CH_aH$_b$); 5.61 (AB, *J* = 14.8 Hz, 1H, CH$_a$$H_b$); 4.60–4.50 (m, 2H, PCCCH_2); 4.21–4.09 (m, 4H, 2×POCH_2CH$_3$); 3.80 (ddd, *J* = 10.7 Hz, *J* = 6.3 Hz, *J* = 3.4 Hz, 1H, PC*H*(OH)); 3.54 (s, 3H, CH_3); 3.40 (s, 3H, CH_3); 3.25 (brs, 1H, OH); 2.37–2.20 (m, 2H, PCCH_2); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); 1.31 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.3 (s, C=O); 151.0 (s, C=O); 147.2; 141.4; 138.9; 124.1; 107.3; 64.1 (d, *J* = 165.7 Hz, PC); 63.1 (d, *J* = 7.1 Hz, POC); 62.9 (d, *J* = 7.1 Hz, POC); 46.6 (d, *J* = 15.8 Hz, PCC*C*); 41.0; 31.9 (d, *J* = 2.6 Hz, PC*C*); 29.9; 28.1; 16.6 (d, *J* = 5.2 Hz, POC*C*); 16.5 (d, *J* = 5.2 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.61 ppm. Anal. Calcd. for $C_{17}H_{25}ClN_7O_6P$: C, 41.68; H, 5.14; N, 20.02. Found: C, 41.79; H, 5.08; N, 20.10.



Diethyl 3-{4-[(3,7-dimethyl-2,6-dioxopurin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26h**. White powder; m.p.: 129–130°C; IR (KBr): ν = 3288, 2984, 1707, 1661, 1233, 1049 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.69 (s, 1H); 7.54 (s, 1H); 5.33 (AB, *J* = 14.5 Hz, 1H, CH_aH_b); 5.28 (AB, *J* = 14.5 Hz, 1H, CH_aH_b); 4.65–4.45 (m, 2H, PCCCH_2); 4.21–4.09 (m, 4H, 2×POCH_2CH$_3$); 4.00 (s, 3H, CH_3); 3.85–3.76 (m, 1H, PC*H*(OH)); 3.57 (s, 3H, CH_3); 2.33–2.16 (m, 3H, PCH_2, OH); 1.32 (t, *J* = 6.4 Hz, 3H, $POCH_2CH_3$); 1.31 (t, *J* = 6.4 Hz, 3H, $POCH_2CH_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 154.5 (s, C=O); 151.0 (s, C=O); 148.6; 143.2; 141.8; 123.7; 107.4; 64.4 (d, *J* = 166.3 Hz, PC); 62.8 (d, *J* = 7.2 Hz, POC); 62.7 (d, *J* = 7.2 Hz, POC); 46.3 (d, *J* = 16.0 Hz, PCC*C*); 35.9; 33.6; 31.9; 29.7; 16.4 (d, *J* = 5.5 Hz, POC*C*); 16.2 (d, *J* = 5.5 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.85 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_6P$: C, 44.84; H, 5.75; N, 21.53. Found: C, 44.71; H, 5.66; N, 21.65.

^1H NMR



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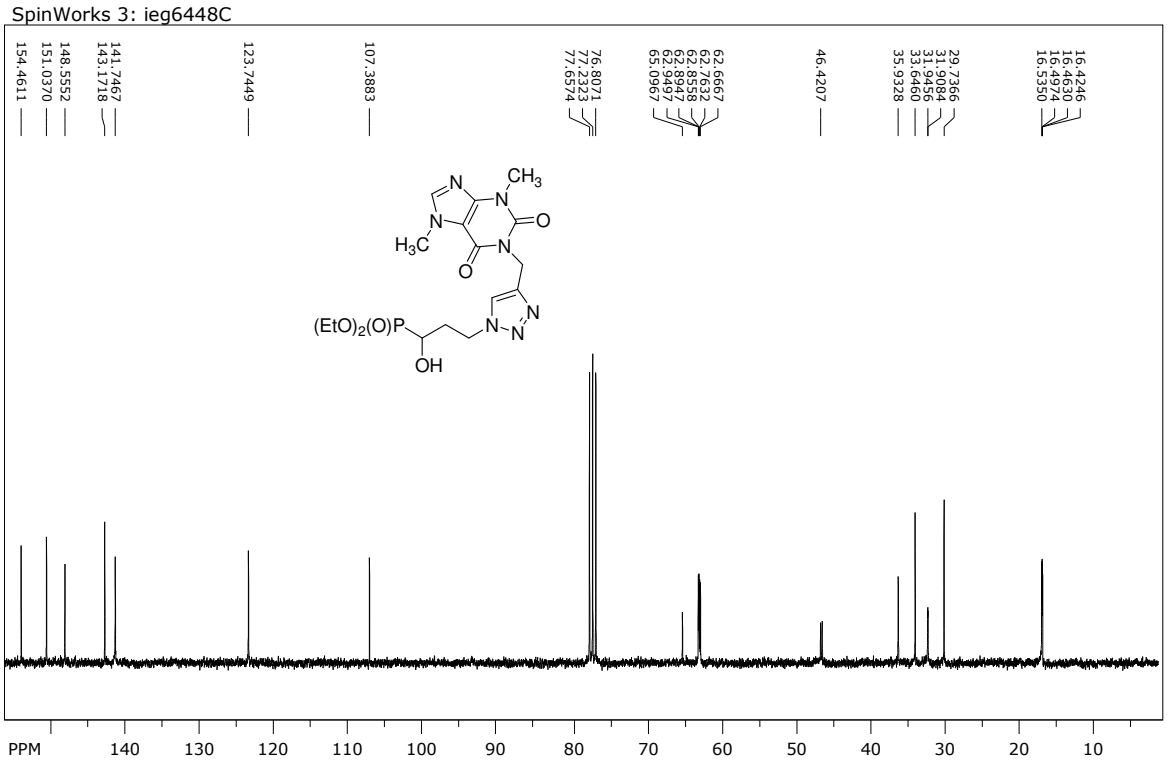
^{13}C NMR



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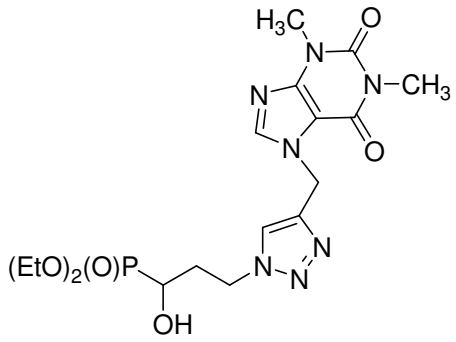
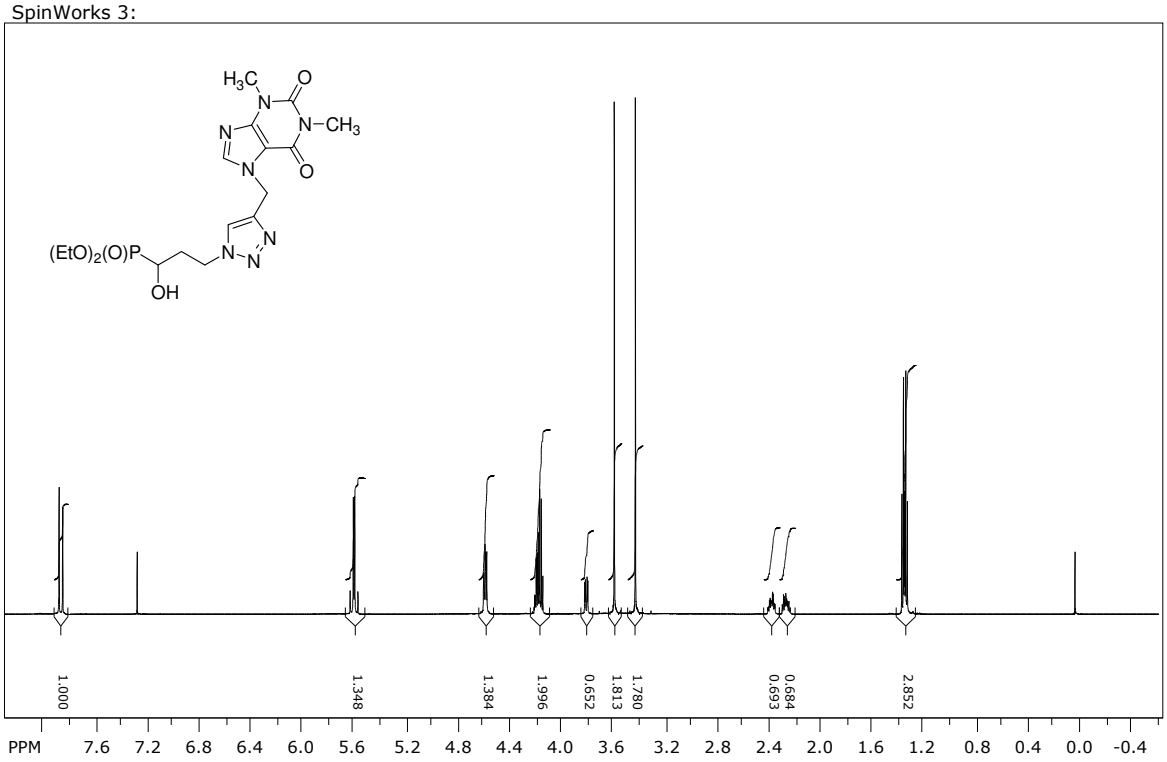


