BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis of ([1,2,4]triazolo[4,3-*a*]pyridin-3-ylmethyl)phosphonates and their benzo derivatives via 5-*exo*-*dig* cyclization

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Experimental procedures, characterization data, and copies of ^{1}H, ^{13}C, and ^{31}P NMR spectra for obtained compounds

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A. General Methods

All reactions were carried out under an inert atmosphere of argon in oven dried glassware with magnetic stirring, unless otherwise noted. All chemicals were purchased from were obtained from commercial suppliers and used without further purification. Column chromatography purifications were performed using Merck silica gel 60. Commercial grade solvents and reagents were used without further purification. Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 silica gel plate. Subsequent to elution, plates were visualized using UV radiation (254 nm). Melting points were uncorrected and were recorded on a Kofler hot-stage (VEB Wägetechnik Rapido, PHMK 81/2969).^{1}H, ^{13}C, ^{15}N and ^{31}P NMR spectra were registered at 400.13, 100.61, 41.50 and 161.98 MHz, respectively, using a Bruker Avance 400 spectrometer. Residual solvent peaks were used as reference. IR spectra were registered on an IRPrestige-21 (Shimadzu) instrument from KBr pellets. HRMS (ESI) analysis was performed on a BrukermicrOTOF mass spectrometer. The X-ray crystal structures were detected on single crystal diffractometers Agilent Technologies (Oxford Diffraction) «Supernova» and «Xcalibur».

B. Typical experimental procedure for the synthesis of dialkyl 2-chloroethynylphosphonates.[1,2]

In a 250 ml round-bottomed flask equipped with an efficient stirrer, thermometer, and reflux condenser a mixture of sodium hydroxide (3 mol), water (150 ml) and benzyltriethylammonium chloride (2 g) was heated with stirring on an oil bath up to 120 ºC. Then, 10 ml of diethyl ether and a solution of trichloroethylene (1 mol) in 100 ml of diethyl ether were added dropwise. Simultaneously the reaction product was distilled off. The distillate consists mainly of the solution of dichloroacetylene in ether. The distillate was dried over calcium chloride, and then over sodium metal. Yield 60%. Trialkylphosphite (0.6 mol) was added dropwise with stirring at 5–20 °C to ether solution of dichloroacetylene obtained. The reaction mixture was kept overnight. Then, diethyl ether was distilled off. The residue was distilled in vacuum (1 mm Hg), collecting the fraction bp 52–60 °C. Yield 68–72%.

Typical experimental procedure for the synthesis of compounds 3-8, 13 and 14. The corresponding 2-hydrazinylpyridines **1a**–**f,g,h** (1 mmol) was added to a mixture of dialkyl chloroacetylenephosphonate **2a**–**c** (1 mmol) and K_2CO_3 (1 mmol) in 5 mL of anhydrous acetonitrile at room temperature. The mixture was stirred at room temperature until the starting chloroethynylphosphonate consumed (monitoring with ^{31}P NMR). After the reaction was completed, the reaction mixture was filtered and evaporated. The oily residue was chromatographed on SiO_2 eluting with 1% MeOH in $CHCl_3$.

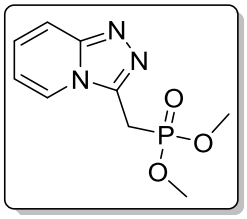
Typical experimental procedure for the synthesis of compounds 10-12. The corresponding 2-hydrazinylpyridines **1i,j** (1 mmol) was added to a mixture of dialkyl chloroacetylenephosphonate **2a,b** (1 mmol) in 5 mL of anhydrous acetonitrile at room temperature. The mixture was stirred (at 60°C for **10**; at reflux for **11** and **12**) until the starting chloroethynylphosphonate consumed (monitoring with ^{31}P NMR). After the reaction was completed, the reaction mixture was filtered and evaporated. The oily residue was chromatographed on SiO_2 eluting with 1% MeOH in $CHCl_3$.

C. References

1. Ionin, B. I.;Petrov, A. A. *Zh. Obshch. Khim.* **1965**, *35*, 1917–1921.
2. Pielichowski, J.; Popielarz, R. *Synthesis (Stuttg).* **1984**, *05*, 433–434.

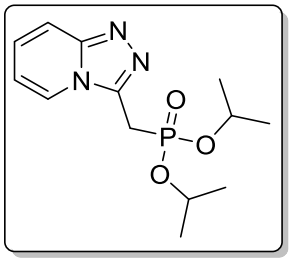
D. Analytical Data

Dimethyl ([1,2,4]triazolo[4,3-a]pyridin-3-ylmethyl)phosphonate 3a



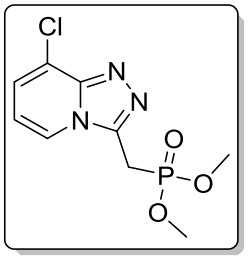
Following the general procedure, **3a** was obtained from **1a** and **2a** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.0 Hz, 1H, 5-$H_{ar.}$), 7.72 (d, *J* = 9.3 Hz, 1H, 8-$H_{ar.}$), 7.39 – 7.17 (m, 1H, 7-$H_{ar.}$), 6.87 (m, 1H, 6-$H_{ar.}$), 3.78 (d, $^{2}J_{HP}$ = 21.5 Hz, 2H, CH_2), 3.73 (d, $^{3}J_{HP}$ = 11.1 Hz, 6H, $2CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.5, 138.8 (d, $^{2}J_{CP}$ = 10.0 Hz), 127.2, 123.2, 116.3, 113.8, 53.4 (d, $^{2}J_{CP}$ = 6.8 Hz), 23.4 (d, $^{1}J_{CP}$ = 143.0 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.85. ν_{max}(KBr)/cm^{-1} 1433, 2951, 1637, 1510, 1388, 1251, 1238, 1188, 1043, 1012, 871, 814, 738. HRMS-ESI (m/z): calcd for $C_9H_{12}N_3O_3P$, $[M+H]^+$: 242.0689, found 242.0694.

Diisopropyl ([1,2,4]triazolo[4,3-a]pyridin-3-ylmethyl)phosphonate 3b



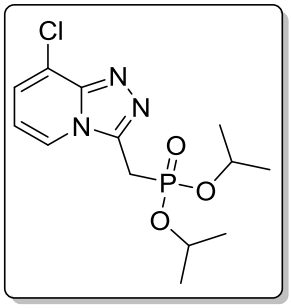
Following the general procedure, **3b** was obtained from **1a** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d,$^{3}J_{HH}$ = 9.3 Hz, 1H, 5-$H_{ar.}$), 7.38 (d,$^{3}J_{HH}$ = 9.3 Hz, 1H, 8-$H_{ar.}$), 7.03 – 6.88 (m, 1H, 7-$H_{ar.}$), 6.56 (m, 1H, 6-$H_{ar.}$), 4.34 (m, $^{3}J_{HP}$ = 12.6 Hz, $^{3}J_{HH}$ = 6.2 Hz, 2H, 2CH), 3.47 (d,$^{3}J_{HP}$ = 20.3 Hz, 2H, CH_2), 0.96 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H, $2CH_3$), 0.92 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H, $2CH_3$).^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 139.2 (d, $^{2}J_{CP}$ = 9.9 Hz), 126.9, 123.6, 115.6, 113.1, 71.6 (d, $^{2}J_{CP}$ = 6.9 Hz), 25.1 (d, $^{1}J_{CP}$ = 143.3 Hz), 23.7 (d, $^{3}J_{CP}$ = 3.9 Hz), 23.5 (d, $^{3}J_{CP}$ = 4.9 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.40. ν_{max}(KBr)/cm^{-1} 3461, 2981, 1637, 1507, 1387, 1376, 1251, 1105, 988, 759. HRMS-ESI (m/z): calcd for $C_{13}H_{20}N_3O_3P$, $[M+H]^+$: 298.1315, found 298.1301.

Dimethyl ((8-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 4a



Following the general procedure, **4a** was obtained from **1b** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, $^{3}J_{HH}$ = 7.0 Hz, 1H, 5-$H_{ar.}$), 7.34 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, 7-$H_{ar.}$), 6.85 (t, $^{3}J_{HH}$ = 7.0 Hz, 1H, 6-$H_{ar.}$), 3.81 (d, *J* = 20.6 Hz, 2H, CH_2), 3.76 (d, $^{3}J_{HP}$ = 11.0 Hz, 6H, $2OCH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 140.5 (d, $^{2}J_{CP}$ = 10.1 Hz), 126.1, 122.5, 122.1, 113.7, 53.5 (d, $^{2}J_{CP}$ = 6.7 Hz), 23.7 (d, $^{1}J_{CP}$ = 142.6 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.33. ν_{max}(KBr)/cm^{-1} 3434, 2952, 1630, 1506, 1383, 1321, 1263, 1239, 1041, 1026, 1009, 945, 865, 818. HRMS-ESI (m/z): calcd for $C_9H_{11}ClN_3O_3P$, $[M+Na]^+$: 298.0119, found 298.0132. M. p. 155 - 160 °C.

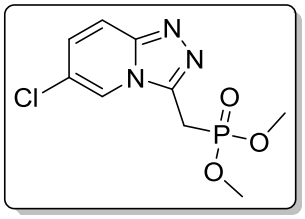
Diisopropyl ((8-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 4b



Following the general procedure, **4b** was obtained from **1b** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, $^{3}J_{HH}$ = 6.9 Hz, 1H, 5-$H_{ar.}$), 7.14 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, 7-$H_{ar.}$), 6.66 (t, $^{3}J_{HH}$ = 7.0 Hz, 1H, 6-$H_{ar.}$), 4.44 (m, 2H, 2CH), 3.59 (d, $^{2}J_{HP}$ = 20.3 Hz, 2H, CH_2), 1.08 (d, $^{3}J_{HH}$ = 6.1 Hz, 6H, $2CH_3$), 1.04 (d,

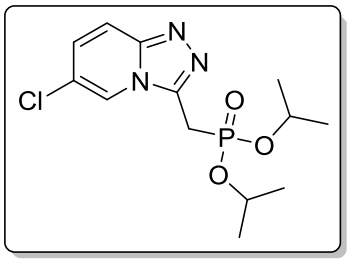
$^{3}J_{HH}$ = 6.2 Hz, 6H, 2CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 141.1 (d, $^{2}J_{CP}$ = 9.9 Hz), 126.1, 122.7, 121.6, 113.2, 72.0 (d, $^{2}J_{CP}$ = 7.0 Hz), 25.3 (d, $^{1}J_{CP}$ = 143.1 Hz), 23.8 (d, $^{3}J_{CP}$ = 4.0 Hz), 23.7 (d, $^{3}J_{CP}$ = 4.9 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.08. ν_{max}(KBr)/cm^{-1} 3464, 2981, 1632, 1502, 1385, ,1249, 1104, 990, 739. HRMS-ESI (m/z): calcd for $C_{13}H_{19}ClN_3O_3P$, $[M+H]^+$: 332.0925, found 332.0925.

Dimethyl ((6-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 5a



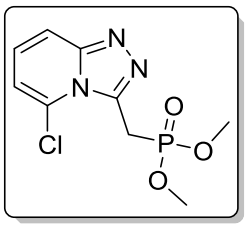
Following the general procedure, **5a** was obtained from **1c** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H, 5-$H_{ar.}$), 7.70 (d, $^{3}J_{HH}$ = 9.7 Hz, 1H, 8-$H_{ar.}$), 7.22 (dd, $^{3}J_{HH}$ = 9.7,$^{4}J_{HH}$= 1.6 Hz, 1H, 7-$H_{ar.}$), 3.76 (d, $^{3}J_{HP}$ = 11.0 Hz, 6H, 2OCH_3),3.75 (d, $^{2}J_{HP}$ = 20.6 Hz, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 139.2 (d, $^{2}J_{CP}$ = 9.9 Hz), 129.2, 122.7, 121.2, 116.9, 53.6 (d, $^{3}J_{CP}$ = 6.7 Hz), 23.6 (d, $^{1}J_{CP}$ = 143.0 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.45. ν_{max}(KBr)/cm^{-1} 3087, 2950, 1635, 1506, 1255, 1239, 1043, 1024, 874, 820. HRMS-ESI (m/z): calcd for $C_9H_{11}ClN_3O_3P$, $[M+H]^+$: 276.0299, found 276.0308. M. p. 144 - 145 °C.

Diisopropyl ((6-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 5b



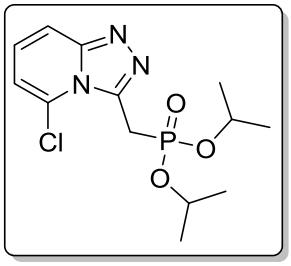
Following the general procedure, **5b** was obtained from **1c** and **2b** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H, 5-$H_{ar.}$), 7.67 (d, $^{3}J_{HH}$ = 9.7 Hz, 1H, 8-$H_{ar.}$), 7.19 (dd, $^{3}J_{HH}$ = 9.7,$^{4}J_{HH}$ 1.8 Hz, 1H, 7-$H_{ar.}$), 4.65 (m, 2H, 2CH), 3.69 (d, $^{2}J_{HP}$ = 20.3 Hz, 2H, CH_2), 1.26 (d, $^{3}J_{HH}$ = 6.1 Hz, 6H, 2CH_3), 1.25 (d, $^{3}J_{HH}$ = 6.1 Hz, 6H, 2CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 139.8 (d, $^{2}J_{CP}$ = 10.2 Hz), 128.9, 122.1, 121.66, 116.8, 72.4 (d, $^{2}J_{CP}$ = 7.2 Hz), 25.7 (d, $^{1}J_{CP}$ = 143.7 Hz), 24.1 (d, $^{3}J_{CP}$ = 4.2 Hz), 24.0 (d, $^{3}J_{CP}$ = 4.7 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.12. ν_{max}(KBr)/cm^{-1} 3075, 2980, 2921, 1634, 1506, 1384, 1238, 1025, 982, 802, 796. HRMS-ESI (m/z): calcd for $C_{13}H_{19}ClN_3O_3P$, $[M+H]^+$: 332.0925, found 332.0929. M. p. 132 - 133 °C.

Dimethyl ((5-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 6a



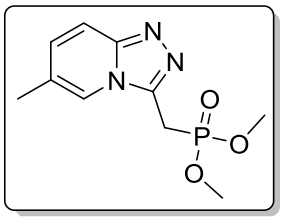
Following the general procedure, **6a** was obtained from **1d** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, $^{3}J_{HH}$ = 7.0 Hz, 1H, 8-$H_{ar.}$), 7.34 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, 7-$H_{ar.}$), 6.85 (t, $^{3}J_{HH}$ = 7.0 Hz, 1H, 6-$H_{ar.}$), 4.19 (d, J = 20.6 Hz, 2H, CH_2), 3.76 (d, $^{3}J_{HP}$ = 11.0 Hz, 6H, 2OCH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 140.5 (d, $^{2}J_{CP}$ = 10.1 Hz), 126.1, 122.5, 122.1, 113.7, 53.5 (d, $^{2}J_{CP}$ = 6.7 Hz), 23.7 (d, $^{1}J_{CP}$ = 142.6 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.33. ν_{max}(KBr)/cm^{-1} 2957, 2360, 1630, 1494, 1404, 1354, 1298, 1267, 1248, 1230, 1138, 1003, 875, 829, 783, 731, 669, 597, 524. HRMS-ESI (m/z): calcd for $C_9H_{11}ClN_3O_3P$, $[M+H]^+$: 276.0299, found 276.0293. M. p. 99 - 100 °C.

