



Supplementary

Diethylphosphonate-containing aminoacyl-adenosine analog as inhibitor of bacterial tRNA-dependent transamidase

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Supplementary Figure

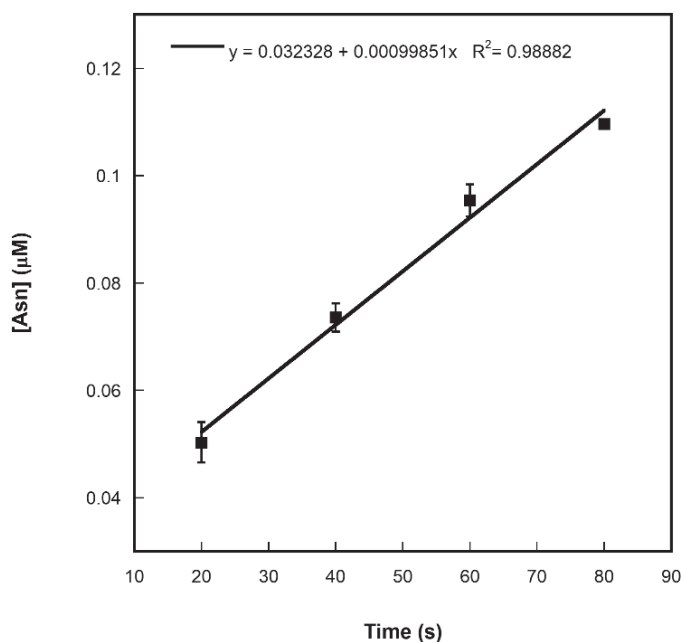


Fig. S1 Initial rate of transamidase reaction in absence of compound 1, where error bars indicate \pm SD and R^2 = coefficient of determination

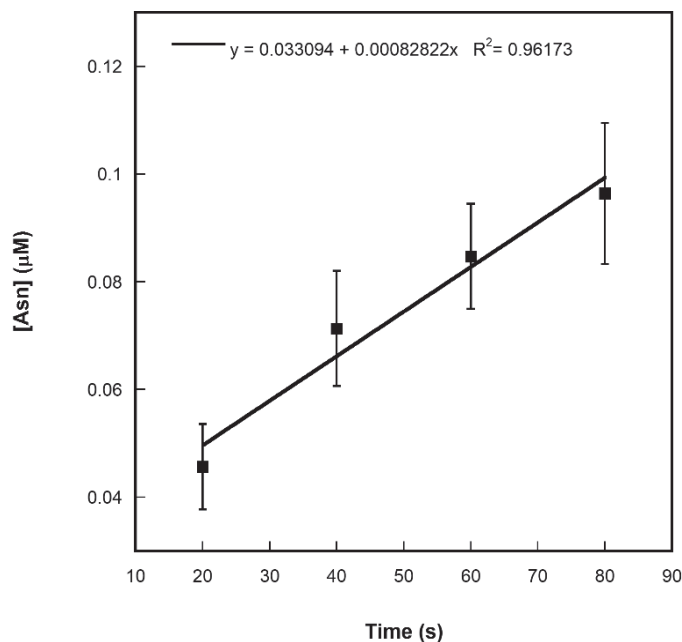


Fig. S2 Initial rate of transamidase reaction in presence of compound 1, where error bars indicate \pm SD and R^2 = coefficient of determination

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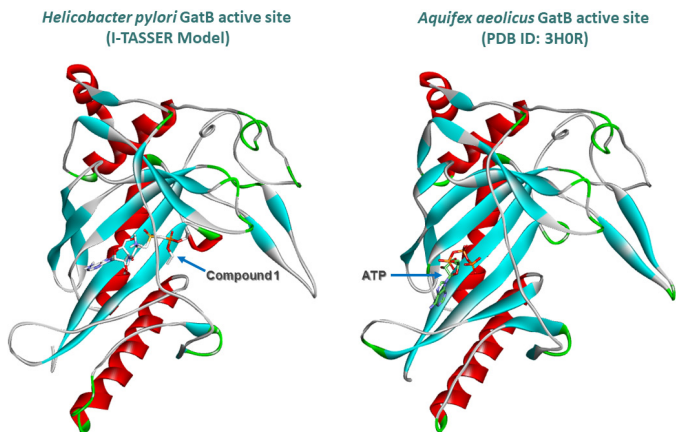