Diethyl 3-{4-[(1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26i**. White powder; m.p.: 123–125°C; IR (KBr): ν = 3365, 2991, 1704, 1658, 1222, 1050 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$): δ = 7.89 (s, 1H); 7.87 (s, 1H); 5.62 (AB, *J* = 14.9 Hz, 1H, CH_aH_b); 5.59 (AB, *J* = 14.9 Hz, 1H, CH_aH_b); 4.63–4.55 (m, 2H, PCCCH_2); 4.22–4.09 (m, 4H, 2×POCH_2CH$_3$); 3.80 (ddd, *J* = 10.9 Hz, *J* = 6.2 Hz, *J* = 3.3 Hz, 1H, PC*H*(OH)); 3.59 (s, 3H, CH_3); 3.43 (s, 3H, CH_3); 2.37 (ddddd, *J* = 14.4 Hz, *J* = 8.0 Hz, *J* = 8.0 Hz, *J* = 6.1 Hz, *J* = 3.3 Hz, 1H, PCCH_aH_b); 2.26 (ddddd, *J* = 14.4 Hz, *J* = 10.9 Hz, *J* = 6.4 Hz, *J* = 5.6 Hz, *J* = 5.6 Hz, 1H, PCCH_aH_b); 1.35 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 155.2 (s, C=O); 151.4 (s, C=O); 148.7; 141.9; 141.6; 124.3; 106.3; 64.0 (d, *J* = 166.1 Hz, PC); 63.1 (d, *J* = 7.1 Hz, POC); 62.9 (d, *J* = 7.1 Hz, POC); 46.6 (d, *J* = 15.8 Hz, PCC*C*); 41.3; 31.9 (d, *J* = 2.8 Hz, PC*C*); 29.9; 28.1; 16.6 (d, *J* = 5.4 Hz, POC*C*); 16.5 (d, *J* = 5.4 Hz, POC*C*); ^{31}P NMR (243 MHz, $CDCl_3$): δ = 23.44 ppm. Anal. Calcd. for $C_{17}H_{26}N_7O_6P$: C, 44.84; H, 5.75; N, 21.53. Found: C, 45.00; H, 5.90; N, 21.40.

^{1}H NMR

SpinWorks 3:



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number of scans: 16

freq. of 0 ppm: 600.260000 MHz
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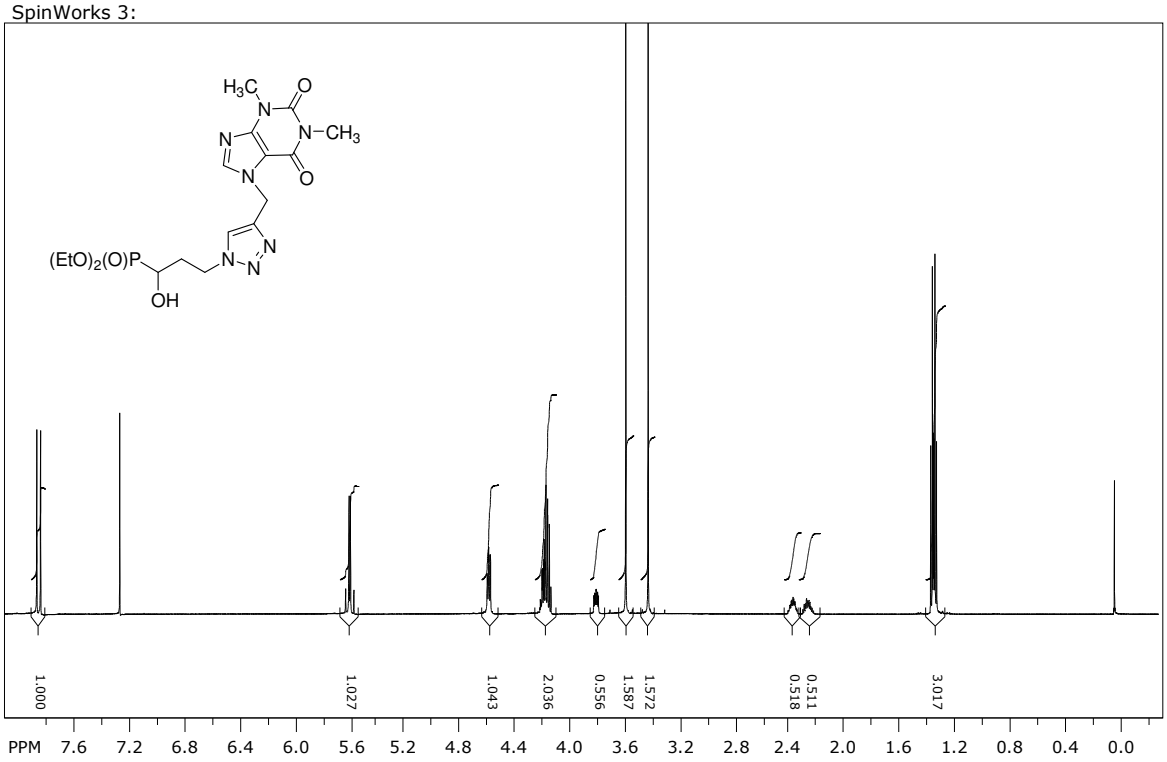
^{1}H NMR

SpinWorks 3:



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number of scans: 16

freq. of 0 ppm: 600.260000 MHz
processed size: 32768 complex points
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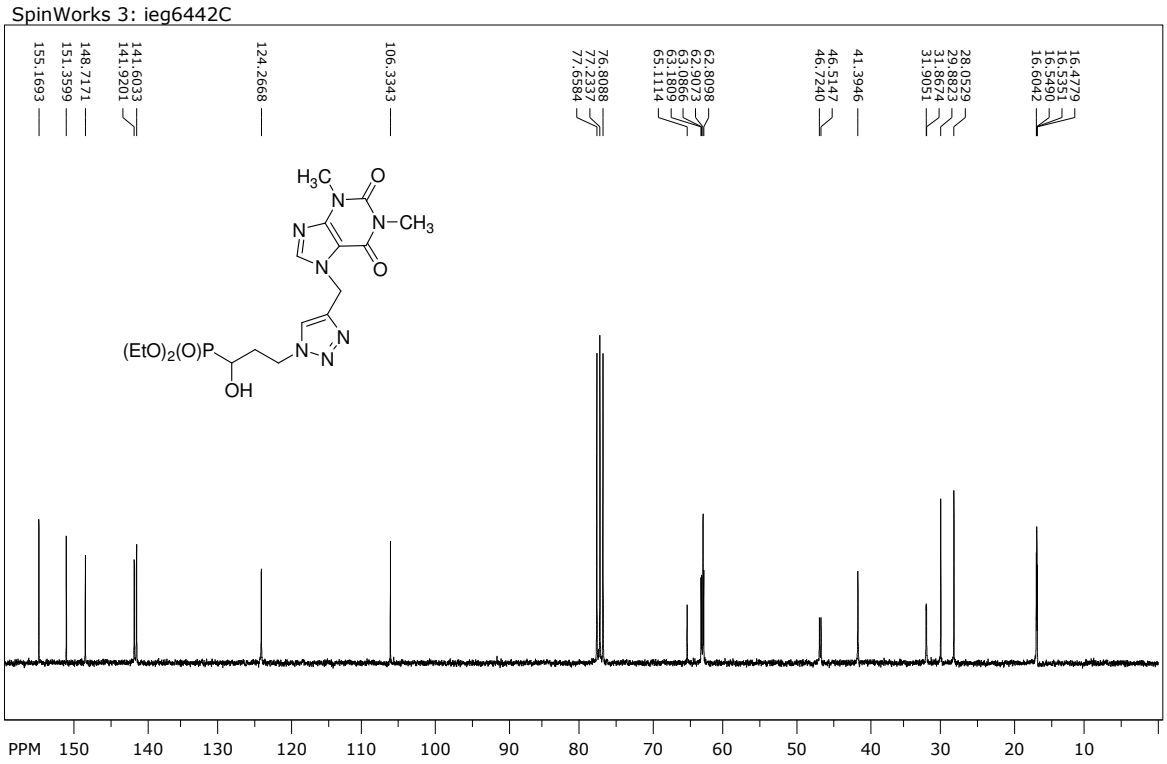
Hz/cm: 202.480 ppm/cm: 0.33732

^{13}C NMR



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number of scans: 704

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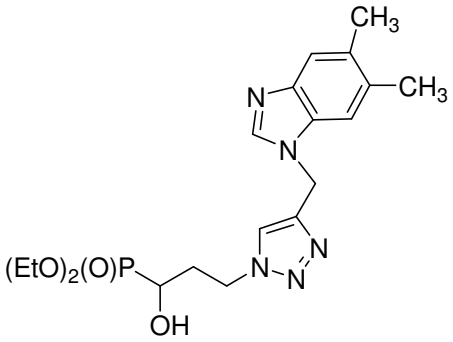
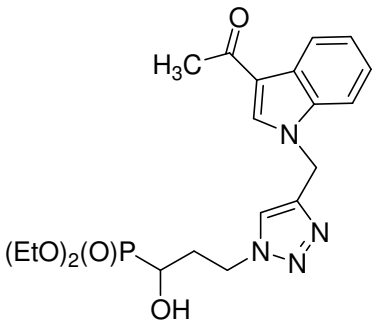
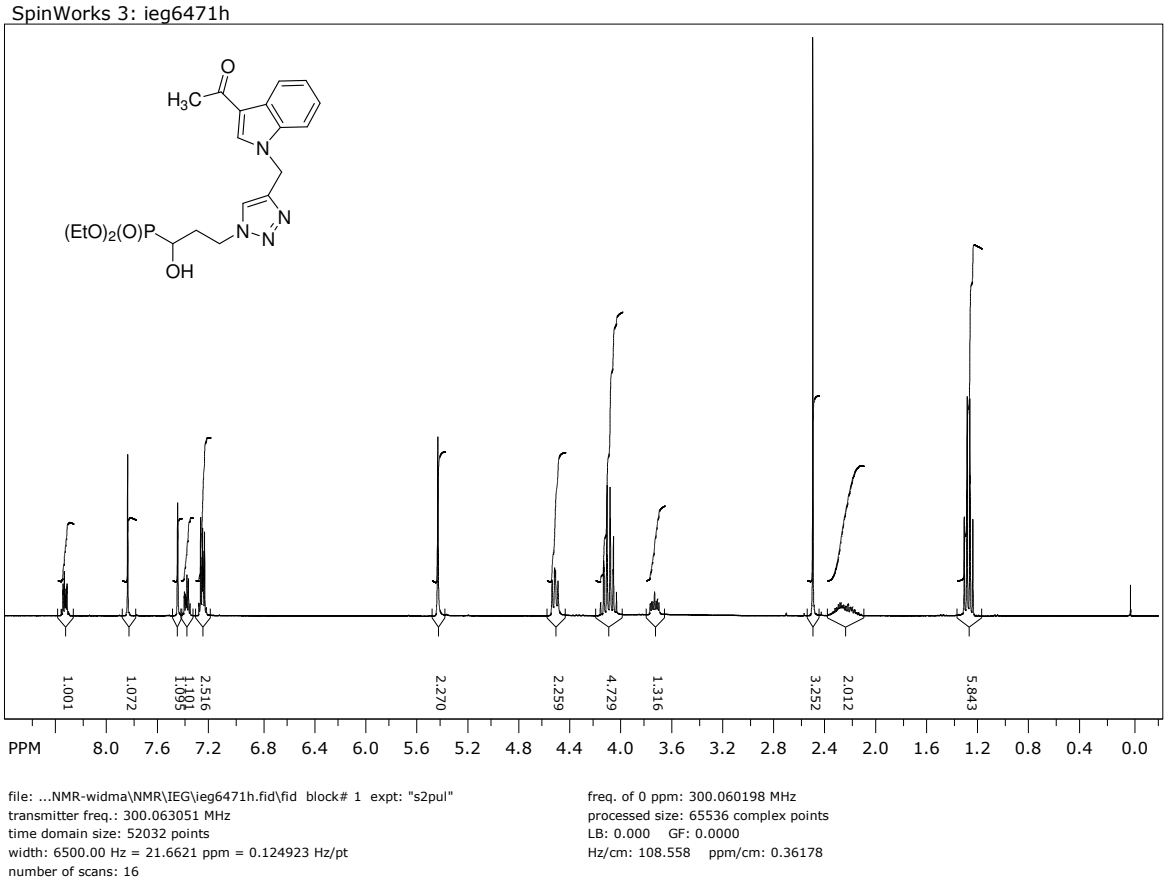