Diisopropyl ((5-chloro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 6b



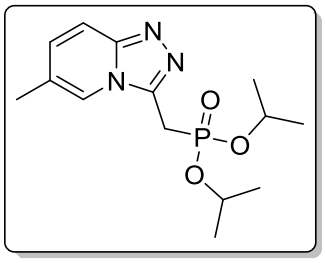
Following the general procedure, **3b** was obtained from **1d** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, $^{3}J_{HH}$ = 9.2,$^{4}J_{HH}$= 0.9 Hz, 1H, 8-$H_{ar.}$), 7.14 (dd, $^{3}J_{HH}$ = 9.2, 7.0 Hz, 1H, 7-$H_{ar.}$), 6.82 (dd, $^{3}J_{HH}$ = 7.0,$^{4}J_{HH}$= 0.8 Hz, 1H, 6-$H_{ar.}$), 4.66 (m, 2H, 2CH), 4.11 (d, $^{2}J_{HP}$ = 20.7 Hz, 2H, CH_2), 1.26 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H), 1.23 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 140.4 (d, $^{2}J_{CP}$ = 11.0 Hz), 127.5, 125.4, 115.2, 115.0, 71.5 (d, $^{2}J_{CP}$ = 7.2 Hz), 27.9 (d, $^{1}J_{CP}$ = 142.9 Hz), 23.8 (d, $^{3}J_{CP}$ = 3.7 Hz), 23.7 (d, $^{3}J_{CP}$ = 5.2 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.20. ν_{max}(KBr)/cm^{-1} 3471, 2981, 1629, 1496, 1387, 1255, 1106, 987, 788. HRMS-ESI (m/z): calcd for $C_{13}H_{19}ClN_3O_3P$, $[M+H]^+$: 332.0925, found 332.0919.

Dimethyl ((6-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 7a



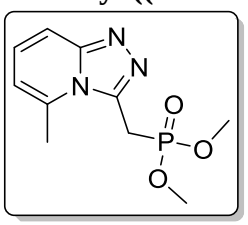
Following the general procedure, 7**a** was obtained from **1e** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, $^{4}J_{HH}$ = 1.4 Hz, 1H, 5-$H_{ar.}$), 7.67 (d, $^{3}J_{HH}$ = 9.4 Hz, 1H, 8-$H_{ar.}$), 7.14 (dd, $^{3}J_{HH}$ = 9.4,$^{4}J_{HH}$= 1.4 Hz, 1H, 7-$H_{ar.}$), 3.77 (d, $^{3}J_{HP}$ = 11.1 Hz, 6H, 2CH_3), 3.77 (d, $^{2}J_{HP}$ = 20.3 Hz, 2H, CH_2), 2.38 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.0, 138.2 (d, $^{2}J_{CP}$ = 9.8 Hz), 130.7, 123.9, 120.2, 115.6, 53.4 (d, $^{2}J_{CP}$ = 6.8 Hz), 23.4 (d, $^{1}J_{CP}$ = 143.2 Hz), 18.3. ^{31}P NMR (162 MHz, $CDCl_3$) δ 22.92. ν_{max}(KBr)/cm^{-1} 3396, 2947, 1649, 1520, 1425, 1256, 1187, 1042, 1020, 876, 822, 759, 773. HRMS-ESI (m/z): calcd for $C_{10}H_{14}N_3O_3P$, $[M+Na]^+$: 278.0665, found 278.0666. M. p. 128 - 130 °C.

Diisopropyl ((6-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 7b



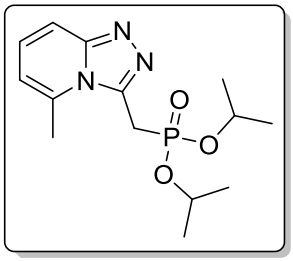
Following the general procedure, **7b** was obtained from **1e** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H, 5-$H_{ar.}$), 7.27 (d,$^{3}J_{HH}$ = 9.4 Hz, 1H, 8-$H_{ar.}$), 6.80 (d, $^{3}J_{HH}$ = 9.4 Hz, 1H, 7-$H_{ar.}$), 4.34 (m, $^{3}J_{HH}$ = 6.2 Hz, 2H, 2CH), 3.42 (d, $^{2}J_{HP}$ = 20.3 Hz, 2H, CH_2), 2.02 (s, 3H, CH_3) 0.96 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H, 2CH_3), 0.92 (d, $^{3}J_{HH}$ = 6.2 Hz, 6H, 2CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4, 138.6 (d, $^{2}J_{CP}$ = 10.1 Hz), 130.3, 122.9, 120.6, 114.9, 71.6 (d, $^{2}J_{CP}$ = 7.0 Hz), 25.1 (d, $^{1}J_{CP}$ = 143.6 Hz), 23.7 (d, $^{3}J_{CP}$ = 3.9 Hz), 23.5 (d, $^{3}J_{CP}$ = 5.0 Hz), 17.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.51. ν_{max}(KBr)/cm^{-1} 3494, 2981, 1646, 1525, 1383, 1274, 1209, 1105, 999, 813. HRMS-ESI (m/z): calcd for $C_{14}H_{22}N_3O_3P$, $[M+H]^+$: 312.1472, found 312.1466.

Dimethyl ((5-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 8a



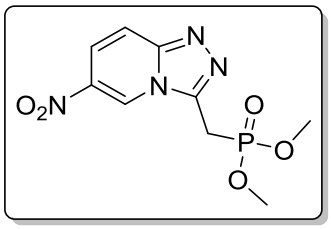
Following the general procedure, **8a** was obtained from **1f** and **2a** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (d, $^{3}J_{HH}$ = 9.2 Hz, 1H, 8-$H_{ar.}$), 6.70 (dd,$^{3}J_{HH}$ = 9.2, 6.7 Hz, 1H, 7-$H_{ar.}$), 6.14 (d, $^{3}J_{HH}$ = 6.7 Hz, 1H, 6-$H_{ar.}$), 3.61 (d, $^{2}J_{HP}$ = 20.6 Hz, 2H, CH_2), 3.35 (d, $^{3}J_{HP}$ = 11.1 Hz, 6H, $2CH_3$), 2.53 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.5, 139.0 (d, $^{2}J_{CP}$ = 9.9 Hz), 134.7, 127.5, 114.4, 113.7, 53.1 (d, $^{2}J_{CP}$ = 6.9 Hz), 25.4 (d, $^{1}J_{CP}$ = 141.8 Hz), 19.3. ^{31}P NMR (162 MHz, $CDCl_3$) δ 23.00. ν_{max}(KBr)/cm^{-1} 3420, 3273, 2360, 1651, 1573, 1518, 1446, 1232, 1199, 1107, 1043, 486, 798, 769, 746, 696. HRMS-ESI (m/z): calcd for $C_{10}H_{14}N_3O_3P$, $[M+H]^+$: 256.0846, found 256.0852.

Diisopropyl ((5-methyl-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 8b



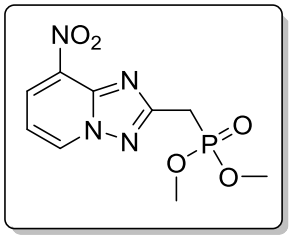
Following the general procedure, **8b** was obtained from **1f** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, $^{3}J_{HH}$ = 9.2 Hz, 1H, 8-$H_{ar.}$), 7.09 (dd, $^{3}J_{HH}$ = 9.2, 6.7 Hz, 1H, 7-$H_{ar.}$), 6.51 (d, $^{3}J_{HH}$ = 6.6 Hz, 1H, 6-$H_{ar.}$), 4.79 – 4.40 (m, 2H, 2OCH), 3.92 (d, $^{2}J_{HP}$ = 20.6 Hz, 2H, CH_2), 2.97 (s, 3H, CH_3) 1.40 – 1.05 (m, 12H, $4CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 139.8 (d, $^{2}J_{CP}$ = 10.5 Hz), 134.9, 127.4, 114.5, 114.5, 71.9 (d, $^{2}J_{CP}$ = 7.0 Hz) 27.7 (d, $^{1}J_{CP}$ = 143.3 Hz), 24.0 (d, $^{3}J_{CP}$ = 3.8 Hz), 23.8 (d, $^{3}J_{CP}$ = 5.1 Hz), 19.9. ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.65. ν_{max} (KBr)/cm^{-1} 2978, 1640, 1512, 1465, 1383, 1245, 1107, 994, 791. HRMS-ESI (m/z): calcd for $C_{14}H_{22}N_3O_3P$, $[M+H]^+$: 312.1472, found 312.1479.

Dimethyl ((6-nitro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 10a



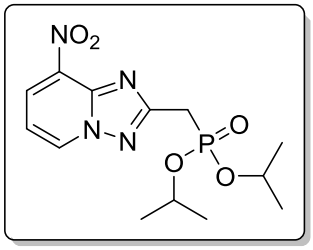
Following the general procedure, **10a** was obtained from **1j** and **2a** as pale yellow oil. ^{1}H NMR (400 MHz, CDCl3) δ 9.48 (s, 1H, 5-$H_{ar.}$), 8.05 (d, $^{3}J_{HH}$ = 10.0 Hz, 1H, 8-$H_{ar.}$), 7.86 (d, $^{3}J_{HH}$ = 10.0 Hz, 1H, 7-$H_{ar.}$), 3.91 (d, $^{2}J_{HP}$ = 20.6 Hz, 2H, CH_2), 3.82 (d, $^{3}J_{HP}$ = 11.1 Hz, 6H, $2CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.9, 141.9 (d, $^{2}J_{CP}$ = 10.1 Hz), 138.4, 124.6, 121.5, 116.6, 53.7 (d, $^{2}J_{CP}$ = 6.7 Hz), 23.6 (d,$^{1}J_{CP}$= 142.5 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 21.88. ν_{max}(KBr)/cm^{-1} 3038, 2361, 1636, 1527, 1473, 1257, 1030, 866, 827, 794, 756, 534. HRMS-ESI (m/z): calcd for $C_9H_{12}N_4O_5P$, $[M+H]^+$: 287.0540, found 287.0548

Dimethyl ((8-nitro-[1,2,4]triazolo[1,5-a]pyridin-3-yl)methyl)phosphonate 11a



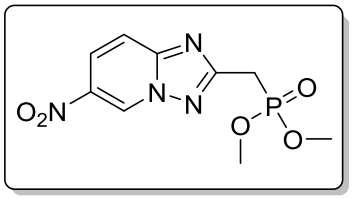
Following the general procedure, **11a** was obtained from **1i** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (dd, $^{3}J_{HH}$ = 6.7,$^{4}J_{HH}$= 1.2 Hz, 1H, 5-$H_{ar.}$), 8.57 (dd, $^{3}J_{HH}$ = 7.9,$^{3}J_{HH}$= 1.2 Hz, 1H, 7-$H_{ar.}$), 7.23 (dd, $^{3}J_{HH}$ = 7.9, 6.7 Hz, 1H, 6-$H_{ar.}$), 3.90 (d, $^{2}J_{HP}$= 11.1 Hz, 6H, $2CH_3$), 3.71 (d, $^{2}J_{HP}$ = 21.6 Hz, 2H, CH_2).^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9 (d, $^{2}J_{CP}$ = 8.1 Hz), 145.5, 136.5, 133.9, 128.1, 111.6, 53.4 (d, $^{2}J_{CP}$ = 6.5 Hz), 27.0 (d, $^{1}J_{CP}$ = 140.2 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 24.68. ν_{max} (KBr)/cm^{-1} 3037, 2361, 1635, 1528, 1474, 1296, 1257, 1215, 1030, 989, 866, 827, 795, 756, 534. HRMS-ESI (m/z): calcd for $C_9H_{12}N_4O_5P$, $[M+H]^+$: 287.0540, found 287.0553. M. p. 104 - 105 °C.

Diisopropyl ((8-nitro-[1,2,4]triazolo[1,5-a]pyridin-3-yl)methyl)phosphonate 11b



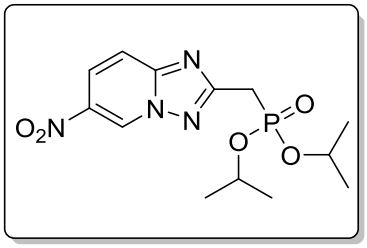
Following the general procedure, **11b** was obtained from **1i** and **2b** as pale solid. ^{1}H NMR (400 MHz, CDCl3) δ 8.88 (dd, $^{3}J_{HH}$ = 6.8,$^{4}J_{HH}$= 1.1 Hz, 1H, 5-H$_{ar.}$), 8.53 (dd, $^{3}J_{HH}$ = 7.8,$^{3}J_{HH}$= 1.1 Hz, 1H, 7-H$_{ar.}$), 7.20 (dd, $^{3}J_{HH}$ = 7.8, 6.8 Hz, 1H, 6-H$_{ar.}$), 4.80 (m, 2H), 3.62 (d, ^{2}J$_{HP}$ = 21.5 Hz, 1H), 1.36 (d, $^{3}J_{HH}$ = 5.6 Hz, 3H, CH$_3$),1.35 (d, $^{3}J_{HH}$ = 5.6 Hz, 3H, CH$_3$).^{13}C NMR (101 MHz, CDCl$_3$) δ 162.4 (d, $^{2}J_{CP}$ = 8.1 Hz), 145.4, 136.4, 133.9, 128.0, 111.4, 71.6 (d, $^{2}J_{CP}$ = 6.6Hz), 28.9 (d, $^{1}J_{CP}$ = 140.5 Hz), 24.1 (d, *J* = 3.6 Hz), 23.9 (d, *J* = 5.2 Hz). ^{31}P NMR (162 MHz, CDCl$_3$) δ 19.71. ν$_{max}$ (KBr)/cm^{-1} 3046, 2982, 2932, 1638, 1528, 1477, 1383, 1255, 1244, 1109, 976, 785, 756, 681, 540. HRMS-ESI (m/z): calcd for $C_{13}H_{19}N_4O_5P$, $[M+H]^+$: 343.2875, found 343.1166. M. p. 89 - 90 °C.