Fig. S3 Best-docked pose of compound 1 for *H. pylori* GatB active site from molecular docking simulations (left) and crystal structure of *A. aeolicus* GatB active site co-crystallized with ATP (PDB ID: 3HOR; right), where I-TASSER = iterative threading assembly refinement and ATP = adenosine triphosphate

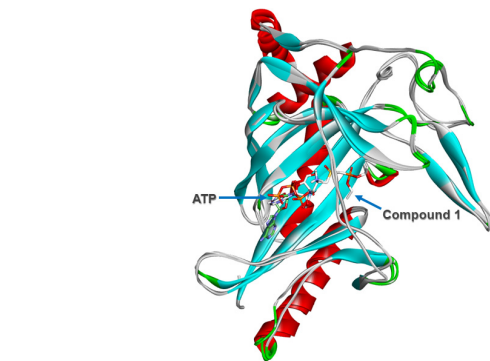


Fig. S4 Superposition of *H. pylori* and *A. aeolicus* GatB active sites (structures from Fig. S3) indicating binding regions of compound 1 and adenosine triphosphate (ATP) molecule overlap at GatB active site

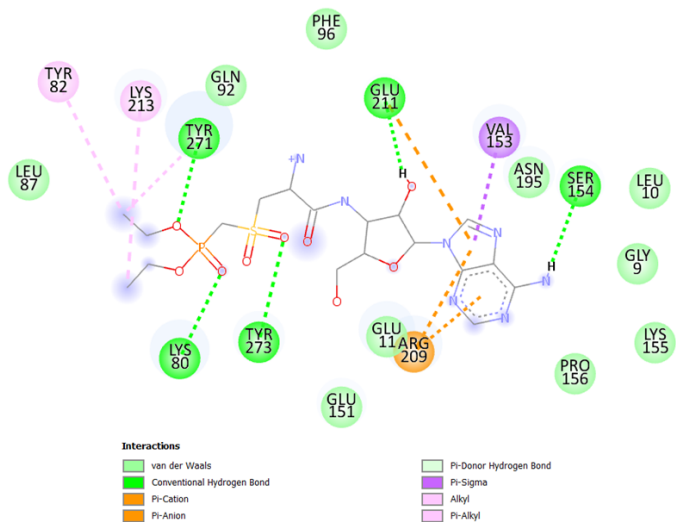


Fig. S5 Binding interactions between compound 1 and *H. pylori* GatB active site

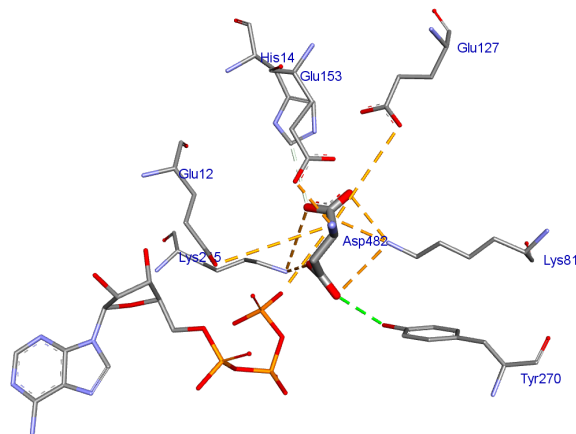


Fig. S6 Binding interactions between aspartate and *A. aeolicus* GatB (PDB ID: 3HOR), with adenosine triphosphate (ATP) illustrated, though its interactions with GatB are omitted for clarity