Diethyl 3-{4-[(5,6-dimethylbenzoimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26j**. Yellow oil; IR (film): ν = 3339, 3140, 2982, 2935, 1222, 1048, 965, 838 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.08 (s, 1H); 7.56 (s, 1H); 7.53 (s, 1H); 7.25 (s, 1H); 5.45 (s, 2H, CH_2); 4.64–4.54 (m, 2H, PCCCH_2); 4.18–4.05 (m, 4H, 2×POCH_2CH$_3$); 3.75 (ddd, *J* = 10.5 Hz, *J* = 6.5 Hz, *J* = 3.2 Hz, 1H, PC*H*(OH)); 3.40 (brs, 1H, OH); 2.37 (s, 3H, CH_3); 2.35 (s, 3H, CH_3); 2.34–2.14 (m, 2H, PCCH_2); 1.29 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); 1.26 (t, *J* = 7.0 Hz, 3H, POCH$_2$CH_3); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 142.7; 142.0; 141.4; 132.6; 131.8; 131.6; 123.1; 119.7; 110.2; 64.0 (d, *J* = 151.2 Hz, PC); 62.8 (d, *J* = 7.1 Hz, POC); 62.8 (d, *J* = 7.1 Hz, POC); 46.7 (d, *J* = 15.7 Hz, PCC*C*); 40.5; 32.0; 20.7; 20.4; 16.6 (d, *J* = 6.3 Hz, POC*C*); 16.6 (d, *J* = 6.3 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.71 ppm. Anal. Calcd. for $C_{19}H_{28}N_5O_4P$: C, 54.15; H, 6.20; N, 16.62. Found: C, 54.00; H, 6.89; N, 16.70 .

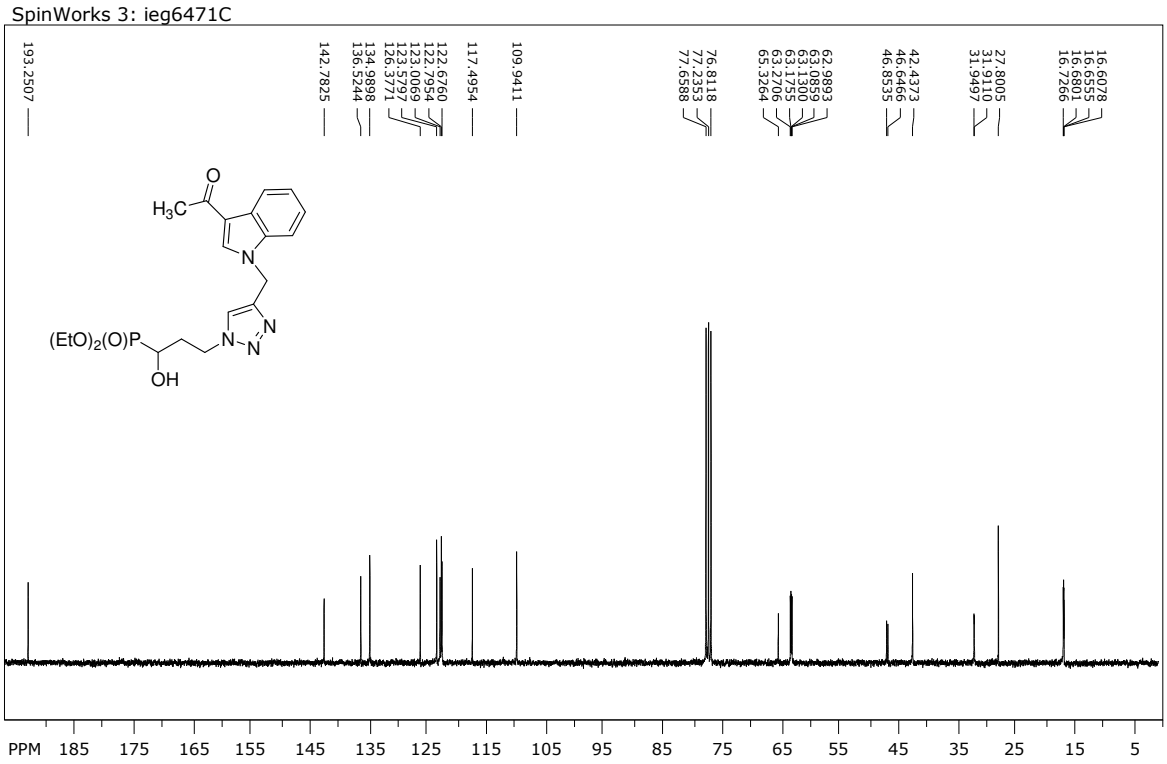


Diethyl 3-{4-[(3-acetylindol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxypropylphosphonate **26k**. Colourless oil; IR (film): ν = 3330, 3140, 2984, 1799, 1527, 1389, 1223, 1022 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ = 8.38–8.33 (m, 1H); 7.86 (s, 1H, *H*C5′); 7.47 (s, 1H); 7.43–7.38 (m, 1H); 7.31–7.25 (m, 2H); 5.41 (s, 2H, CH_2); 4.60–4.45 (m, 2H, PCCC*H*$_2$); 4.16–4.03 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.72 (ddd, *J* = 10.8 Hz, *J* = 6.4 Hz, *J* = 3.5 Hz, 1H, PC*H*(OH)); 2.49 (s, 3H, CH_3); 2.36–2.11 (m, 2H, PCC*H*$_2$); 1.29 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); 1.26 (t, *J* = 7.0 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 193.3 (s, C=O); 142.8; 136.5; 135.0; 126.4; 123.6; 123.0; 122.8; 122.7; 117.5; 109.9; 64.2 (d, *J* = 165.9 Hz, PC); 63.2 (d, *J* = 6.3 Hz, POC); 62.9 (d, *J* = 6.3 Hz, POC); 46.7 (d, *J* = 15.6 Hz, PCC*C*); 42.4; 31.9 (d, *J* = 2.9 Hz, PC*C*); 27.8 (s, CH_3); 16.7 (d, *J* = 6.0 Hz, POC*C*); 16.6 (d, *J* = 6.0 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.60 ppm. Anal. Calcd. for $C_{20}H_{27}N_4O_5P$: C, 55.29; H, 6.26; N, 12.90. Found: C, 55.40; H, 6.10; N, 13.03.

^1H NMR



^{13}C NMR



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number of scans: 1024

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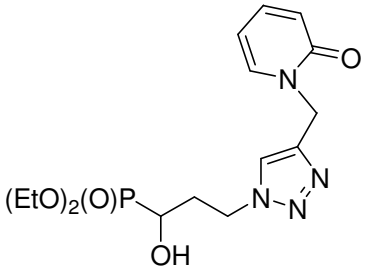
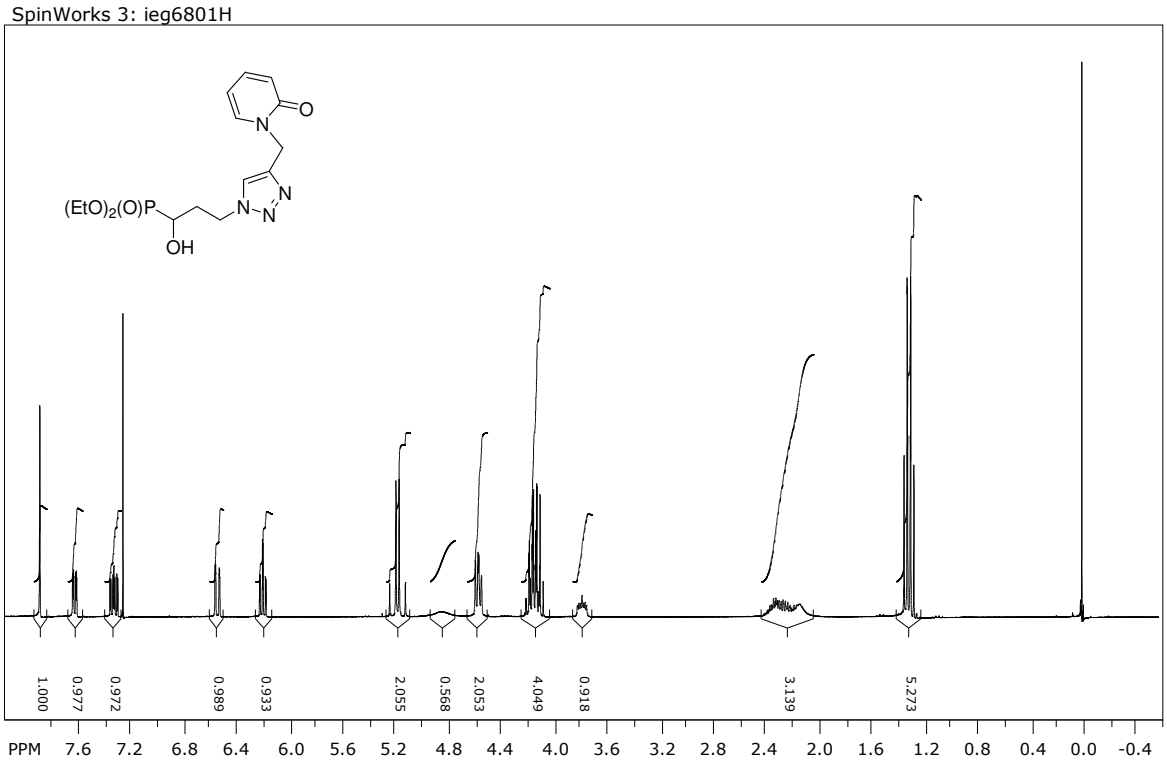