Dimethyl ((6-nitro-[1,2,4]triazolo[1,5-a]pyridin-3-yl)methyl)phosphonate 12a



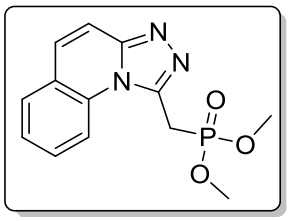
Following the general procedure, **12a** was obtained from **1j** and **2a** as pale yellow oil. 1H NMR (400 MHz, CDCl$_3$) δ 9.61 (d, $^{4}J_{HH}$ = 2.1 Hz, 1H, 5-H$_{ar.}$), 8.34 (dd, $^{3}J_{HH}$ = 9.8 Hz,$^{4}J_{HH}$ = 2.1 Hz, 1H, 7-H$_{ar.}$), 7.82 (d, $^{3}J_{HH}$ = 9.8 Hz, 1H, 8-H$_{ar.}$), 3.87 (d, $^{3}J_{HP}$ = 21.6 Hz, 2H, CH$_2$), 3.63 (d, $^{2}J_{HP}$ = 11.1 Hz, 6H, 2CH$_3$). ^{13}C NMR (101 MHz, CDCl$_3$) δ 163.3 (d, $^{2}J_{CP}$ = 8.6 Hz), 152.7, 137.9, 127.7, 124.2, 115.9, 53.3 (d, $^{2}J_{CP}$ = 6.1 Hz), 27.0 (d,$^{1}J_{CP}$= 140.1 Hz).^{31}P NMR (162 MHz, CDCl3) δ 24.53. ν$_{max}$ (KBr)/cm^{-1} 3075, 2918, 2361, 2342, 1643, 1526, 1472, 1389, 1350, 1252, 1022, 862, 798, 735, 532. HRMS-ESI (m/z): calcd for $C_9H_{12}N_4O_5P$, $[M+H]^+$: 287.1812, found 287.0540.

Diisopropyl ((6-nitro-[1,2,4]triazolo[4,3-a]pyridin-3-yl)methyl)phosphonate 12b



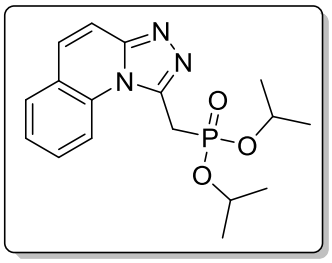
Following the general procedure, **12b** was obtained from **1j** and **2b** as pale yellow oil. ^{1}H NMR (400 MHz, CDCl$_3$) δ 9.60 (dd, $^{3}J_{HH}$ = 2.2, $^{4}J_{HH}$ = 0.8 Hz, 1H, 5-H$_{ar.}$), 8.32 (dd, $^{3}J_{HH}$ = 9.8, $^{3}J_{HH}$ = 2.2 Hz, 1H, 7-H$_{ar.}$), 7.80 (dd, $^{3}J_{HH}$ = 9.8, 0.8 Hz, 1H, 6-H$_{ar.}$), 4.80 (m, 2H), 3.56 (d, ^{2}J$_{HP}$ = 21.6 Hz, 2H, CH$_2$), 1.36 (d, $^{3}J_{HH}$ = 6.1 Hz, 3H, CH$_3$), 1.34 (d, $^{3}J_{HH}$ = 6.1 Hz, 3H, CH$_3$).^{13}C NMR (101 MHz, CDCl$_3$) δ 163.9 (d, $^{2}J_{CP}$ = 8.5 Hz), 152.6, 137.8, 127.6, 124.0, 115.8, 71.5 (d, $^{2}J_{CP}$ = 6.6 Hz), 29.2 (d, $^{1}J_{CP}$ = 140.4 Hz), 24.1 (d, *J* = 3.7 Hz), 23.9 (d, *J* = 5.1 Hz). ^{31}P NMR (162 MHz, CDCl$_3$) δ 19.65. ν$_{max}$ (KBr)/cm^{-1} 3078, 2982, 1639, 1558, 1529, 1476, 1348, 1234, 1107, 982, 783, 761, 734, 529. HRMS-ESI (m/z): calcd for $C_{13}H_{19}N_4O_5P$, $[M+H]^+$: 343.2875, found 343.1166

Dimethyl ([1,2,4]triazolo[4,3-a]quinolin-1-ylmethyl)phosphonate 13a



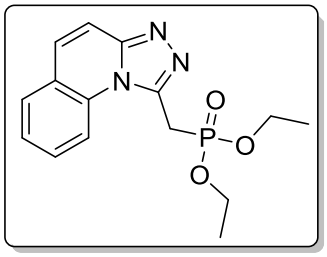
Following the general procedure, 1**3a** was obtained from **1g** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 – 8.48 (m, 1H), 7.99 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H), 7.81 – 7.56 (m, 3H), 7.10 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H), 3.80 (d, $^{2}J_{HP}$ = 20.4 Hz, 2H, CH_2), 3.77 (d, $^{3}J_{HP}$ = 11.1 Hz, 6H, 2OCH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 140.6 (d, $^{2}J_{CP}$ = 9.8 Hz), 130.2, 129.7, 129.1, 127.1, 123.9, 121.4, 119.8, 115.2, 53.5 (d, $^{2}J_{CP}$ = 6.7 Hz), 23.4 (d, $^{1}J_{CP}$ = 142.6 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.75. ν_{max}(KBr)/cm^{-1} 3473, 2941, 1661, 1643, 1524, 1453, 1401, 1130, 1063, 1023, 898, 885, 839, 808, 790. HRMS-ESI (m/z): calcd for $C_{13}H_{14}N_3O_3P$, $[M+H]^+$: 292.0846, found 292.0839. M. p. 108 - 109 °C.

Diisopropyl ([1,2,4]triazolo[4,3-a]quinolin-1-ylmethyl)phosphonate 13b



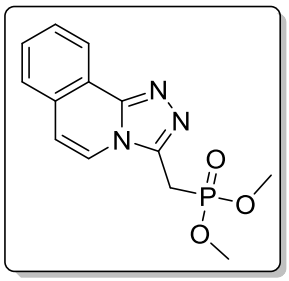
Following the general procedure, **13b** was obtained from **1g** and **2b** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.79 – 8.68 (m, 1H), 8.10 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H), 7.89 – 7.57 (m, 3H), 7.10 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H), 4.67 (m, 2H, 2OCH), 3.75 (d, $^{2}J_{HP}$ = 20.4 Hz, 2H, CH_2), 1.29 (d, $^{3}J_{HH}$= 6.5 Hz, 6H), 1.28 (d, , $^{3}J_{HH}$ = 6.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 141.2 (d, $^{2}J_{CP}$ = 9.6 Hz), 130.1, 129.7, 129.0, 127.1, 124.0, 121.5, 120.4, 114.7, 72.1 (d, $^{2}J_{CP}$ = 6.9 Hz), 25.5 (d, $^{1}J_{CP}$ = 143.2 Hz), 24.0 (d, $^{3}J_{CP}$ = 4.2 Hz), 24.1 (d, $^{3}J_{CP}$ = 4.8 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.40. ν_{max} (KBr)/cm^{-1} 3464, 2977, 1642, 1524, 1460, 1377, 1242, 1107, 999, 976, 794. HRMS-ESI (m/z): calcd for $C_{17}H_{22}N_3O_3P$, $[M+H]^+$: 348.1472, found 348.1486. M. p. 90 - 91 °C.

Diethyl ([1,2,4]triazolo[4,3-a]quinolin-1-ylmethyl)phosphonate 13c



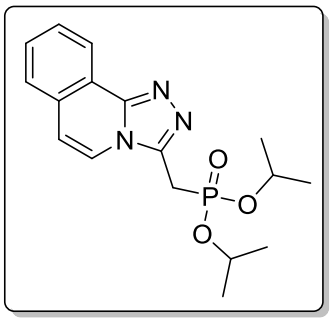
Following the general procedure, **13c** was obtained from **1g** and **2c** as pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, ,$^{3}J_{HH}$ = 7.9Hz, 1H), 7.77 (d, $^{3}J_{HH}$ = 7.9 Hz, 1H), 7.67 (t, $^{3}J_{HH}$ = 7.9 Hz, 1H), 7.58 (dd, $^{3}J_{HH}$ = 7.9 Hz, 1H), 7.55 – 7.46 (m,2H), 4.18– 4.08 (m, 2H, CH_2), 4.14 (d, $^{2}J_{HP}$ = 20.3 Hz, 4H, 2OCH_2), 1.22 (d, $^{3}J_{HH}$ = 7.1 Hz, 3H, CH_3),1.20 (d, $^{3}J_{HH}$ = 7.1 Hz, 3H, CH_3).^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 142.0 (d, $^{2}J_{CP}$ = 9.7 Hz), 131.8, 129.3, 129.2, 126.3, 124.6, 116.9, 114.9, 63.1 (d, $^{2}J_{CP}$ = 7.0 Hz), 27.8 (d, $^{1}J_{CP}$ = 142.4 Hz), 16.2 (d, $^{2}J_{CP}$ = 6.4 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 19.71. ν_{max} (KBr)/cm^{-1} 3421, 2982, 1657, 1605, 1504, 1447, 1372, 1232, 1050, 1026, 969, 830, 811, 758. HRMS-ESI (m/z): calcd for $C_{15}H_{18}N_3O_3P$, $[M+Na]^+$: 342.0978, found 342.0991.

Dimethyl ([1,2,4]triazolo[4,3-a]isoquinolin-3-ylmethyl)phosphonate 14a



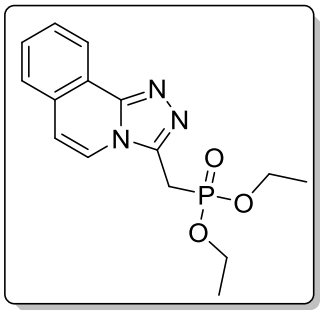
Following the general procedure, **14a** was obtained from **1h** and **2a** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, $^{3}J_{HH}$ = 8.6 Hz, 1H), 7.83 (dd, $^{3}J_{HH}$= 8.6, $^{4}J_{HH}$= 1.4 Hz, 1H), 7.78 – 7.69 (m, 1H), 7.65 (d, $^{3}J_{HH}$ = 8.6 Hz, 1H), 7.61 – 7.53 (m, 1H), 4.19 (d, $^{2}J_{HP}$ = 20.5 Hz, 2H, CH_2), 3.82 (d, $^{2}J_{HP}$ = 11.1 Hz, 6H, $2OCH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 141.8 (d, $^{2}J_{CP}$ = 9 Hz), 131.9, 129.8, 129.4, 126.4, 124.8, 116.6, 115.1, 53.6 (d, $^{2}J_{CP}$ = 7.2 Hz), 27.2 (d, $^{1}J_{CP}$ = 143.2 Hz).^{31}P NMR (162 MHz, $CDCl_3$) δ 22.23. ν_{max}(KBr)/cm^{-1} 4422, 2957, 1622, 1561, 1412, 1260, 1244, 1049, 1014, 864, 822. HRMS-ESI (m/z): calcd for $C_{13}H_{14}N_3O_3P$, $[M+H]^+$: 292.0846, found 292.0836. M. p. 132 - 133 °C.

Diisopropyl ([1,2,4]triazolo[4,3-a]isoquinolin-3-ylmethyl)phosphonate 14b



Following the general procedure, **14b** was obtained from **1h** and **2b** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.6 Hz, 1H), 7.78 (d, $^{3}J_{HH}$ = 8.6 Hz, 1H), 7.68 (t, $^{3}J_{HH}$ = 8.6 Hz, 1H), 7.60 (d, $^{3}J_{HH}$= 8.6 Hz, 1H), 7.56 – 7.48 (m, 2H), 4.89 – 4.55 (m, 2H), 4.12 (d, $^{2}J_{HP}$ = 20.3 Hz, 2H, CH_2), 1.23 (d, $^{3}J_{HH}$ = 6.2 Hz, 12H, $4CH_3$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 142.4 (d, $^{2}J_{CP}$ = 10.0 Hz), 132.0, 129.6, 129.2, 129.1, 126.2, 124.6, 117.3, 115.1, 72.1 (d,$^{2}J_{CP}$= 7.2 Hz), 29.0 (d, $^{1}J_{CP}$ = 143.6 Hz), 23.9 (d, *J* = 5.2 Hz), 23.8 (d, *J* = 5.2 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 18.40. ν_{max}(KBr)/cm^{-1} 3442, 2976, 1656, 1625, 1563, 1539, 1411, 1376, 1276, 1224, 1105, 1022, 1001, 810. HRMS-ESI (m/z): calcd for $C_{17}H_{22}N_3O_3P$, $[M+H]^+$: 348.1472, found 348.1476. M. p. 117 - 118 °C.

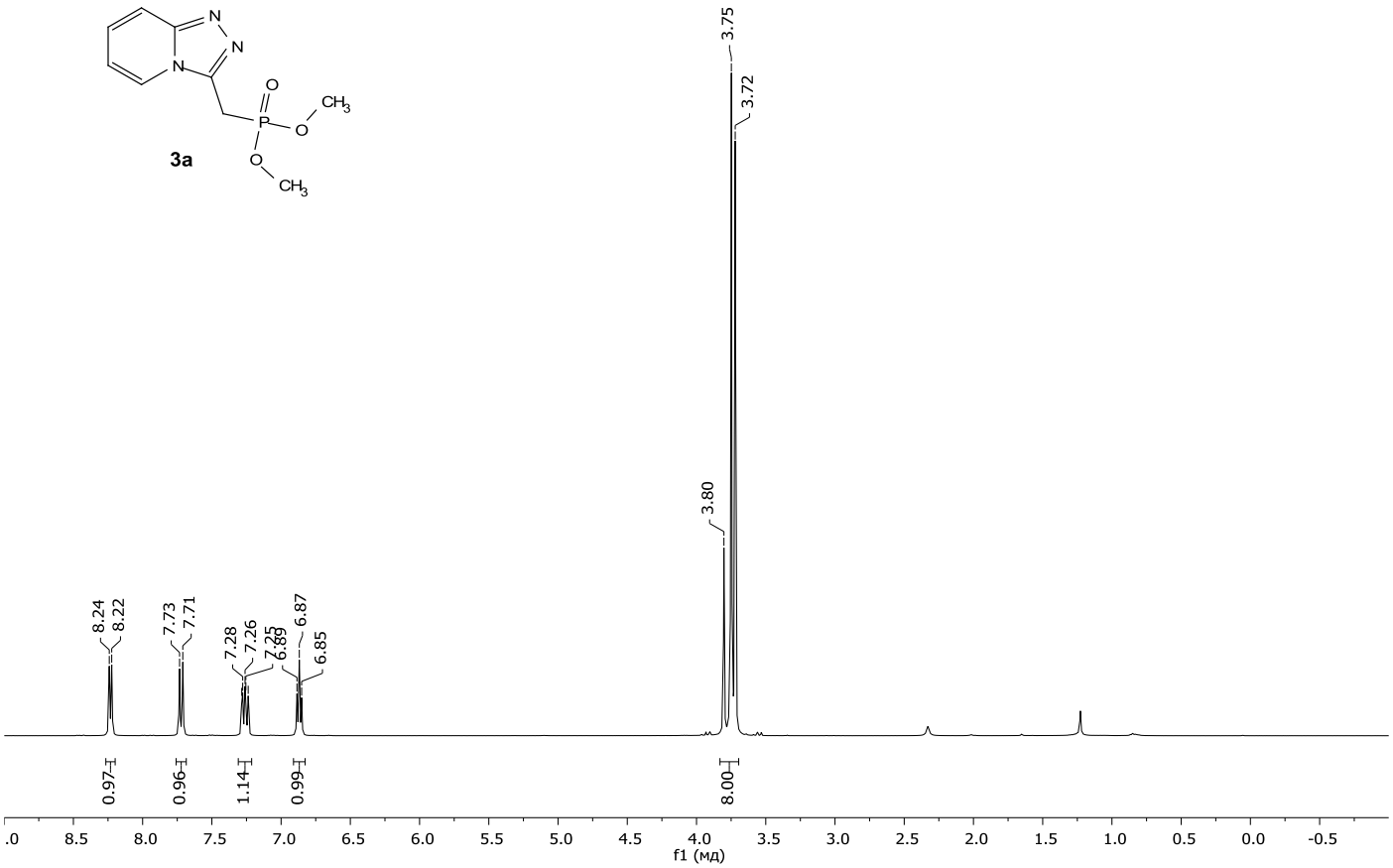
Diethyl ([1,2,4]triazolo[4,3-a]isoquinolin-3-ylmethyl)phosphonate 14c