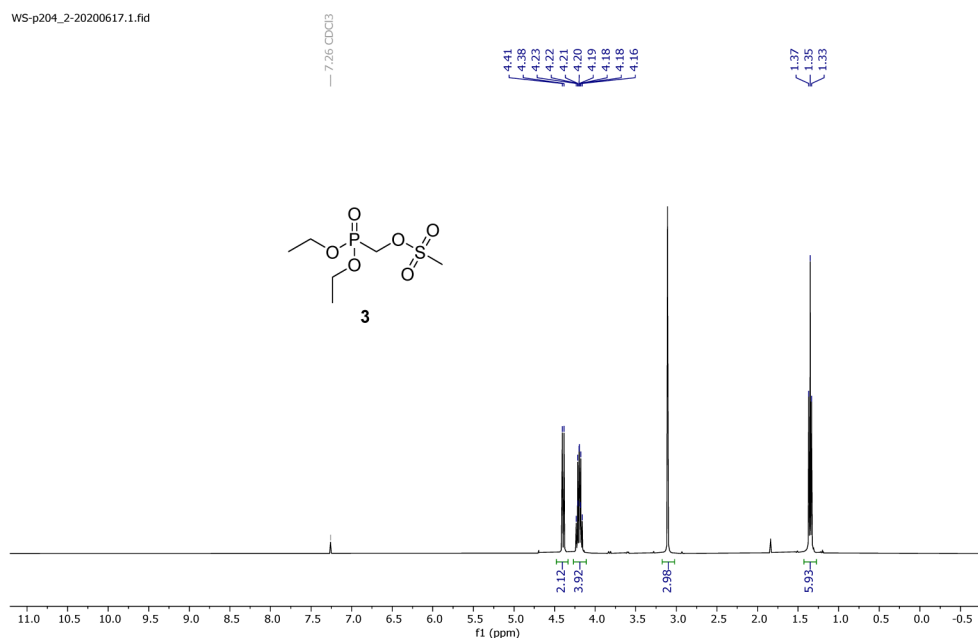


Fig. S7 ¹H Nuclear magnetic resonance spectrum of compound **3** (400 MHz, CDCl₃), where ppm = parts per million

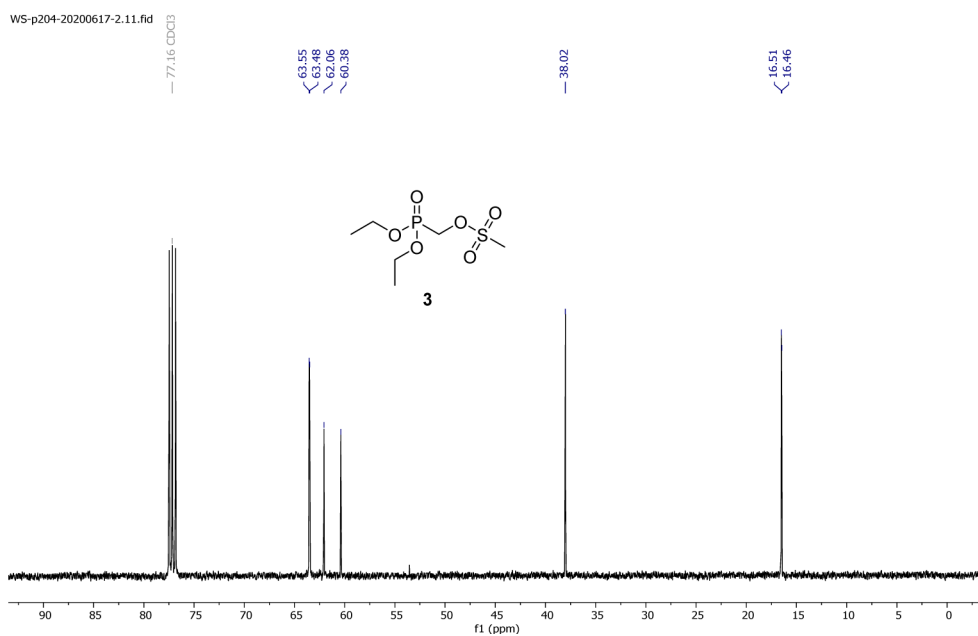


Fig. S8 ¹³C Nuclear magnetic resonance spectrum of compound **3** (100 MHz, CDCl₃), where ppm = parts per million