Diethyl 1-hydroxy-3-{4-[(2-oxopyridin-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonate **26l**. Brown oil; IR (film): ν = 3401, 2986, 2912, 1656, 1224; 1025 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.90 (s, 1H, *H*C5′); 7.63 (ddd, *J* = 6.8 Hz, *J* = 2.0 Hz, *J* = 0.6 Hz, 1H); 7.34 (ddd, *J* = 9.1 Hz, *J* = 6.8 Hz, *J* = 2.0 Hz, 1H); 6.55 (ddd, *J* = 9.1 Hz, *J* = 1.3 Hz, *J* = 0.6 Hz, 1H); 6.21 (dt, *J* = 6.8 Hz, *J* = 1.3 Hz, 1H); 5.22 (AB, *J* = 14.3 Hz, 1H, C*H*$_a$H$_b$); 5.16 (AB, *J* = 14.3 Hz, 1H, CH$_a$*H*$_b$); 4.86 (s, brs, 1H, OH); 4.60–4.45 (m, 2H, PCCC*H*$_2$); 4.22–4.09 (m, 4H, 2×POC*H*$_2$CH$_3$); 3.79 (ddd, *J* = 10.8 Hz, *J* = 6.2 Hz, *J* = 3.2 Hz, 1H, PC*H*(OH)); 2.41–2.16 (m, 2H, PCC*H*$_2$); 1.33 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); 1.30 (t, *J* = 6.9 Hz, 3H, POCH$_2$C*H*$_3$); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 162.4 (s, C=O); 142.3 (s, H*C*=C); 140.3; 137.9; 124.9 (s, HC=*C*); 120.6; 106.9; 64.0 (d, *J* = 165.8 Hz, PC); 63.1 (d, *J* = 7.1 Hz, POC); 62.9 (d, *J* = 7.1 Hz, POC); 46.6 (d, *J* = 16.0 Hz, PCC*C*); 44.8; 31.9 (d, *J* = 3.1 Hz, PC*C*); 16.7 (d, *J* = 5.2 Hz, POC*C*); 16.6 (d, *J* = 5.2 Hz, POC*C*); ^{31}P NMR (121.5 MHz, $CDCl_3$): δ = 24.85 ppm. Anal. Calcd. for $C_{15}H_{23}N_4O_5P$: C, 48.65; H, 6.26; N, 15.13. Found: C, 48.76; H, 6.12; N, 15.03.

^{1}H NMR



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number of scans: 16

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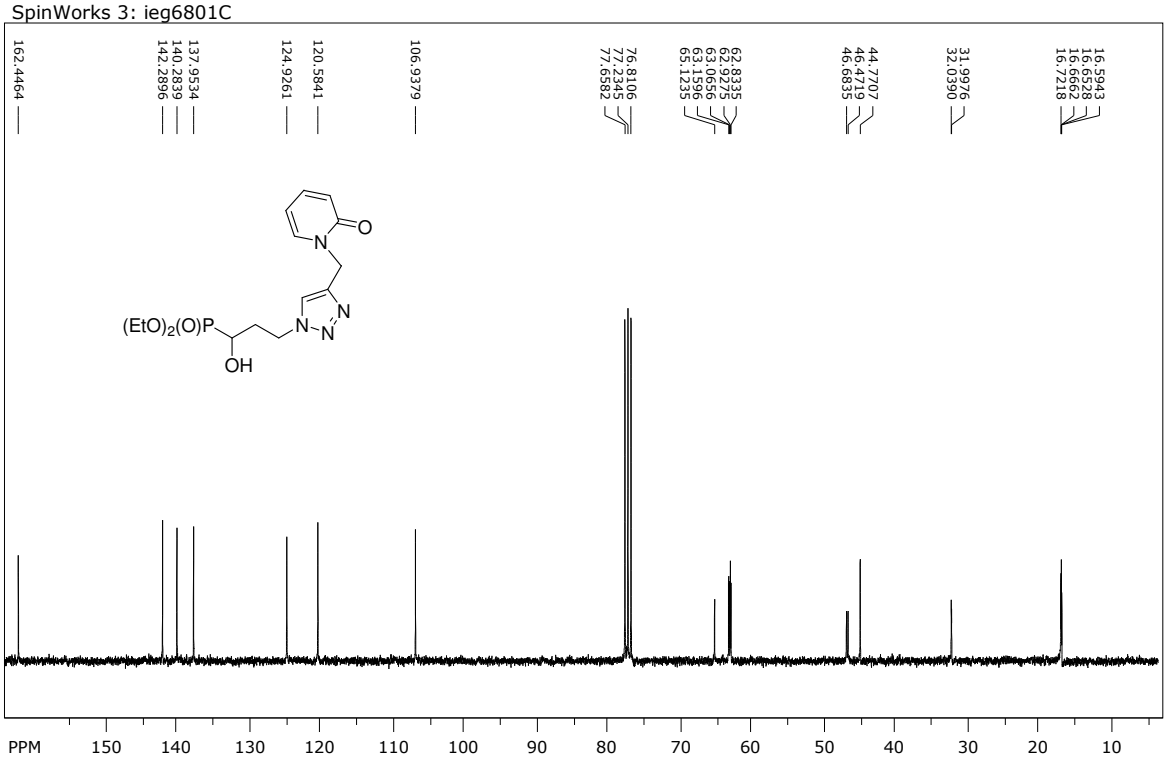
^{13}C NMR

SpinWorks 3: ieg6801C



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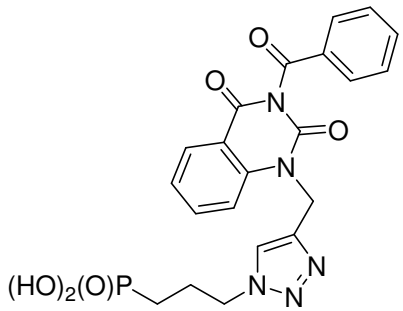
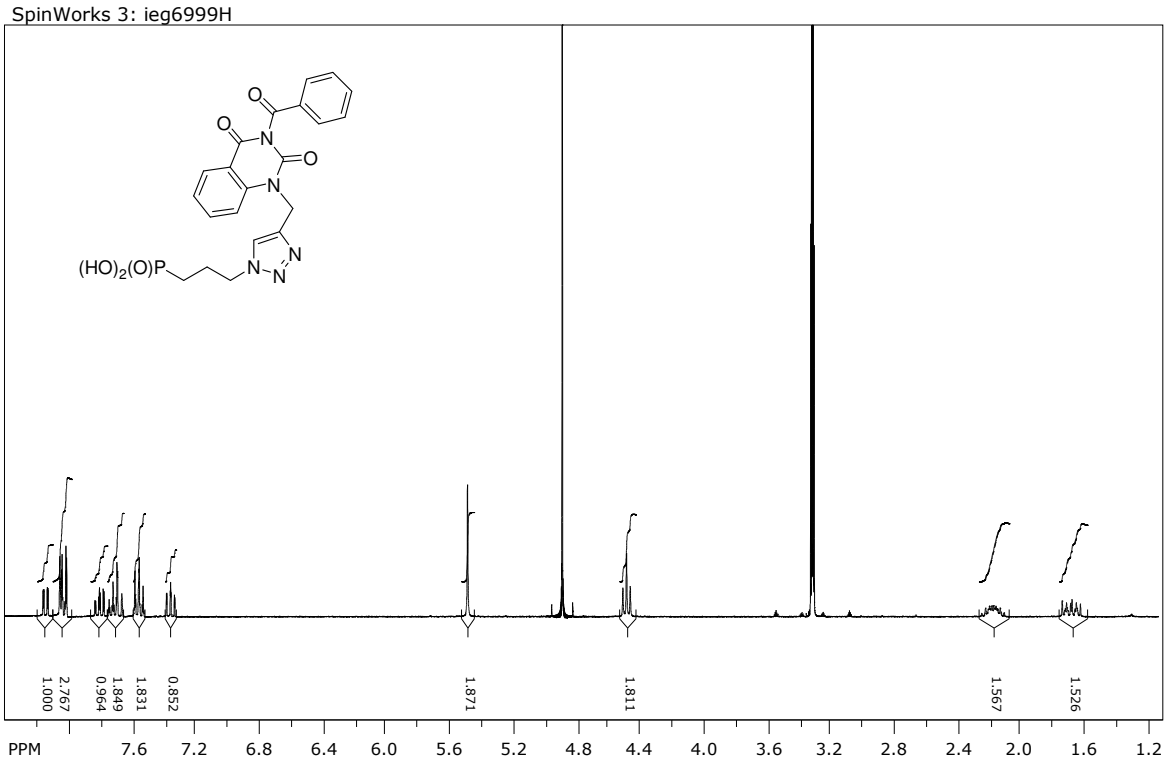