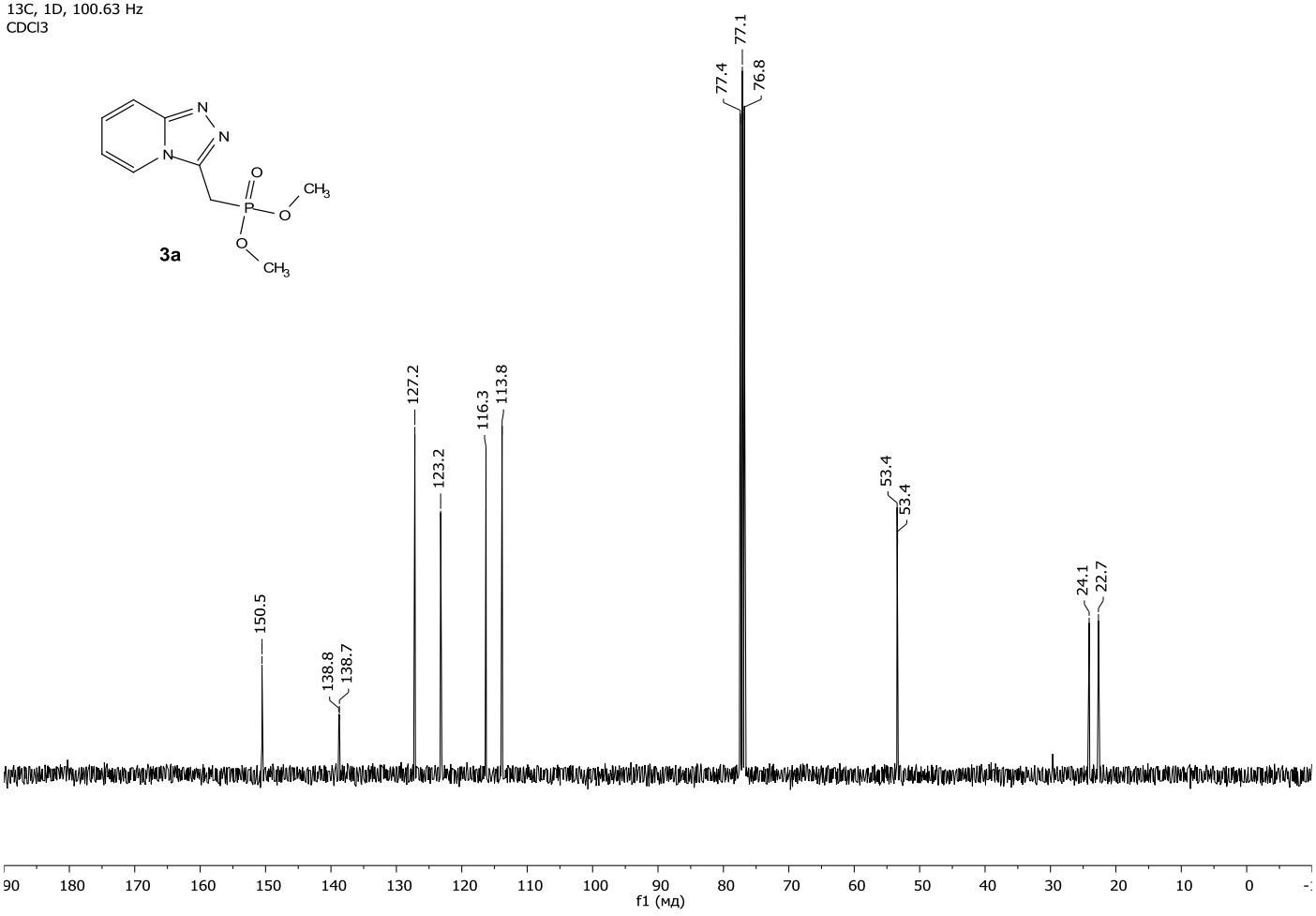
Following the general procedure, **14c** was obtained from **1h** and **2c** as pale solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, ,$^{3}J_{HH}$ = 8.7 Hz, 1H), 7.82 (dd, $^{3}J_{HH}$ = 7.5, $^{4}J_{HH}$ = 1.6 Hz, 1H), 7.75 – 7.70 (m,$^{3}J_{HH}$ = 8.7, $^{3}J_{HH}$ = 7.5,$^{4}J_{HH}$ = 1.6 Hz, 1H), 7.64 (d, $^{3}J_{HH}$ = 8.7 Hz, 1H), 7.60 – 7.52 (m, 2H), 4.74 (m, $^{3}J_{HP}$ = 7.5 Hz, $^{3}J_{HH}$ = 6.2 Hz, 2H, CH_2), 4.15 (d, $^{2}J_{HP}$ = 20.2 Hz, 4H, $2OCH_2$), 1.26 (d, $^{3}J_{HH}$= 6.2 Hz, 6H, $2CH_3$).^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 142.4 (d, $^{2}J_{CP}$ = 9.7 Hz), 132.0, 129.6, 129.1, 126.3, 124.7, 117.3, 115.1, 72.1 (d, $^{2}J_{CP}$ = 7.1 Hz), 29.0 (d, $^{1}J_{CP}$ = 143.8 Hz), 24.0 (d, $^{2}J_{CP}$ = 5.2 Hz), 23.8 (d, $^{2}J_{CP}$ = 5.2 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ 17.83. ν_{max} (KBr)/cm^{-1} 3501, 3328, 3234, 2982, 2888, 1643, 1529, 1235, 1047, 1023, 958, 782. HRMS-ESI (m/z): calcd for $C_{13}H_{14}N_3O_3P$, $[M+H]^+$: 320.1159, found 320.1150. M. p. 58 - 59 °C.