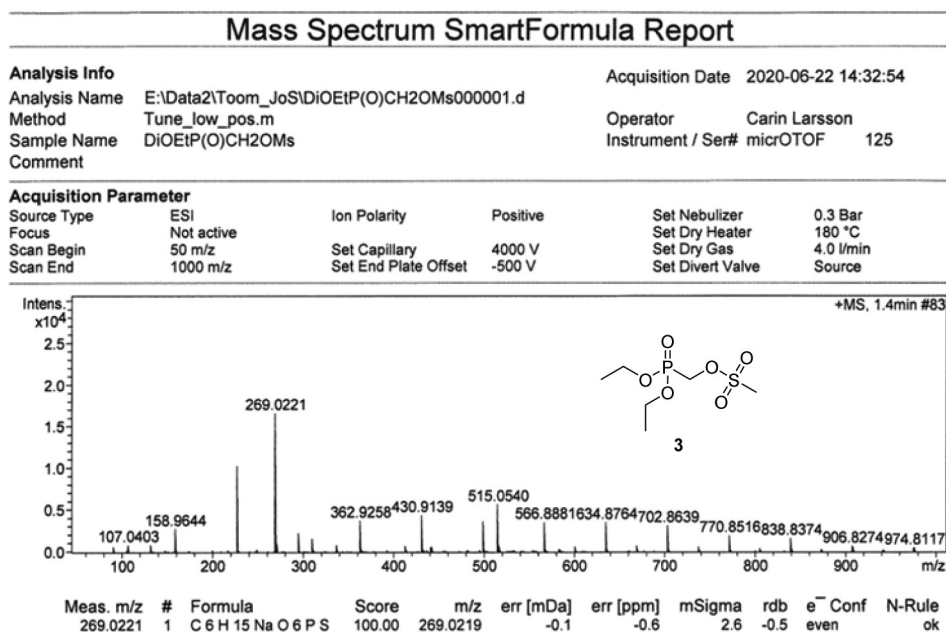


Fig. S9 High-resolution mass spectrum (HRMS) of compound 3

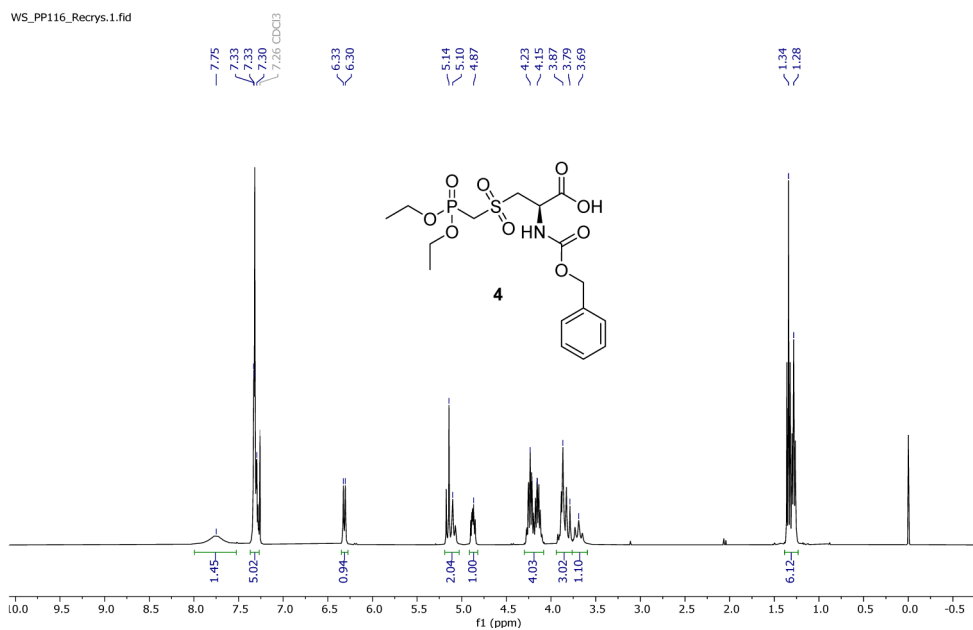


Fig. S10 ¹H Nuclear magnetic resonance spectrum of compound 4 (400 MHz, CDCl₃), where ppm = parts per million