3-(4-{[3-Benzoyl-2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)propylphosphonic acid **31e**. White powder; m.p.: 130–133°C; IR (KBr): ν = 3341, 3014, 2939, 1746, 1699, 1662; 1478; 1240, 987; 756; 674 cm^{-1}; ^{1}H NMR (300 MHz, CD_3OD): δ = 8.16 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 8.07 (s, 1H, *H*C5′); 8.06–8.03 (m, 2H, 2×*o*-CH); 7.82 (ddd, *J* = 8.6 Hz, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H); 7.77–7.68 (m, 2H, *p*-CH, H8); 7.60–7.54 (m, 2H, 2×*m*-CH); 7.32 (dt, *J* = 7.9 Hz, *J* = 0.9 Hz, 1H); 5.49 (s, 2H, CH_2); 4.49 (t, *J* = 7.0 Hz, 2H, PCCCH_2); 2.29–2.10 (m, 2H, PCCH_2); 1.73–1.67 (m, 2H, PCH_2); ^{13}C NMR (151 MHz, CD_3OD): δ = 168.6 (s, C=O); 161.4 (s, C=O); 149.6 (s, C=O); 141.2 (s, H*C*=C); 140.2; 136.2; 135.1; 131.6; 130.3; 129.1; 128.2; 125.3 (s, HC=*C*); 123.7; 115.5; 114.9; 51.2 (d, *J* = 17.8 Hz, PCC*C*); 37.7; 23.4 (d, *J* = 3.7 Hz, PC*C*); 23.4 (d, *J* = 140.7 Hz, P*C*); ^{31}P NMR (121 MHz, CD_3OD): δ = 29.05 ppm. Anal. Calcd. for $C_{21}H_{20}N_5O_6P$: C, 53.73; H, 4.29; N, 14.92. Found: C, 53.55; H, 4.12; N, 15.13.

^{1}H NMR



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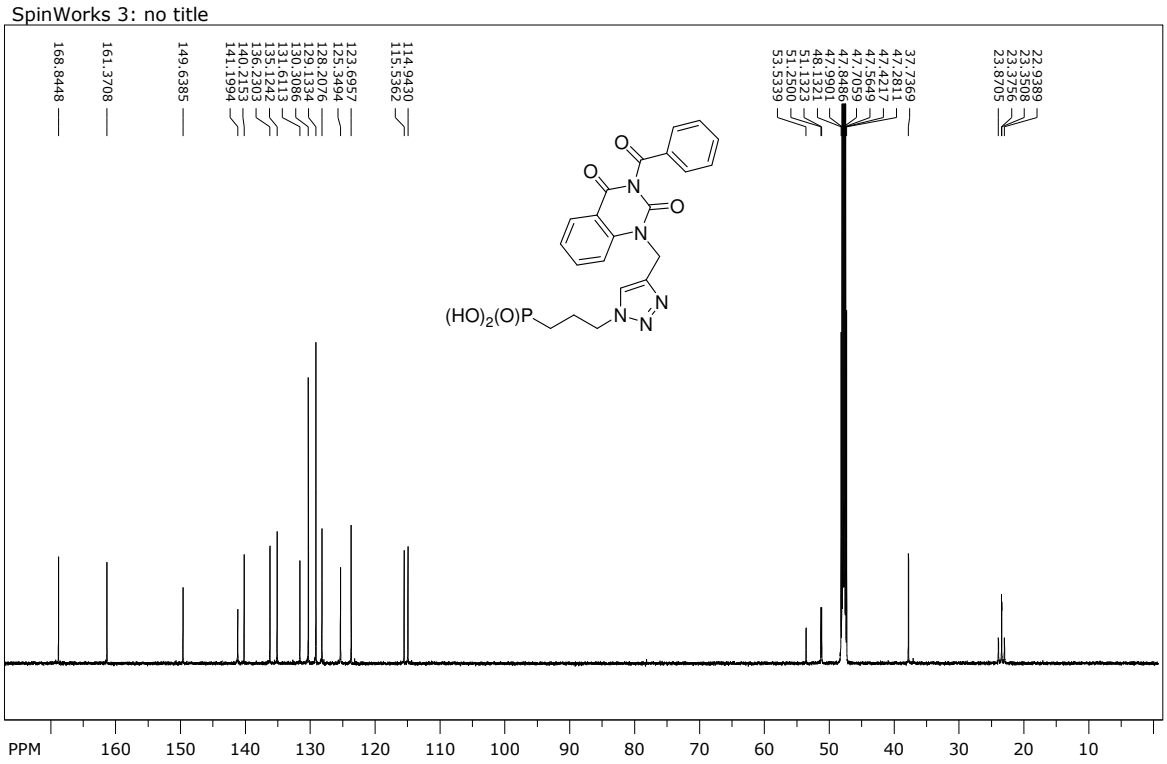
Hz/cm: 87.633 ppm/cm: 0.29205

^{13}C NMR



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number of scans: 1024

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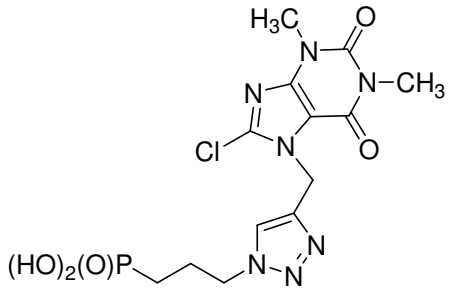
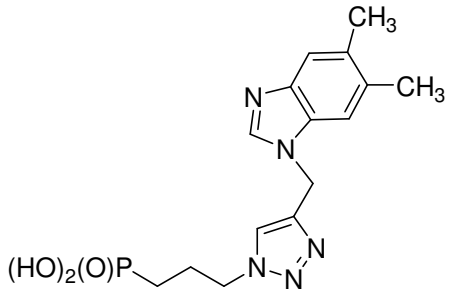
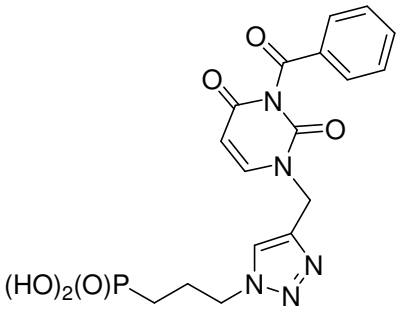


3-{4-[(8-Chloro-1,3-dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonic acid **31g**. White powder; m.p.: 216–220°C; solubility of **31g** in methanol or water was insufficient to measure the ^{13}C NMR spectrum; IR (KBr): ν = 3124, 2998, 2978, 1608, 1463, 1220, 1028, 968 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 8.09 (s, 1H); 5.70 (s, 2H, CH_2); 4.51 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 3.37 (s, 3H, CH_3); 3.34 (s, 3H, CH_3); 2.17 (dqv, *J* = 14.0 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.70 (dt, *J* = 19.2 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); ^{31}P NMR (243 MHz, CD_3OD): δ = 27.81 ppm. Anal. Calcd. for $C_{13}H_{17}ClN_5O_5P$: C, 37.38; H, 4.10; N, 23.47. Found: C, 37.60; H, 4.32; N, 23.33.