E. NMR Spectra

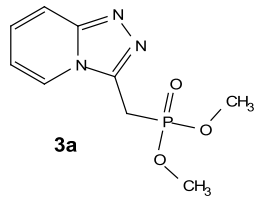
1H, 1D, 400.17 Hz
CDCl3



13C, 1D, 100.63 Hz
CDCl3

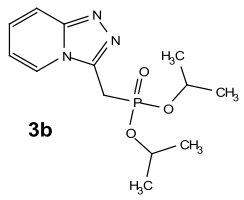


31P, 1D, 162.01 Hz
CDCl3



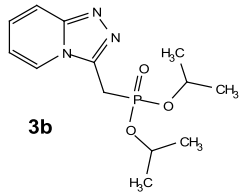
3a

1H, 1D, 400.17 Hz
CDCl3



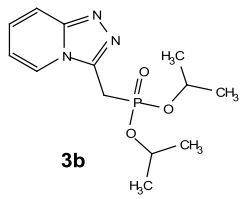
3b

13C, 1D, 100.63 Hz
Chloroform



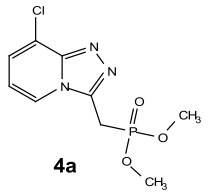
3b

31P, 1D, 162.01 Hz
CDCl3

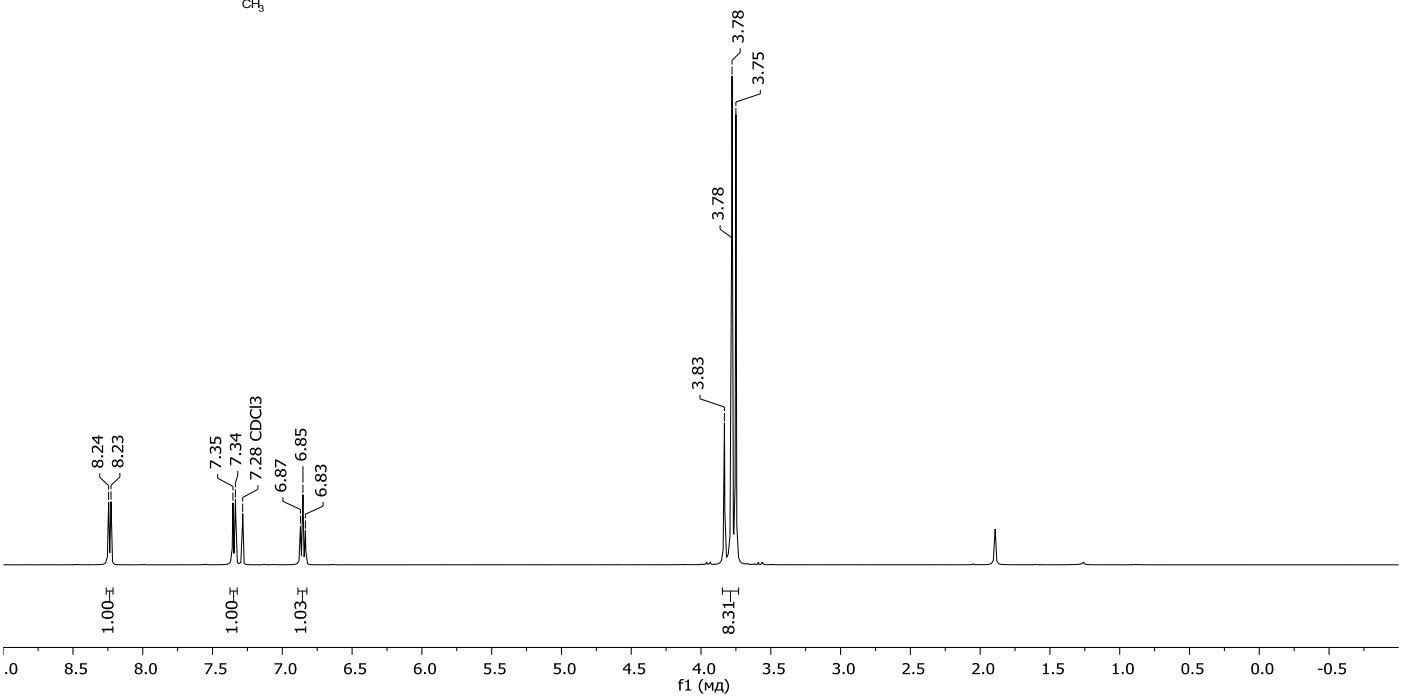


3b

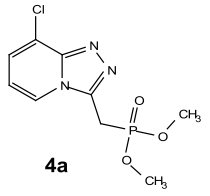
1H, 1D, 400.17 Hz
CDCl3



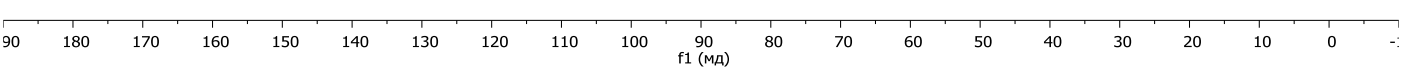
4a



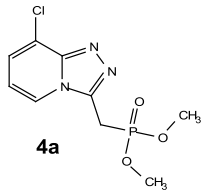
13C, 1D, 100.63 Hz
CDCl3



4a

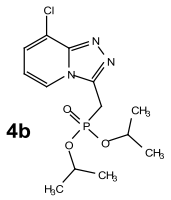


31P, 1D, 162.01 Hz
CDCl3



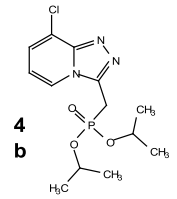
4a

1H, 1D, 400.17 Hz
CDCl3



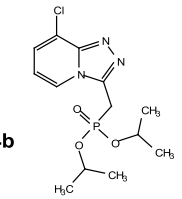
4b

13C, 1D, 100.63 Hz
CDCl3



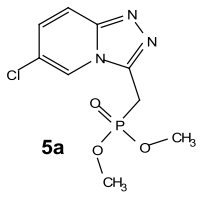
4b

31P, 1D, 162.01 Hz
CDCl3



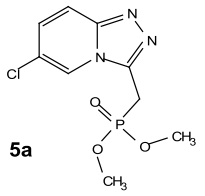
4b

1H, 1D, 400.17 Hz
CDCl3



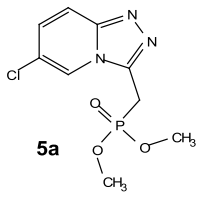
5a

13C, 1D, 100.63 Hz
CDCl3

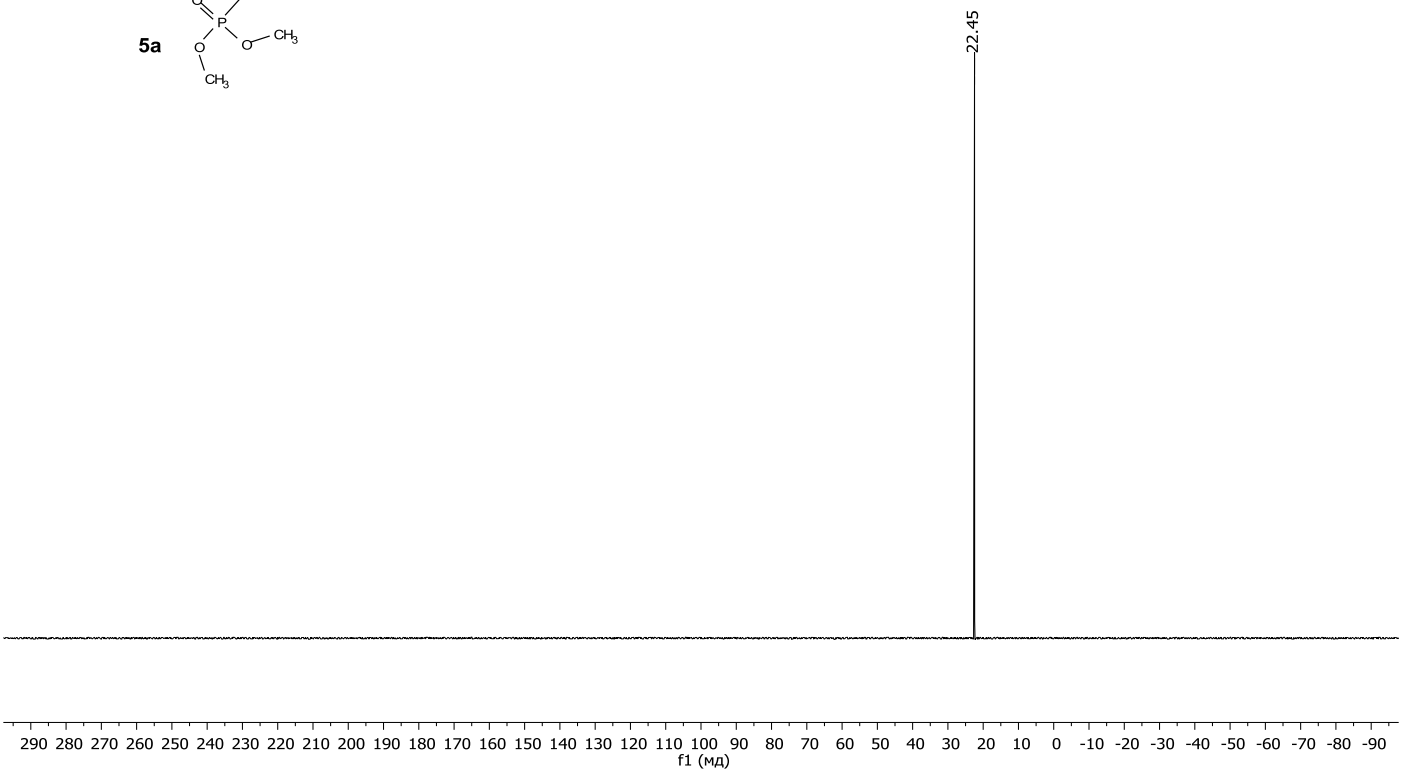


5a

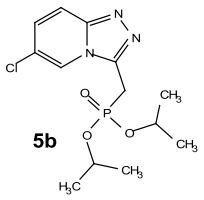
31P, 1D, 162.01 Hz
CDCl3



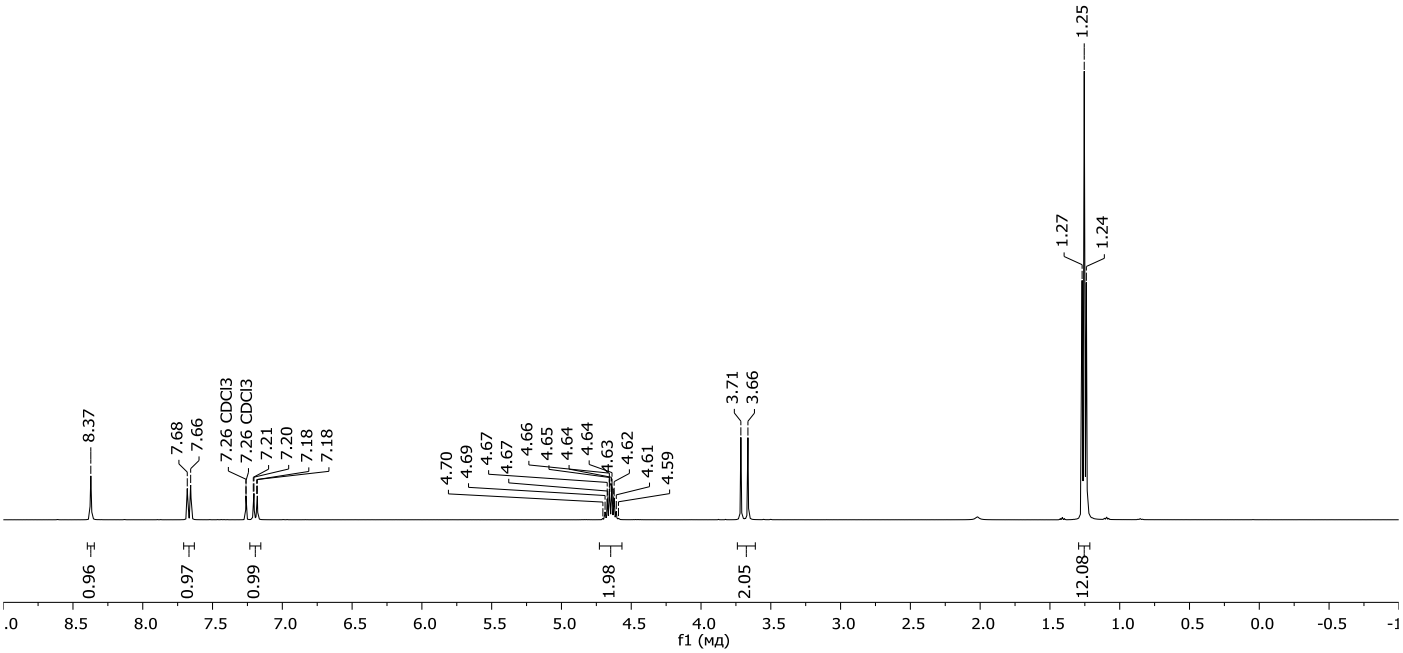
5a



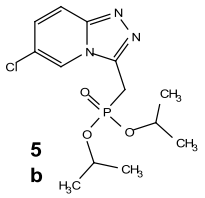
1H, 1D, 400.17 Hz
CDCl3



5b

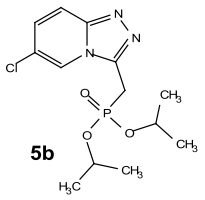


13C, 1D, 100.63 Hz
CDCl3



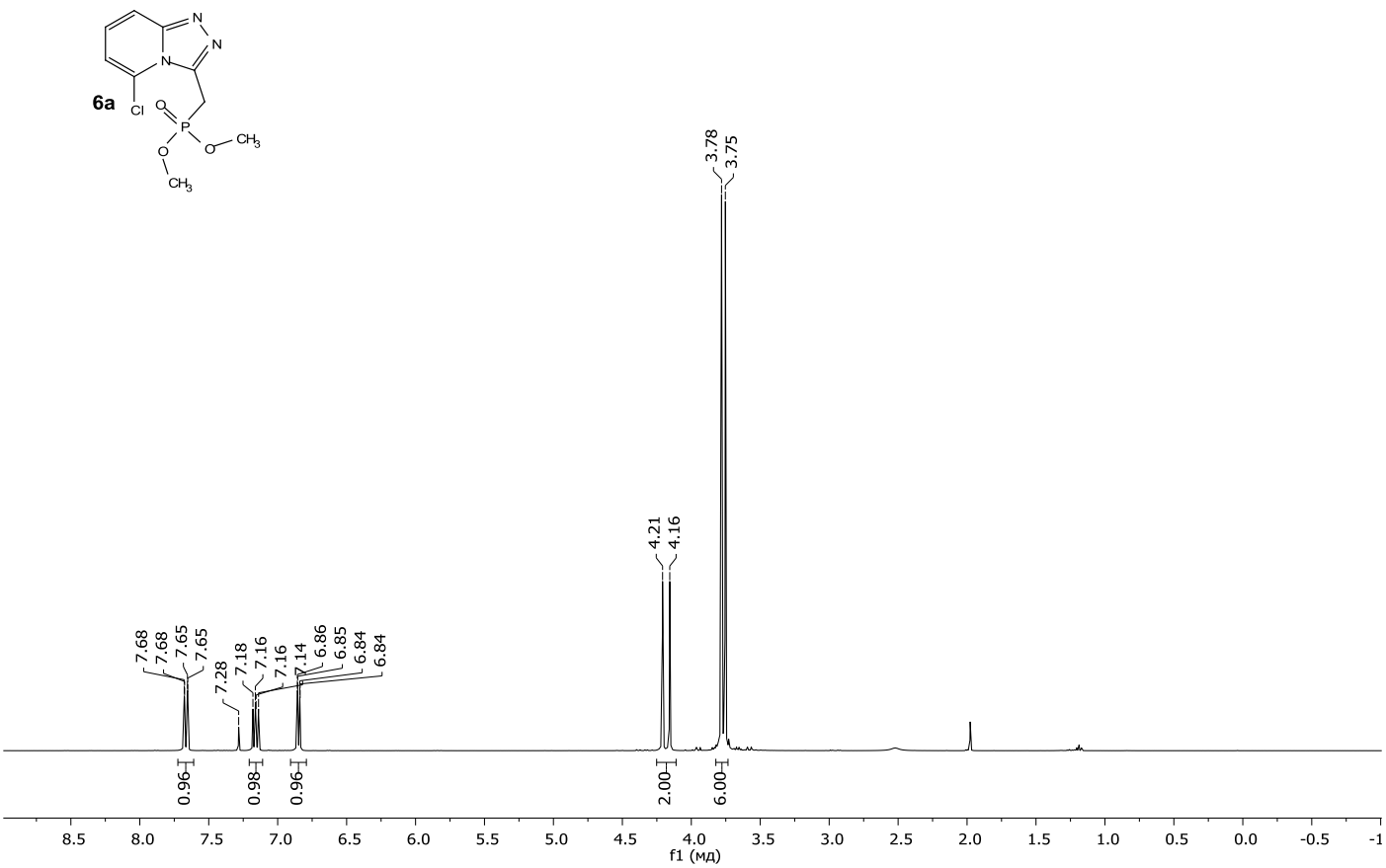
5