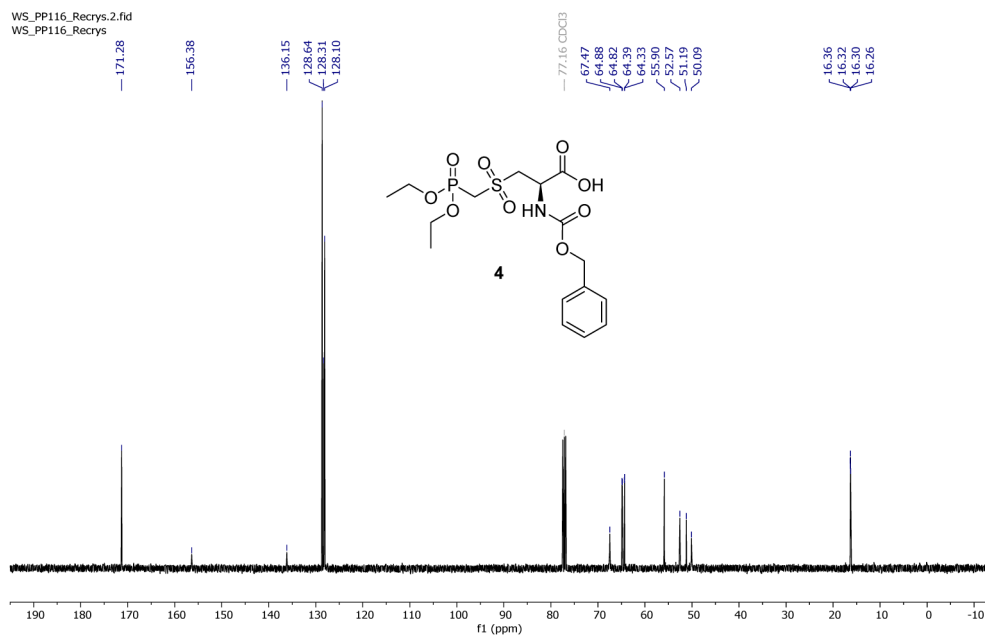


Fig. S11 ^{13}C Nuclear magnetic resonance spectrum of compound 4 (100 MHz, CDCl_3), where ppm = parts per million