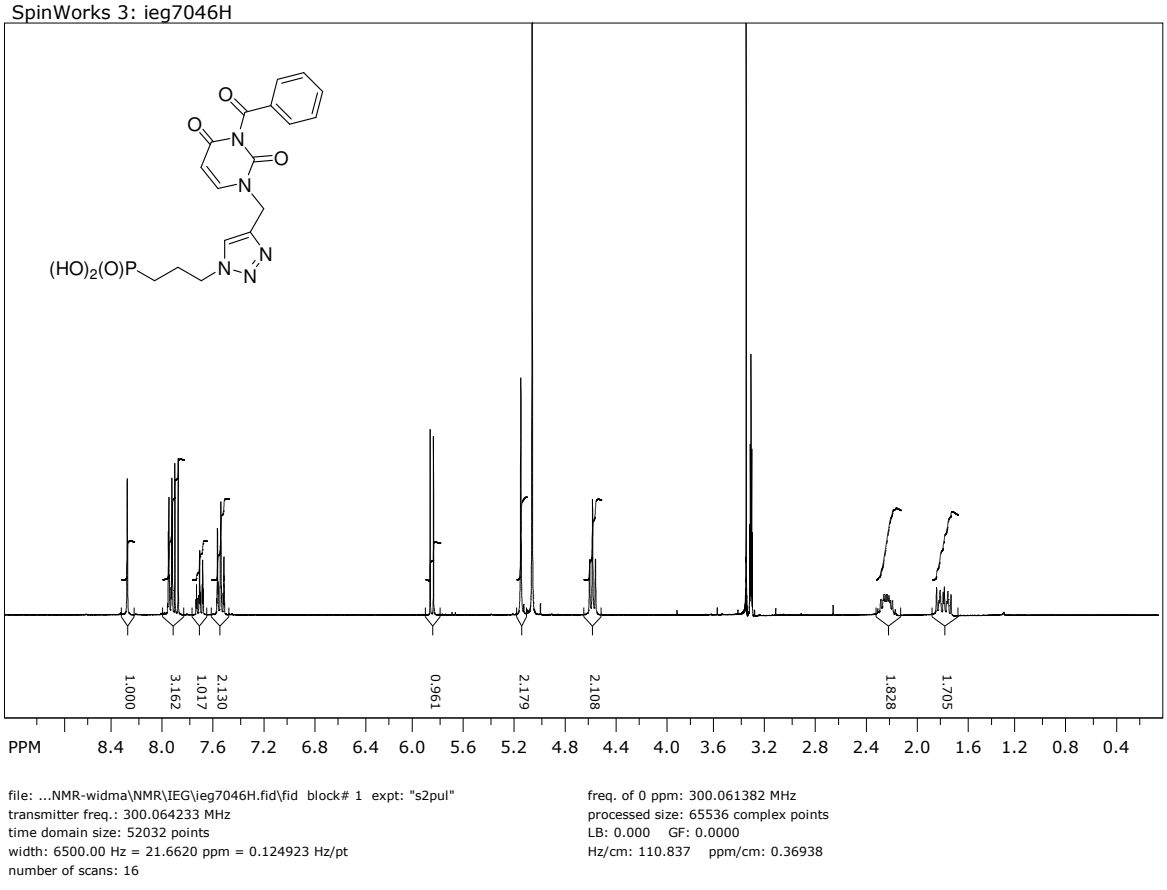


3-{4-[(5,6-Dimethyl-benzimidazol-1-yl)methyl]-1H-1,2,3-triazol-1-yl}propylphosphonic acid **31j**. White powder; m.p.: 148–151°C; IR (KBr): ν = 3100, 2999, 2948, 2889, 1244, 1040, 965 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 9.44 (s, 1H); 8.31 (s, 1H); 7.78 (s, 1H); 7.63 (s, 1H); 5.86 (s, 2H, CH_2); 4.55 (t, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 2.50 (s, 3H, CH_3); 2.47 (s, 3H, CH_3); 2.22 (dqv, *J* = 14.3 Hz, *J* = 7.0 Hz, 2H, PCC*H*$_2$); 1.70 (dt, *J* = 18.7 Hz, *J* = 7.0 Hz, 2H, PC*H*$_2$); ^{13}C NMR (151 MHz, CD_3OD): δ = 140.1; 139.6; 137.4; 137.1; 129.5; 129.4; 125.1; 114.0; 112.7; 50.4 (d, *J* = 18.1 Hz, PCC*C*); 41.6; 23.6 (d, *J* = 4.0 Hz, PC*C*); 23.5 (d, *J* = 139.2 Hz, P*C*); 19.3; 19.1; ^{31}P NMR (243 MHz, CD_3OD): δ = 28.08 ppm. Anal. Calcd. for $C_{15}H_{20}N_5O_3P$: C, 51.57; H, 5.77; N, 20.05. Found: C, 51.80; H, 5.52; N, 19.92.

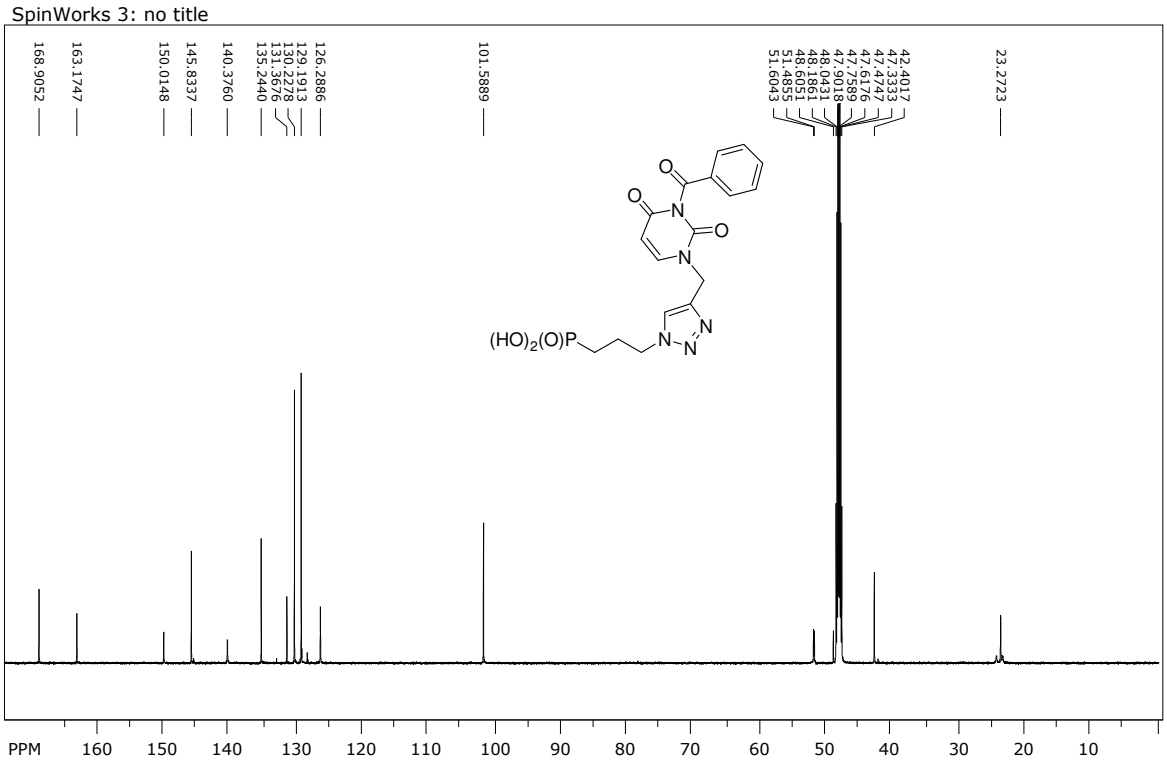


3-(4-{[3-Benzoyl-2,4-dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)propylphosphonic acid **31m**. Colourless oil; IR (film): ν = 3396, 3010, 2983, 2967, 1665, 1654, 1436; 1237, 978, 782, 701 cm^{-1}; ^{1}H NMR (300 MHz, CD_3OD): δ = 8.30 (s, 1H, *H*C5′); 7.98–7.94 (m, 2H, H_{aromat}); 7.91 (d, *J* = 8.0 Hz, 1H, *H*C=CH); 7.75–7.69 (m, 1H, H_{aromat}); 7.58–7.52 (m, 2H, H_{aromat}); 5.86 (d, *J* = 8.0 Hz, 1H, HC=C*H*); 5.15 (s, 2H, CH_2); 4.60 (t, *J* = 7.1 Hz, 2H, PCCCH_2); 2.29–2.18 (m, 2H, PCCH_2); 1.83–1.71 (m, 2H, PCH_2); ^{13}C NMR (151 MHz, CD_3OD): δ = 168.9 (s, C=O); 163.1 (s, C=O); 150.0 (s, C=O); 145.8; 140.4; 135.2; 131.4; 130.2; 129.2; 129.1; 128.3; 126.3; 101.6;101.6; 51.5 (d, *J* = 17.9 Hz, PCC*C*); 42.4; 23.3 (s, *J* = 1.4 Hz, PC*C*); 23.4 (d, *J* = 146.8 Hz, P*C*); ^{31}P NMR (121 MHz, CD_3OD): δ = 29.63 ppm. Anal. Calcd. for $C_{15}H_{18}N_5O_6P \times H_2O$: C, 46.69; H, 4.61; N, 16.01. Found: C, 46.74; H, 4.70; N, 15.94.

^{1}H NMR



^{13}C NMR



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number of scans: 1024

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processed size: 32768 complex points
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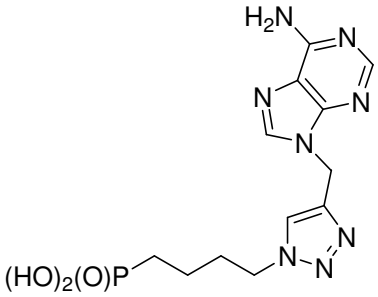
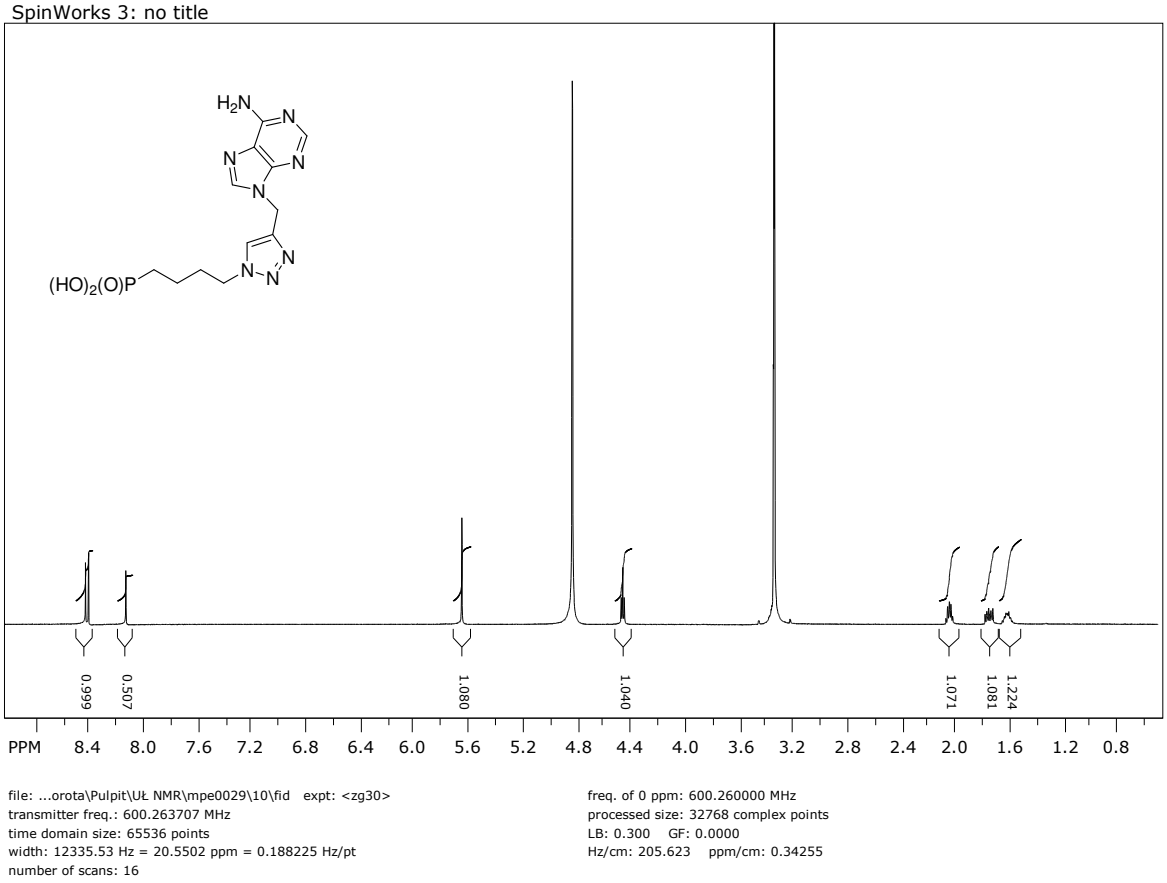
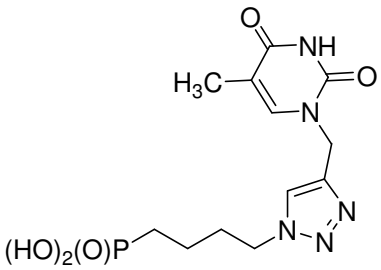