b

31P, 1D, 162.01 Hz
CDCl3

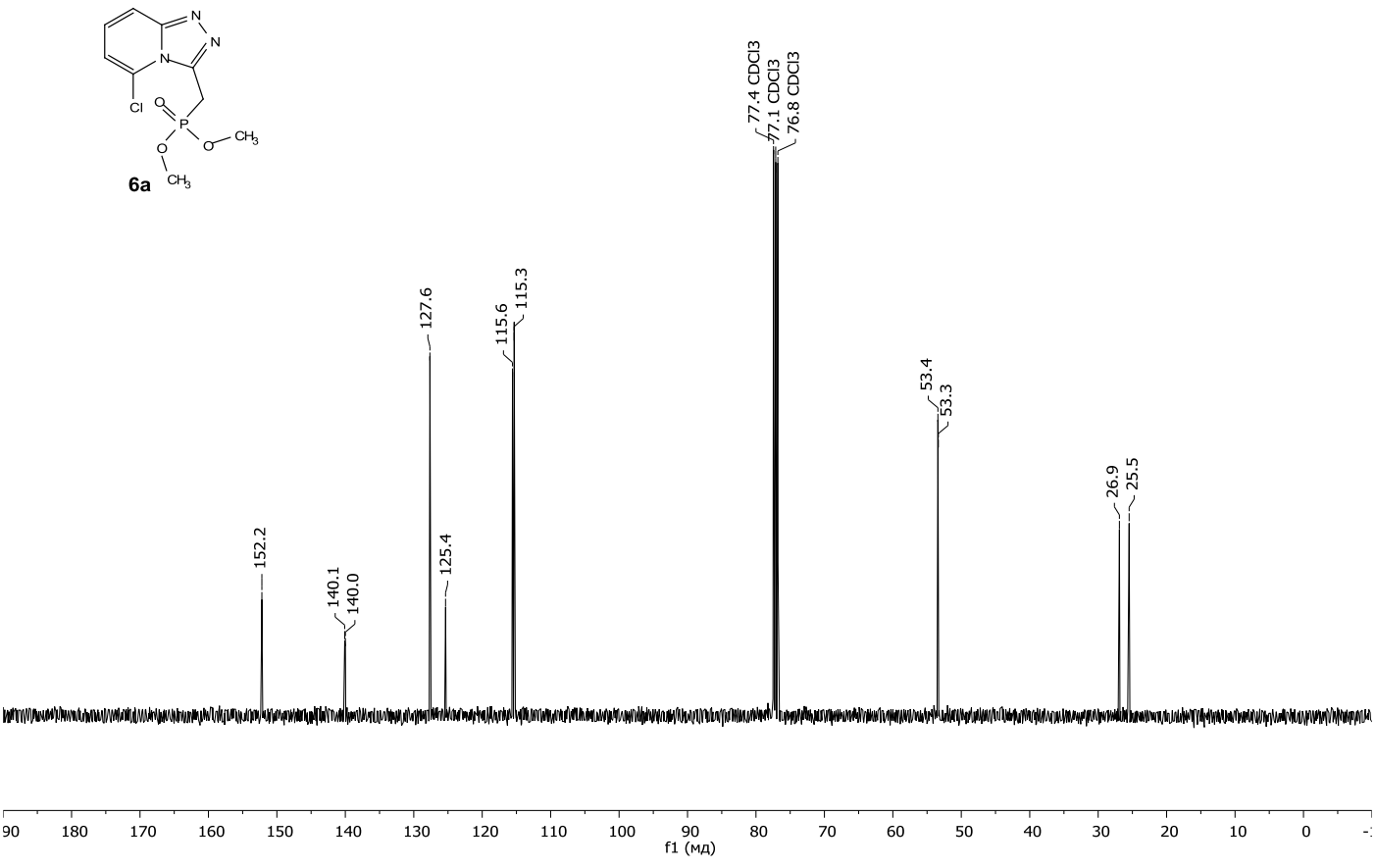


5b

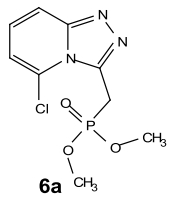
1H, 1D, 400.17 Hz
CDCl3



13C, 1D, 100.63 Hz
CDCl3

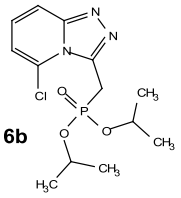


31P, 1D, 162.01 Hz
CDCl3

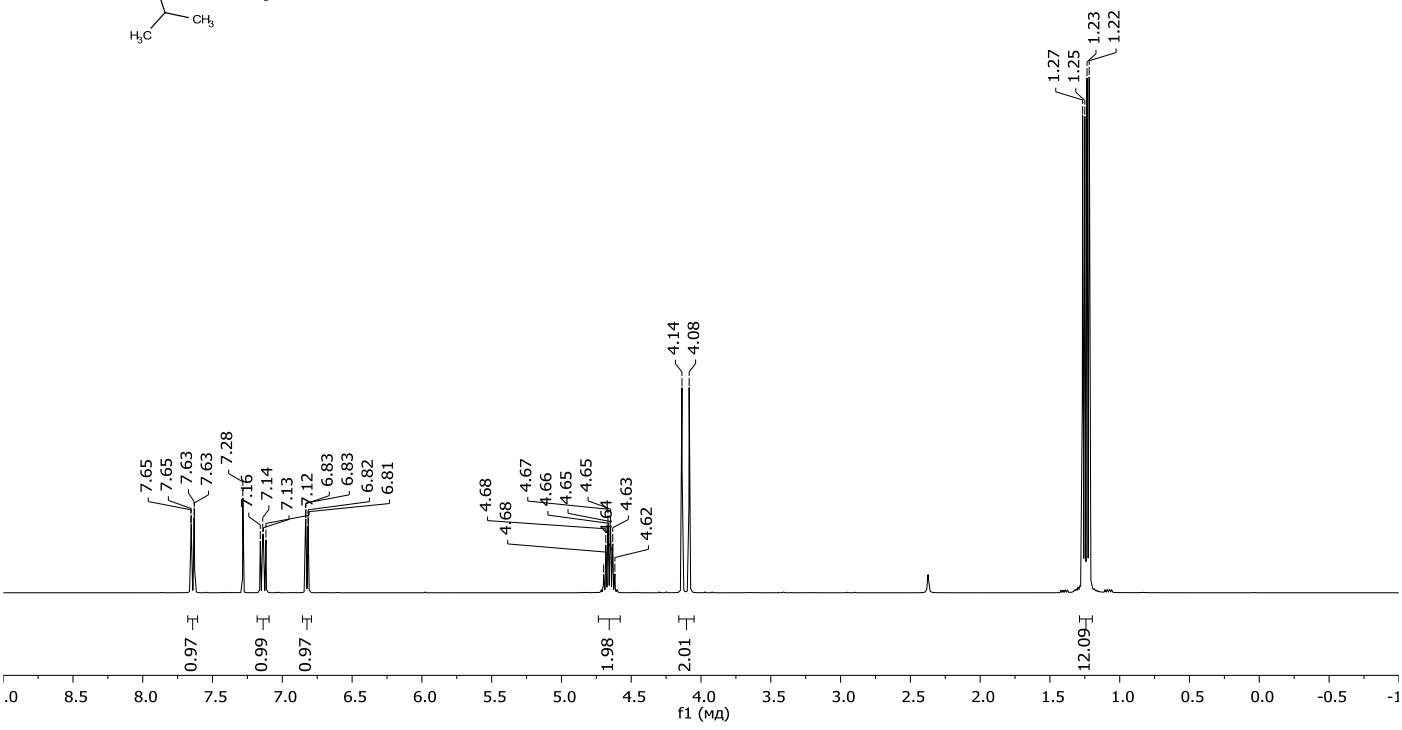


6a

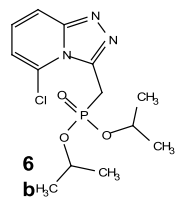
1H, 1D, 400.17 Hz
CDCl3



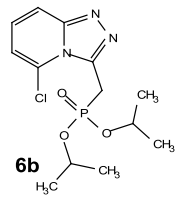
6b



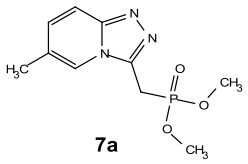
13C, 1D, 100.63 Hz
CDCl3



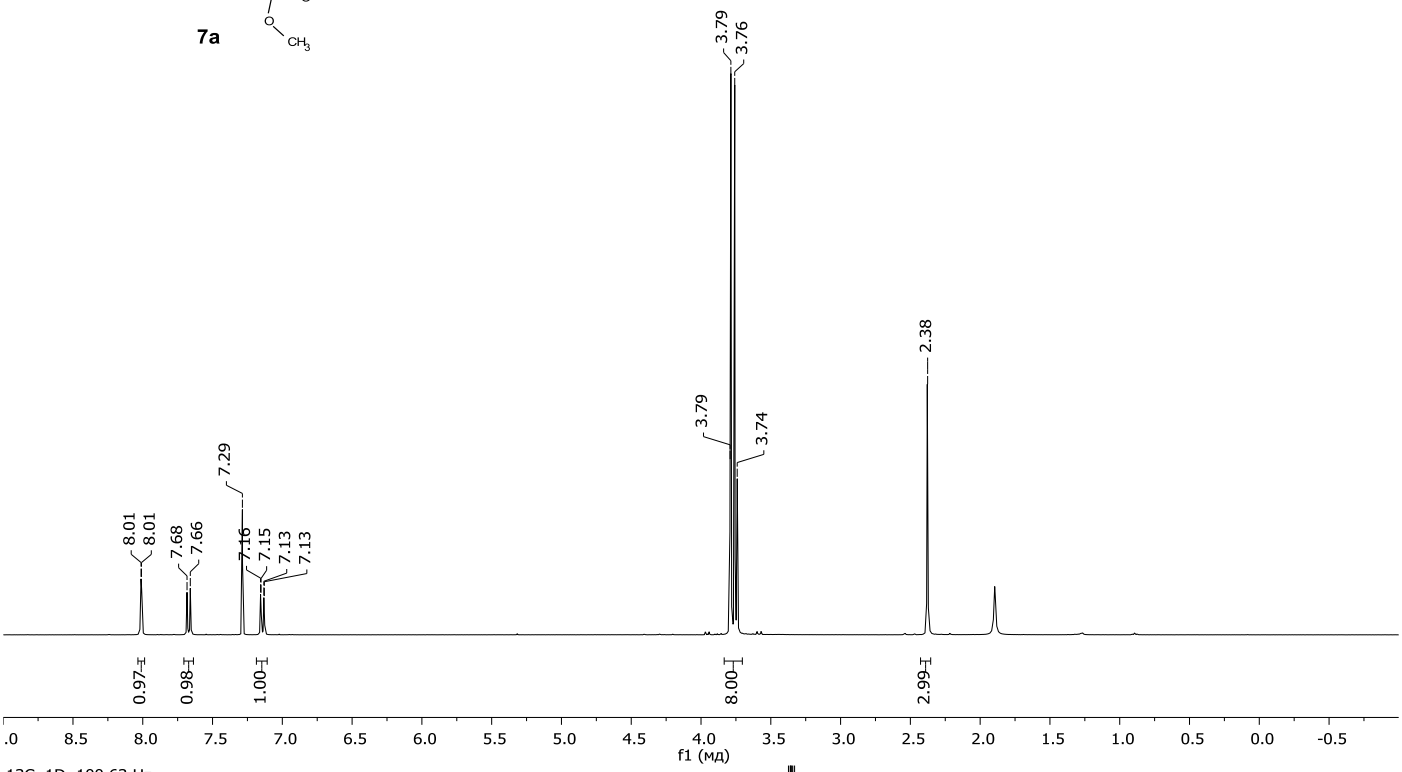
31P, 1D, 162.01 Hz
CDCl3



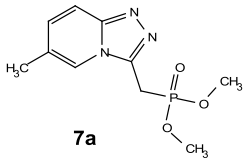
1H, 1D, 400.17 Hz
CDCl3



7a

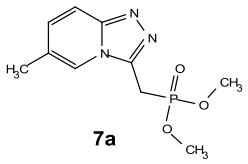


13C, 1D, 100.63 Hz
CDCl3



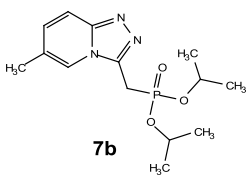
7a

31P, 1D, 162.01 Hz
CDCl3



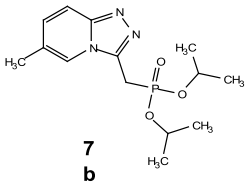
7a

1H, 1D, 400.17 Hz
CDCl3



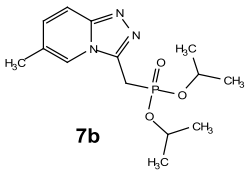
7b

13C, 1D, 100.63 Hz
CDCl3



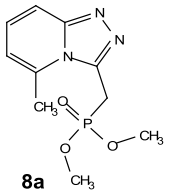
7
b

31P, 1D, 162.01 Hz
CDCl3



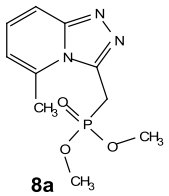
7b

1H, 1D, 400.17 Hz
CDCl3



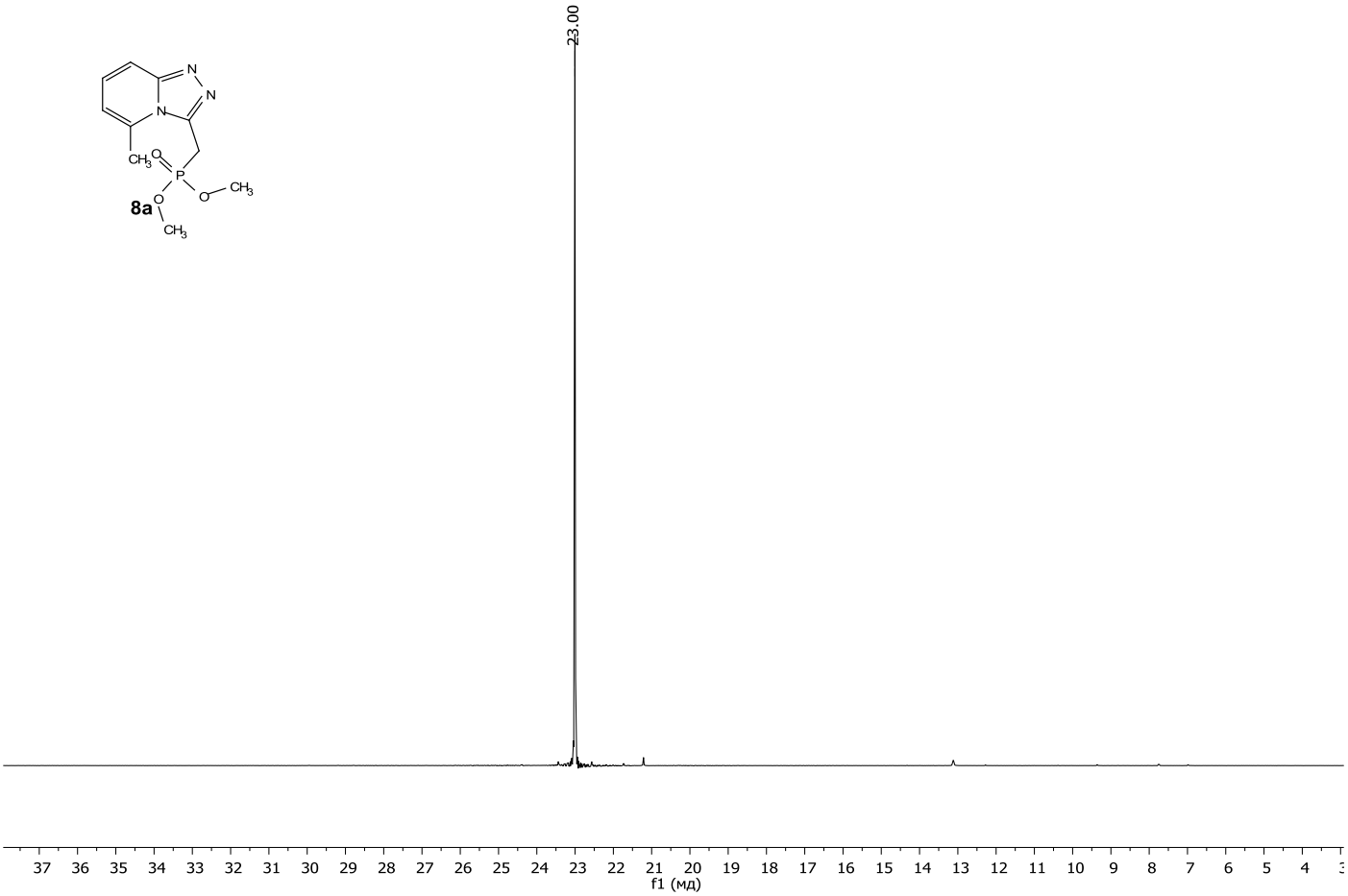
8a

13C, 1D, 100.63 Hz
CDCl3



8a

31P, 1D, 162.01 Hz
CDCl3



1H, 1D, 400.17 Hz
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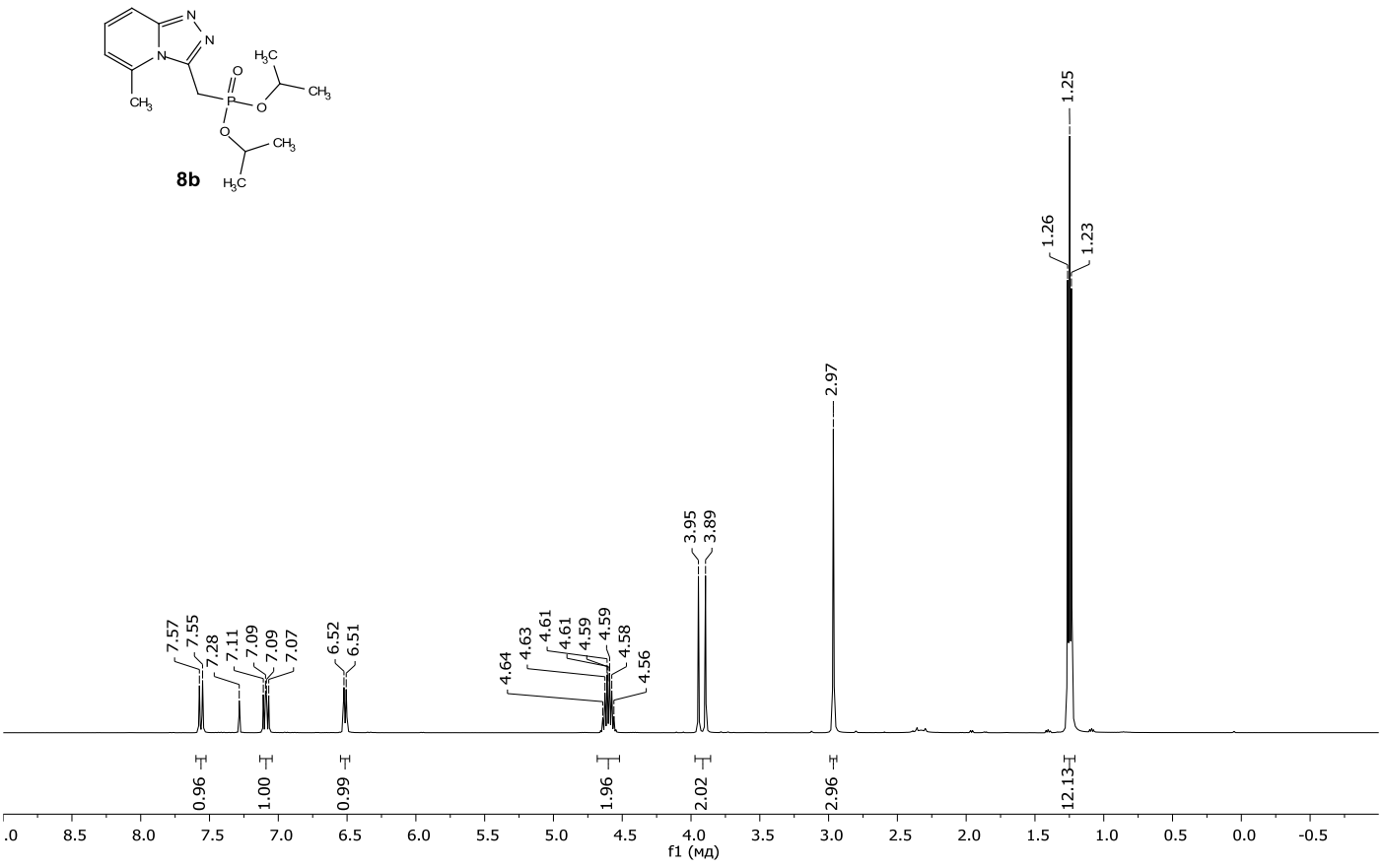

13C, 1D, 100.63 Hz
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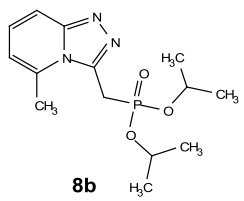
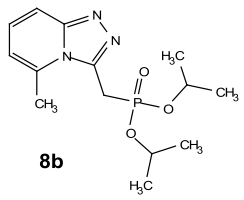