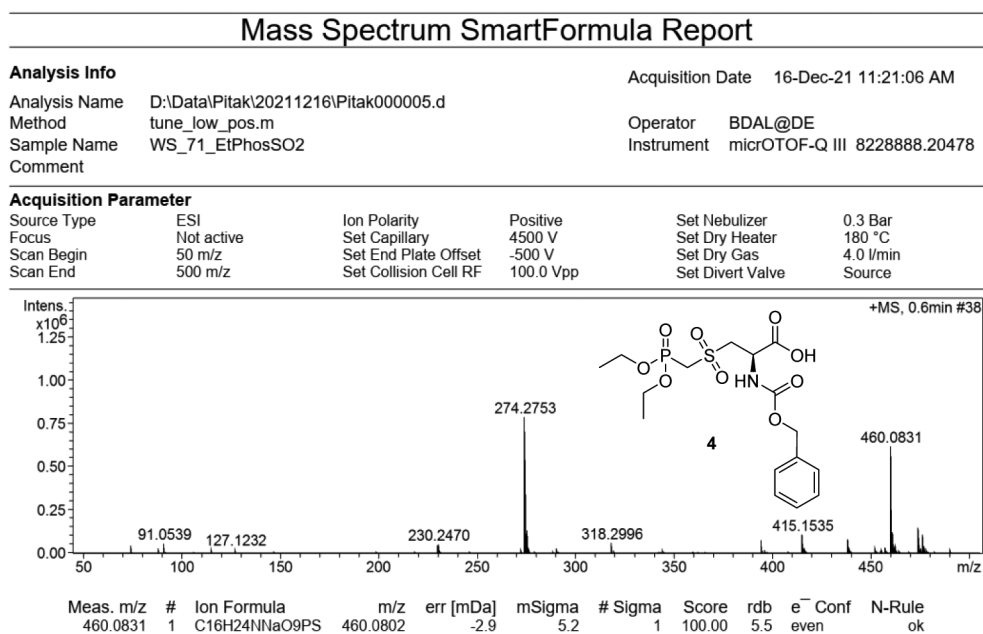


Fig. S12 High-resolution mass spectrum (HRMS) of compound 4

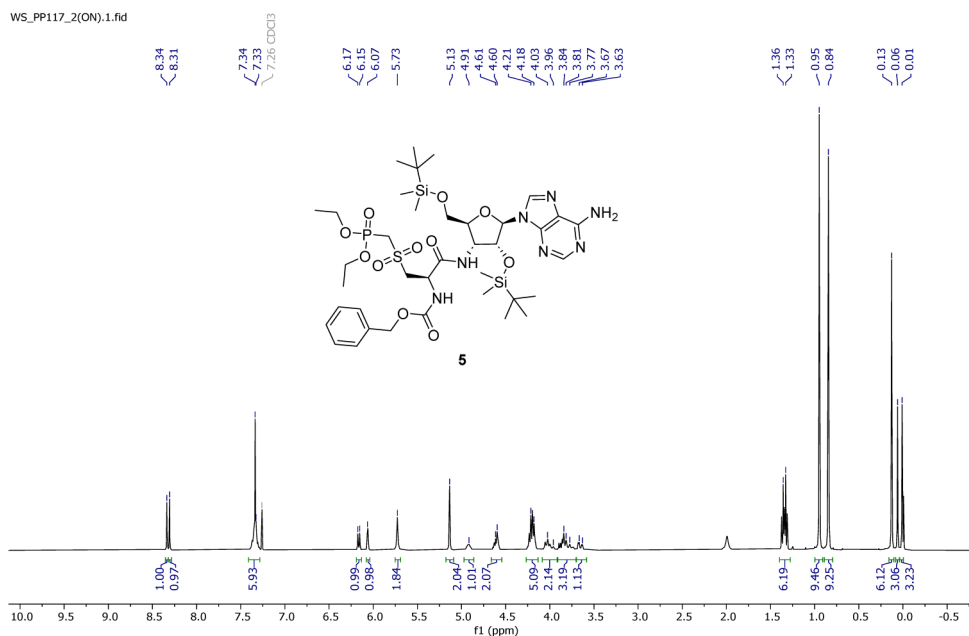


Fig. S13 ¹H Nuclear magnetic resonance spectrum of compound 5 (400 MHz, CDCl₃), where ppm = parts per million