4-(4-{[6-Aminopurin-9-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonic acid **32a**. White powder; m.p.: 217–220ºC; solubility of **32a** in methanol or water was insufficient to measure the ^{13}C NMR spectrum; IR (KBr): ν = 3460, 3300, 3100, 2981, 2910, 2880, 1660, 1647, 1240, 1023 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 8.45 (s, 1H); 8.42 (s, 1H); 8.15 (s, 1H); 5.65 (s, 2H, CH_2); 4.46 (t, *J* = 7.0 Hz, 2H, PCCCC*H*$_2$); 2.03 (qv, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 1.77–1.72 (m, 2H, PC*H*$_2$); 1.64–1.57 (m, 2H, PCC*H*$_2$); ^{31}P NMR (243 MHz, CD_3OD): δ = 29.02 ppm. Anal. Calcd. for $C_{12}H_{17}N_8O_3P$: C, 40.91; H, 4.86; N, 31.81. Found: C, 40.79; H, 4.99; N, 31.69.

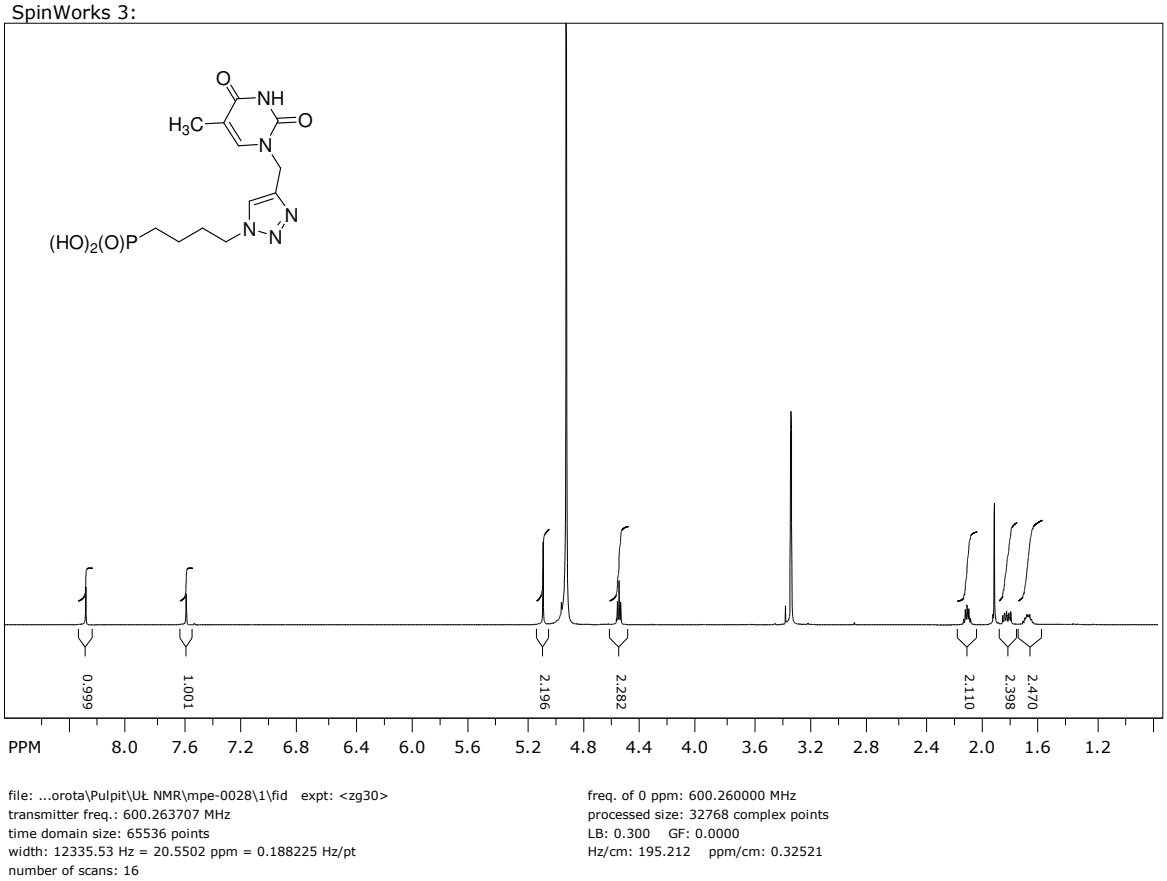
^{1}H NMR

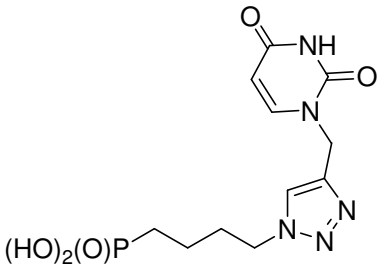




4-(4-{[6-Aminopurin-9-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonic acid **31b**. Amorphous solid; m.p.: 224–226°C; Solubility of **32b** in methanol or water was insufficient to measure the ^{13}C NMR spectrum; IR (KBr): ν = 3445, 3102, 2980, 2910, 1668, 1223, 1025 cm^{-1}; ^{1}H NMR (600 MHz, CD_3OD): δ = 8.30 (s, 1H, *H*C5′); 7.60 (d, *J* = 1.0 Hz, 1H, *H*C=CCH$_3$); 5.08 (s, 2H, CH_2); 4.55 (t, *J* = 7.1 Hz, 2H, PCCCC*H*$_2$); 2.09 (qv, *J* = 7.0 Hz, 2H, PCCC*H*$_2$); 1.90 (d, *J* = 1.0 Hz, 3H, HC=CC*H*$_3$); 1.84–1.79 (m, 2H, PC*H*$_2$); 1.70–1.63 (m, 2H, PCC*H*$_2$); ^{31}P NMR (243 MHz, CD_3OD): δ = 29.86 ppm. Anal. Calcd. for $C_{12}H_{18}N_5O_5P$: C, 41.99; H, 5.29; N, 20.40. Found: C, 42.12; H, 5.03; N, 20.34.