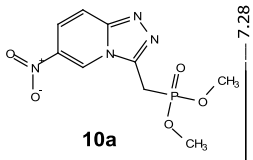
8b

31P, 1D, 162.01 Hz
CDCl3



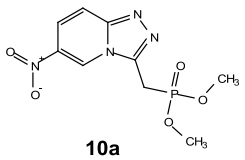
8b

1H, 1D, 400.17 Hz
CDCl3



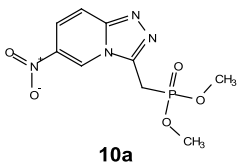
10a

13C, 1D, 100.63 Hz
CDCl3



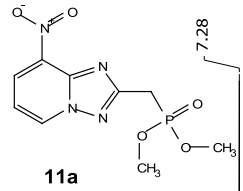
10a

31P, 1D, 162.01 Hz
CDCl3



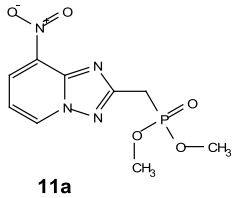
10a

1H, 1D, 400.17 Hz
CDCl3



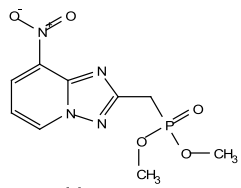
11a

13C, 1D, 100.63 Hz
CDCl3



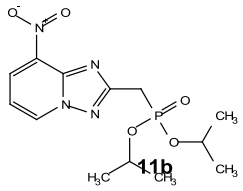
11a

31P, 1D, 162.01 Hz
CDCl3



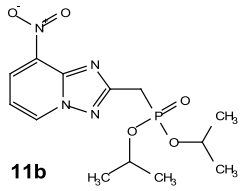
11a

1H, 1D, 400.17 Hz
CDCl3



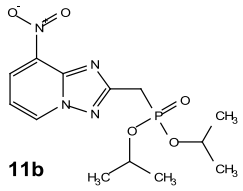
11b

13C, 1D, 100.63 Hz
CDCl3

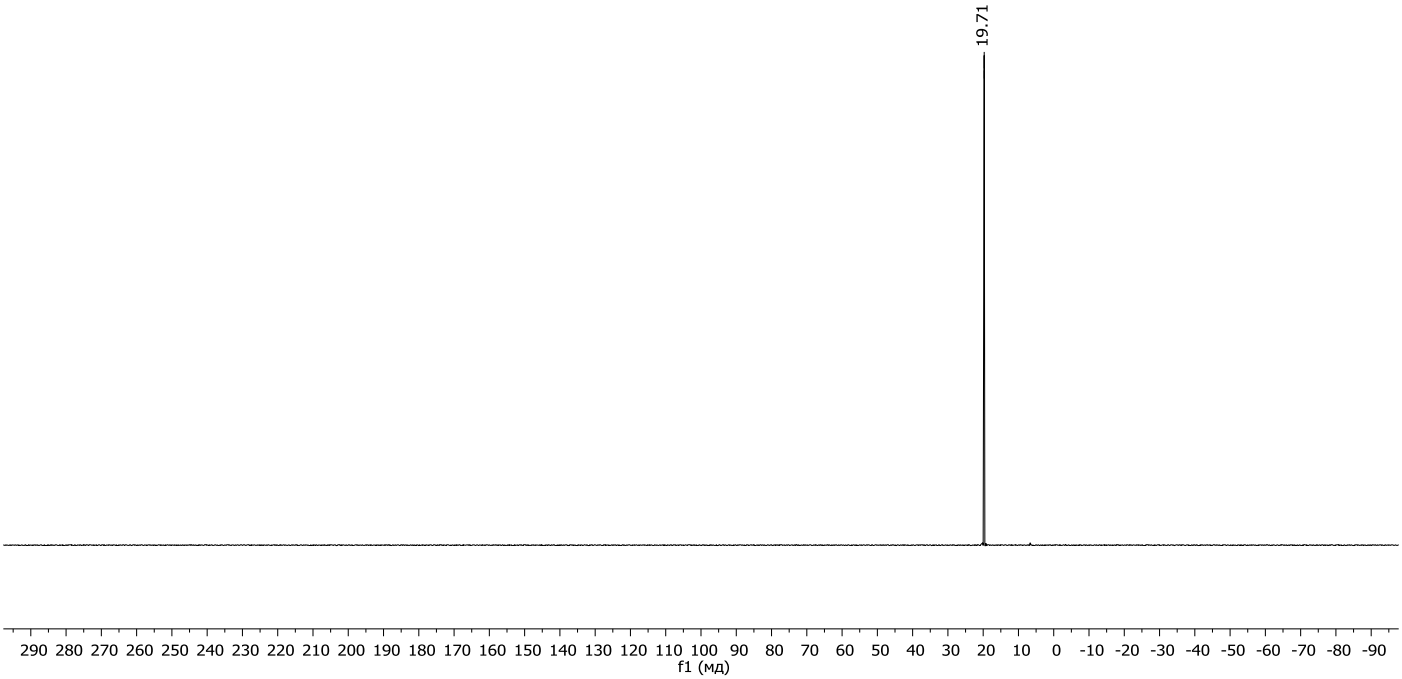


11b

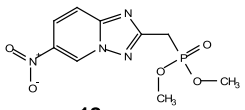
31P, 1D, 162.01 Hz
CDCl3



11b

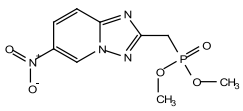


1H, 1D, 400.17 Hz
CDCl3



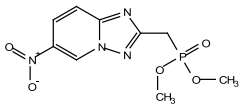
12a

13C, 1D, 100.63 Hz
CDCl3



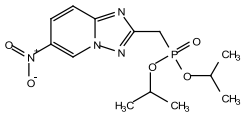
12a

31P, 1D, 162.01 Hz
CDCl3



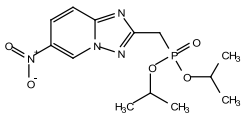
12a

1H, 1D, 400.17 Hz
CDCl3



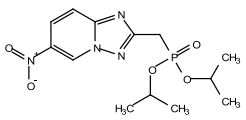
12b

13C, 1D, 100.63 Hz
CDCl3

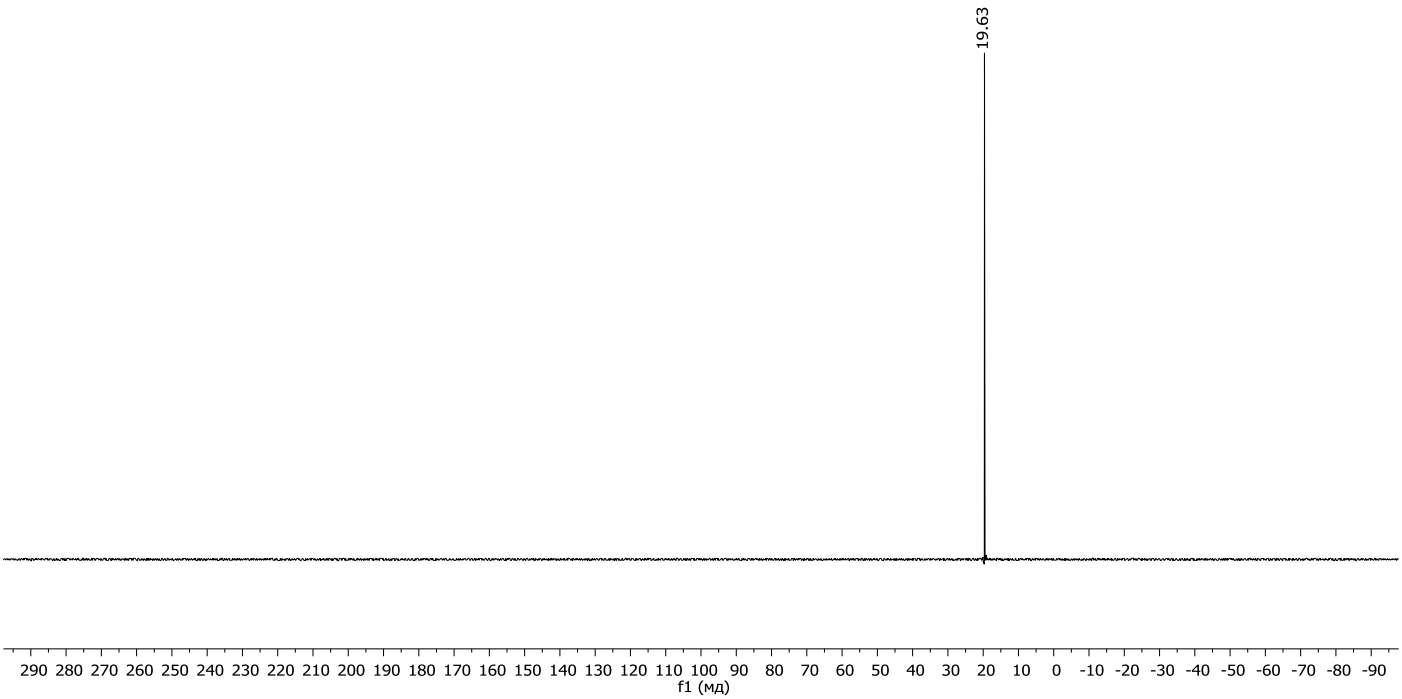


12b

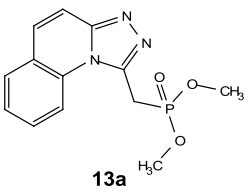
31P, 1D, 162.01 Hz
CDCl3



12b