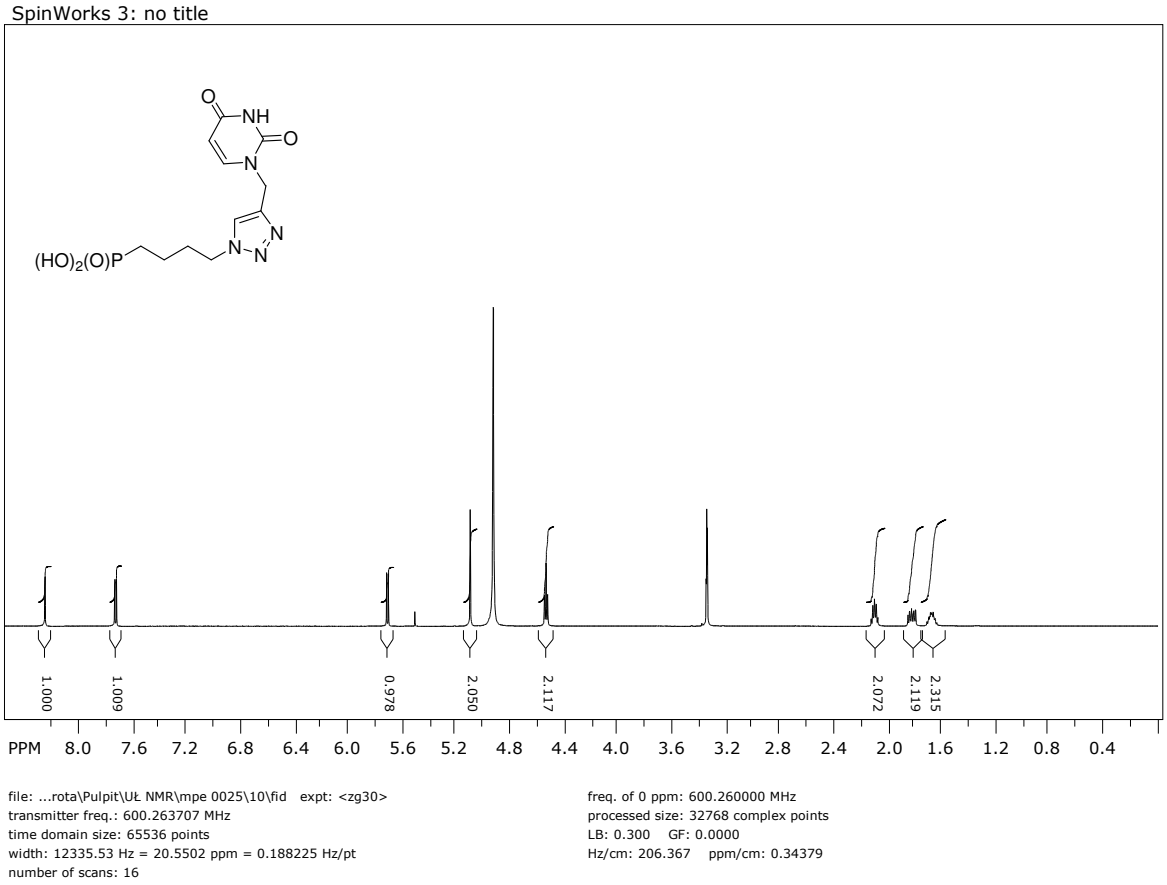
^{1}H NMR



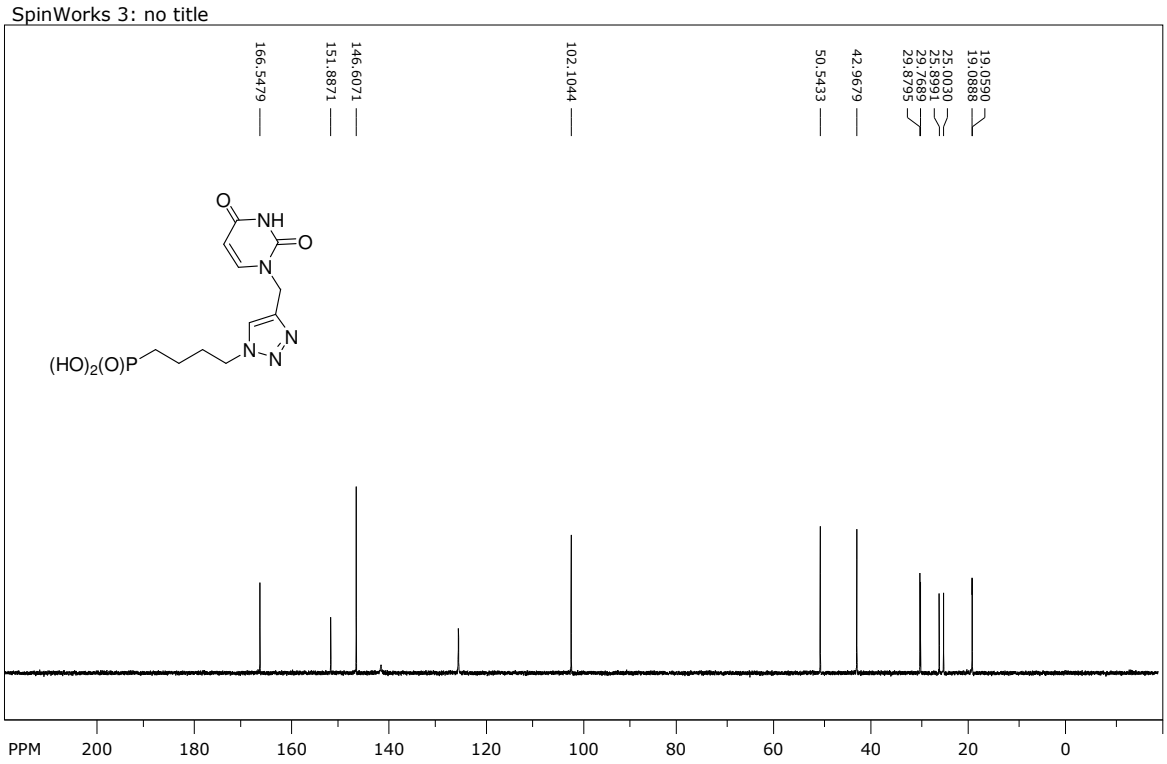


4-(4-{[2,4-Dioxopyrimidin-1-yl]methyl}-1H-1,2,3-triazol-1-yl)butylphosphonic acid **32c**. Amorphous solid; m.p.: 204–206°C; IR (KBr): ν = 3440, 3112, 2980, 2942, 1667, 1219, 1020 cm^{-1}; ^1H NMR (600 MHz, CD_3OD): δ = 8.27 (s, 1H, *H*C5′); 7.74 (d, *J* = 7.9 Hz, 1H, *H*C=CH); 5.71 (d, *J* = 7.9 Hz, 1H, HC=C*H*); 5.01 (s, 2H, CH_2); 4.39 (t, *J* = 7.0 Hz, 2H, PCCCCH_2); 2.06 (qv, *J* = 7.3 Hz, 2H, PCCCH_2); 1.84–1.78 (m, 2H, PCCH_2); 1.70–1.62 (m, 2H, PCH_2); ^{13}C NMR (151 MHz, CD_3OD): δ = 166.5 (s, C=O); 151.9 (s, C=O); 146.6; 141.5; 125.5; 102.1; 50.5; 43.0; 30.6 (d, *J* = 16.7 Hz, PCC*C*); 25.5 (d, *J* = 135.3 Hz, PC); 19.0 (d, *J* = 4.5 Hz, PC*C*); ^{31}P NMR (243 MHz, CD_3OD): δ = 29.81 ppm. Anal. Calcd. for $C_{11}H_{16}N_5O_5P$: C, 40.13; H, 4.90; N, 21.27. Found: C, 40.35; H, 4.68; N, 21.50.

^1H NMR



^{13}C NMR



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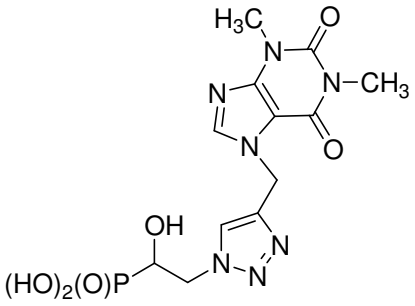
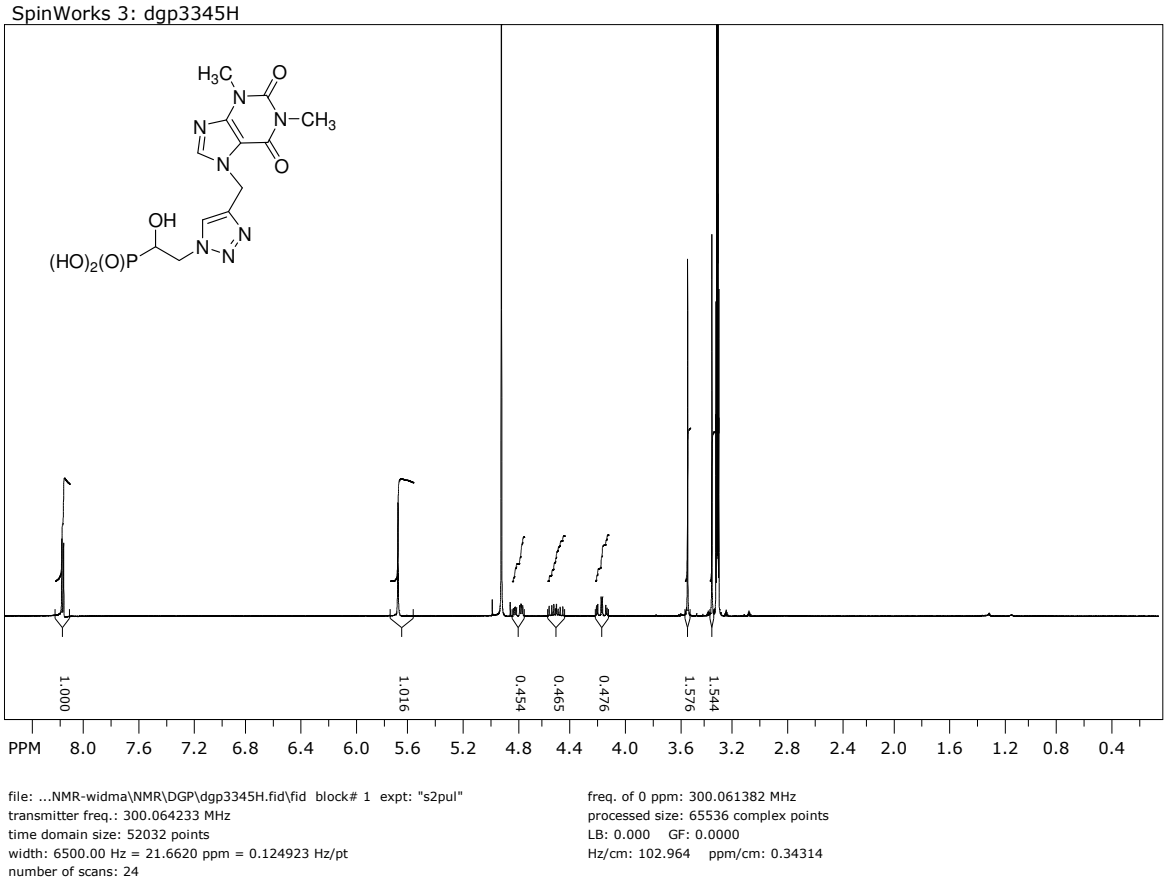


3-{4-[(1,3-Dimethyl-2,6-dioxopurin-7-yl)methyl]-1H-1,2,3-triazol-1-yl}-1-hydroxyethyphosphonic acid **33i**. White powder; m.p.: <244°C; solubility of **33i** in methanol or water was insufficient to measure the ^{13}C NMR spectrum; IR (KBr): ν = 3344, 3102, 2986, 1699, 1672, 1220, 1015 cm^{-1}; ^{1}H NMR (300 MHz, CD_3OD): δ = 8.19 (s, 1H); 8.17 (s, 1H); 5.69 (s, 2H, CH_2); 4.80 (ddd, *J* = 14.2 Hz, *J* = 4.0 Hz, *J* = 2.7 Hz, 1H, PCCH_aH$_b$); 4.51 (ddd, *J* = 14.2 Hz, *J* = 10.3 Hz, *J* = 5.8 Hz, 1H, PCCH$_a$$H_b$); 4.17 (dt, *J* = 10.3 Hz, *J* = 2.7 Hz, 1H, PC*H*(OH)); 3.53 (s, 3H, CH_3); 3.35 (s, 3H, CH_3); ^{31}P NMR (121 MHz, CD_3OD): δ = 19.61 ppm. Anal. Calcd. for $C_{12}H_{16}N_7O_6P$: C, 37.41; H, 4.19; N, 25.45. Found: C, 37.56; H, 4.28; N, 25.30.

^{1}H NMR



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