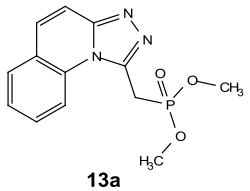


1H, 1D, 400.17 Hz
CDCl3



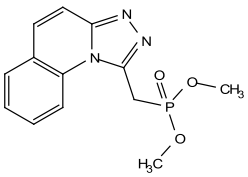
13a

13C, 1D, 100.63 Hz
CDCl3



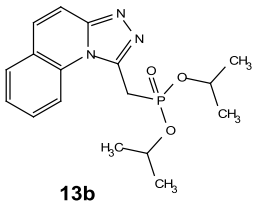
13a

31P, 1D, 162.01 Hz
CDCl3



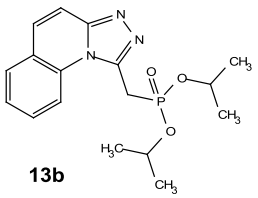
13a

1H, 1D, 400.17 Hz
CDCl3



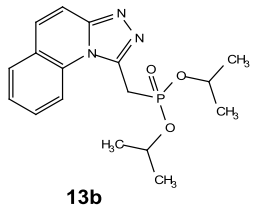
13b

13C, 1D, 100.63 Hz
CDCl3

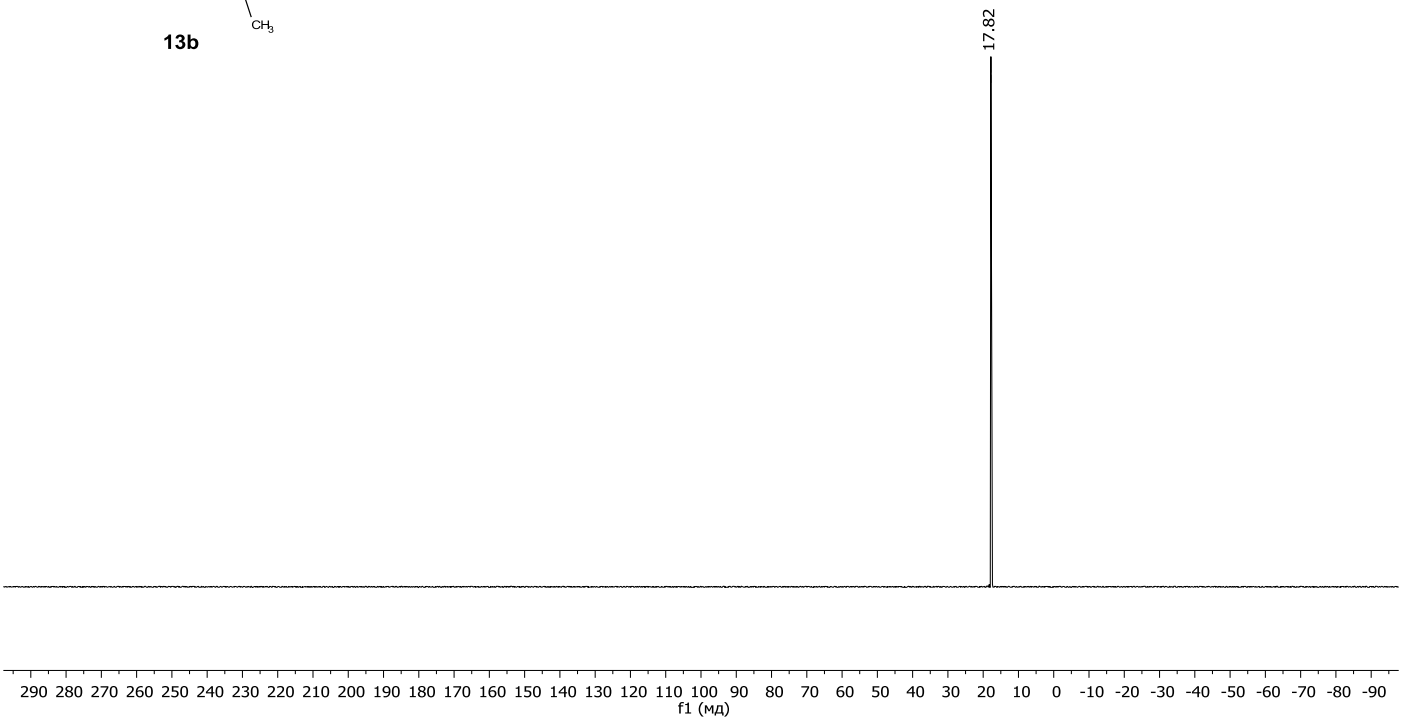


13b

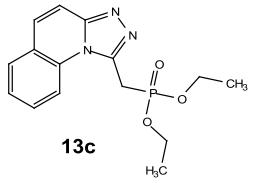
31P, 1D, 162.01 Hz
CDCl3



13b

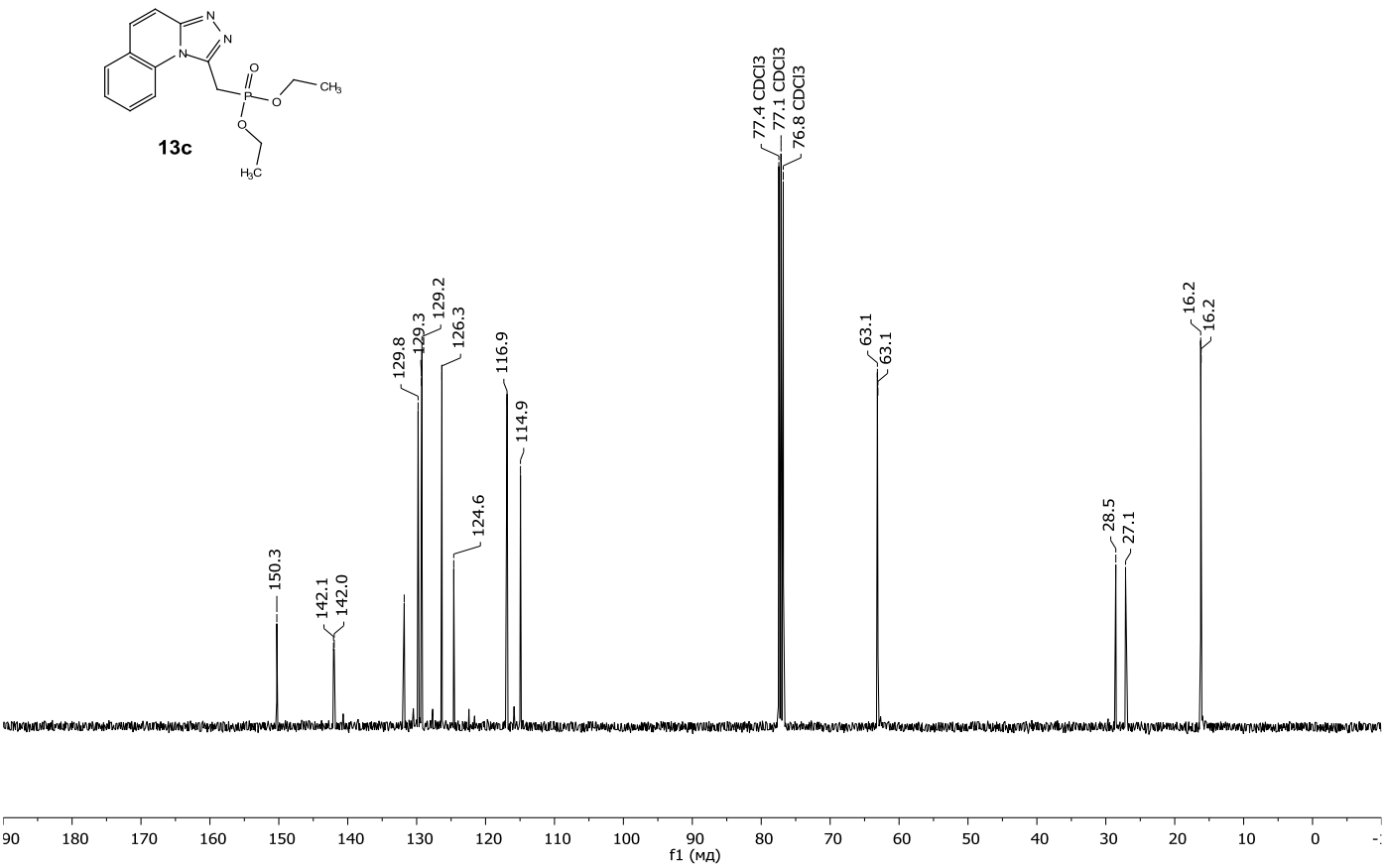


1H, 1D, 400.17 Hz
CDCl3

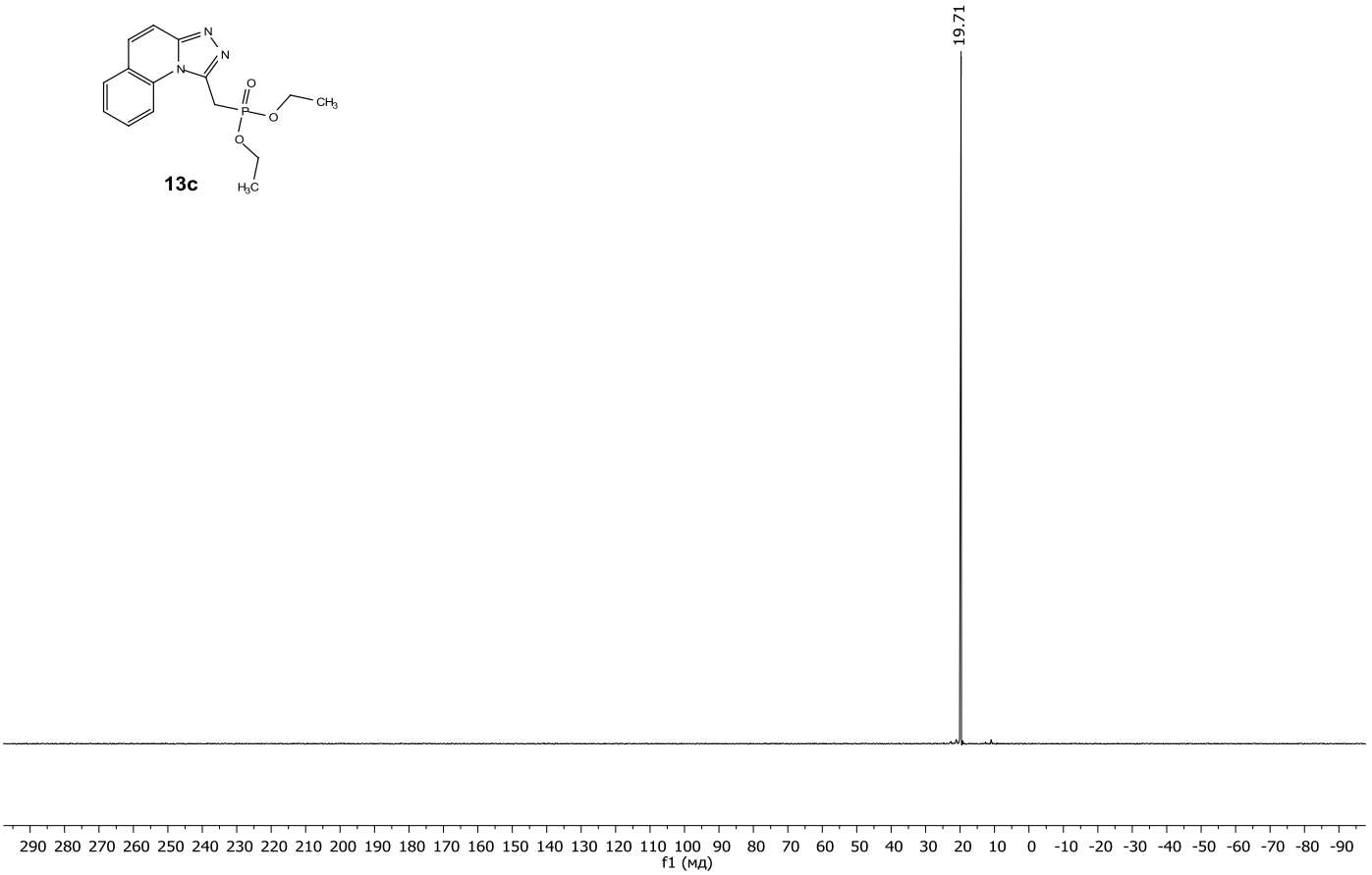


13c

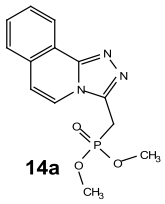
13C, 1D, 100.63 Hz
CDCl3



31P, 1D, 162.01 Hz
CDCl3

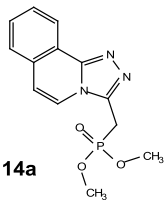


1H, 1D, 400.17 Hz
CDCl3



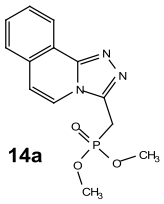
14a

13C, 1D, 100.63 Hz
CDCl3

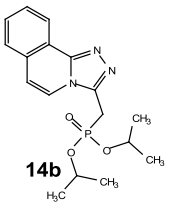


14a

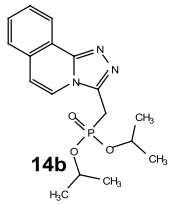
31P, 1D, 162.01 Hz
CDCl3



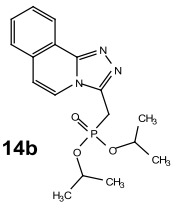
1H, 1D, 400.17 Hz
CDCl3



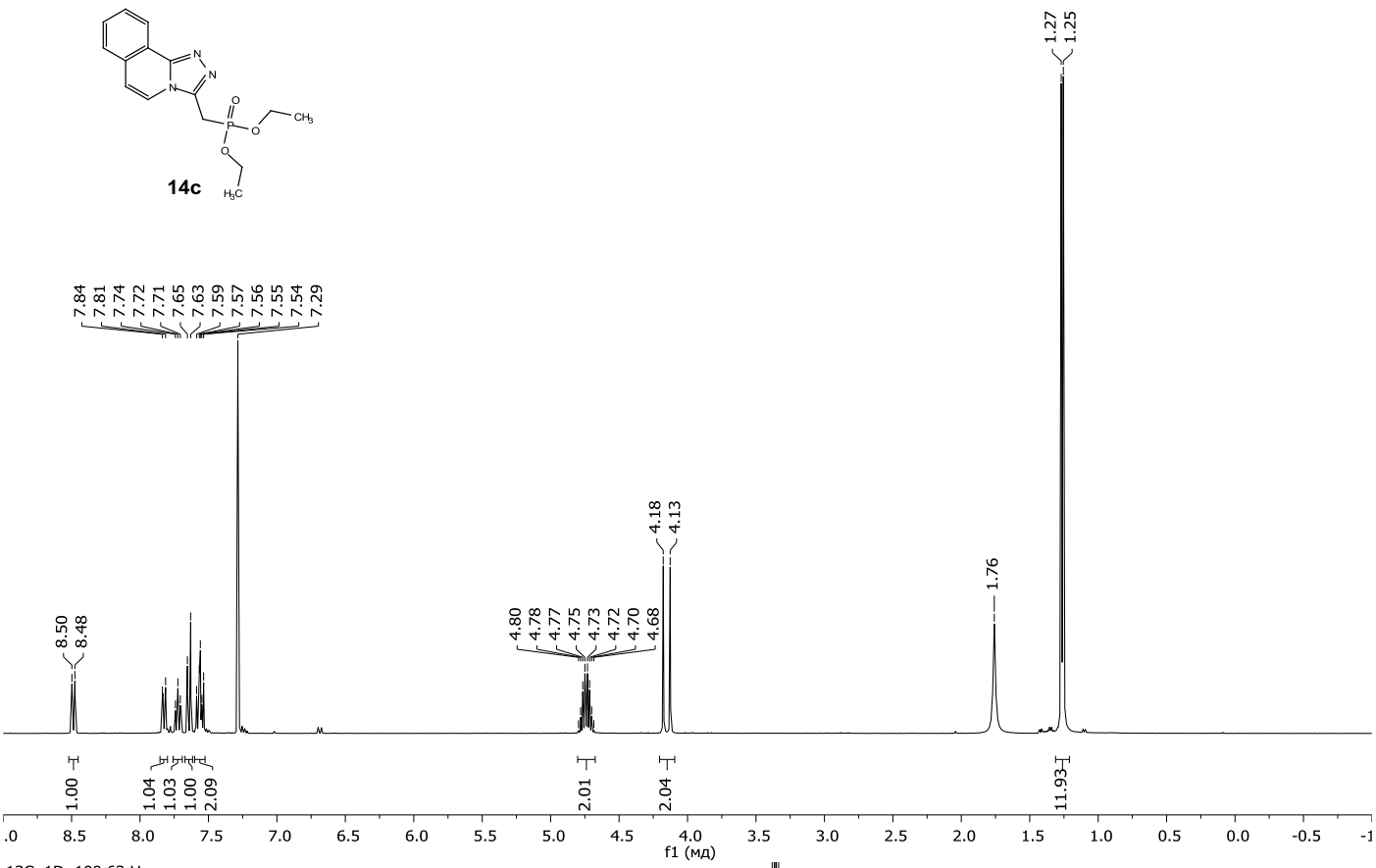
13C, 1D, 100.63 Hz
CDCl3



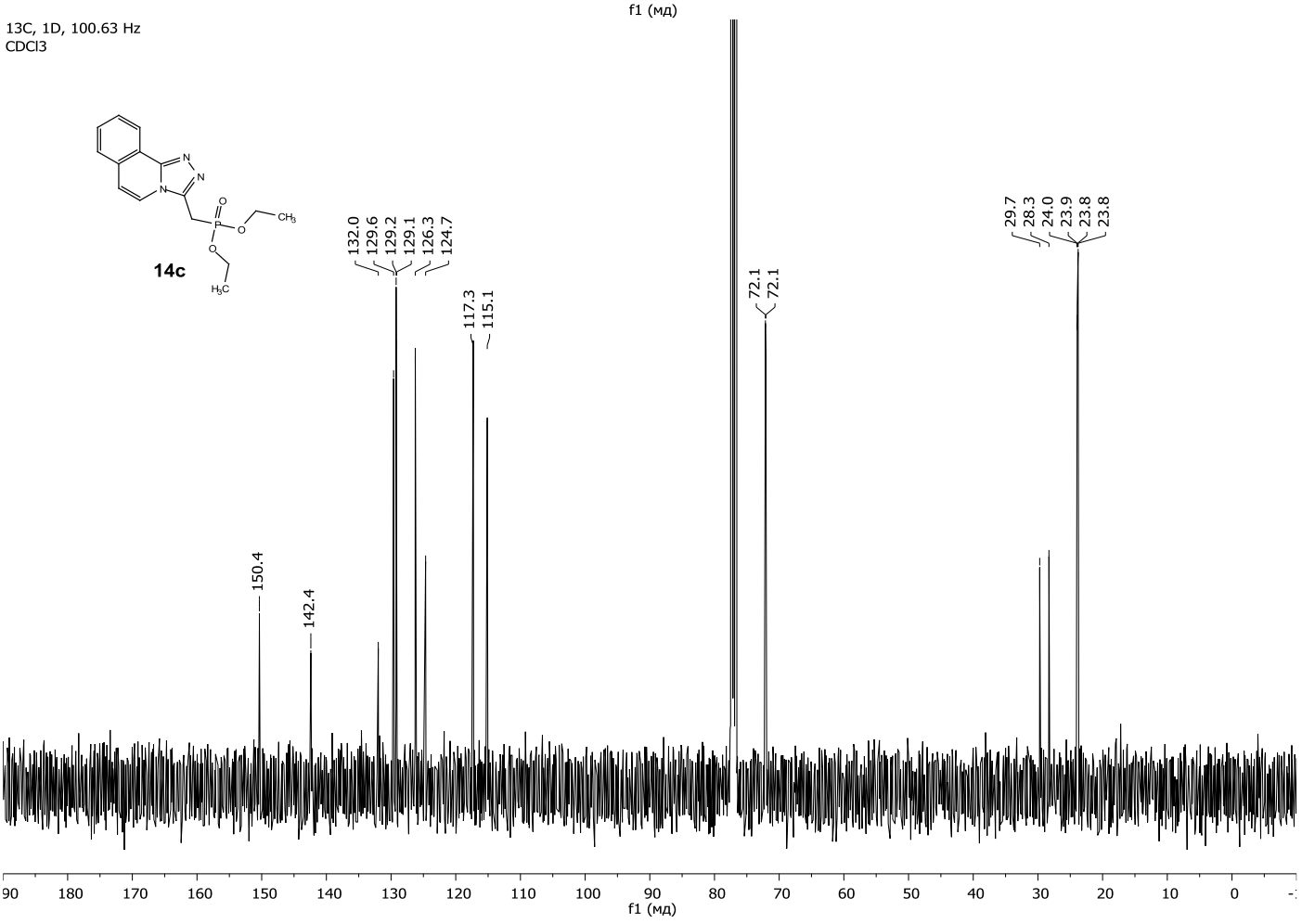
31P, 1D, 162.01 Hz
DMSO



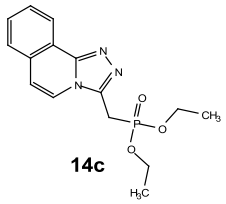
1H, 1D, 400.17 Hz
CDCl3



13C, 1D, 100.63 Hz
CDCl3



31P, 1D, 162.01 Hz
CDCl3



14c