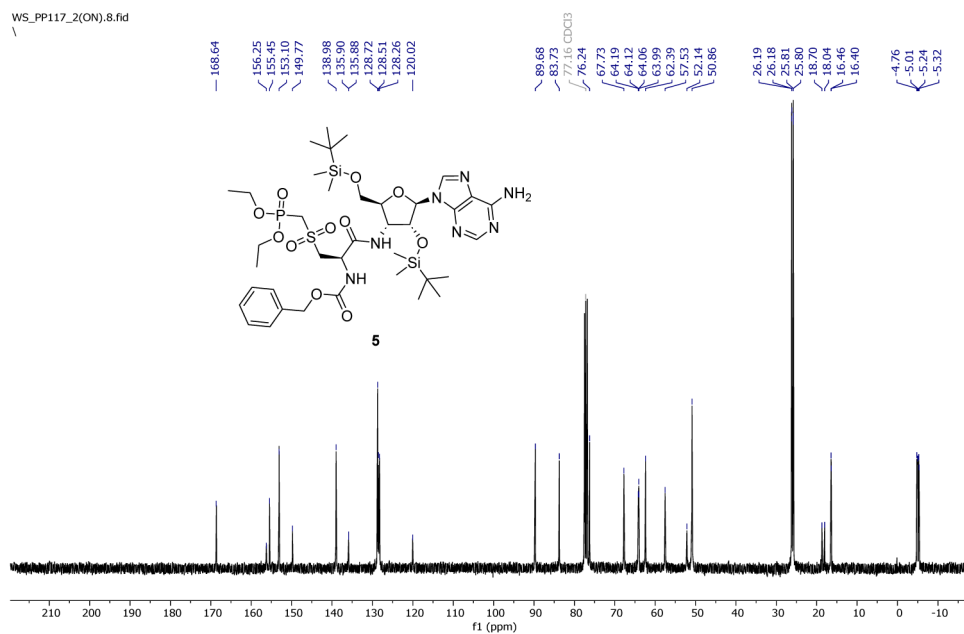


Fig. S14 ¹³C Nuclear magnetic resonance spectrum of compound 5 (100 MHz, CDCl₃), where ppm = parts per million

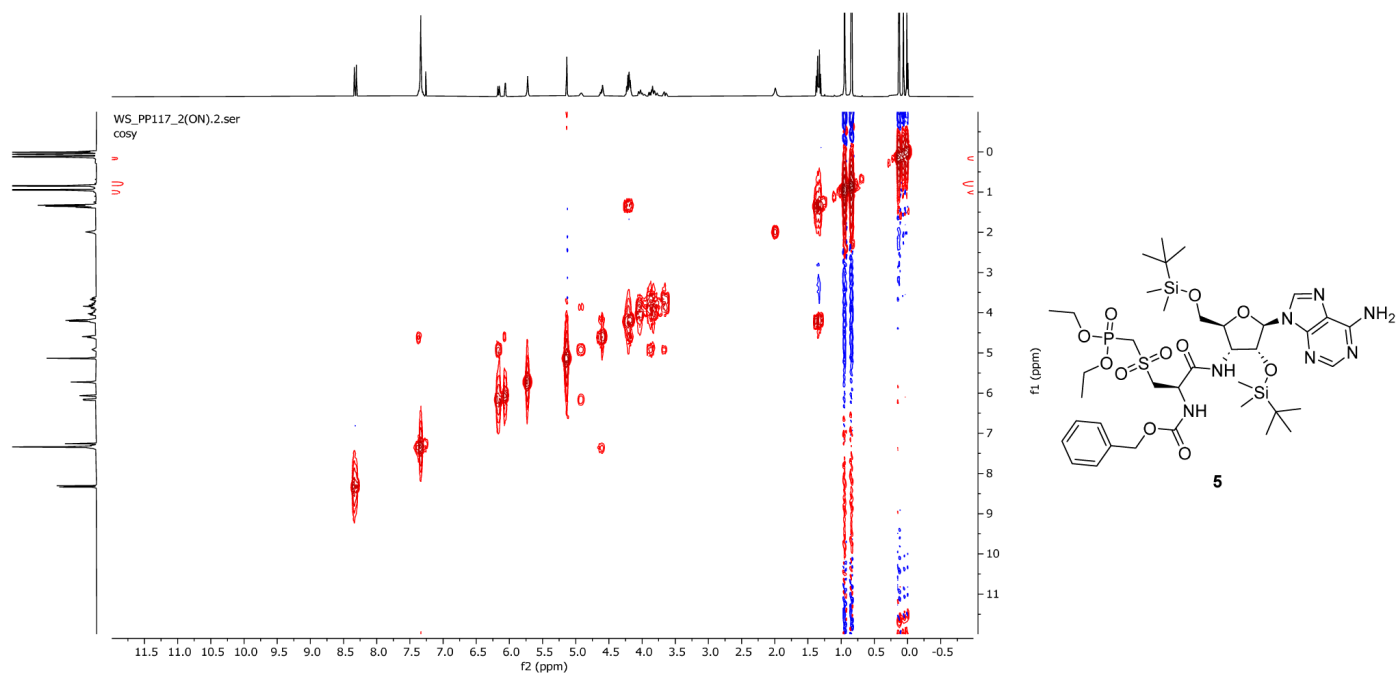


Fig. S15 Correlated spectrum of compound 5 (400 MHz, CDCl₃), where ppm = parts per million

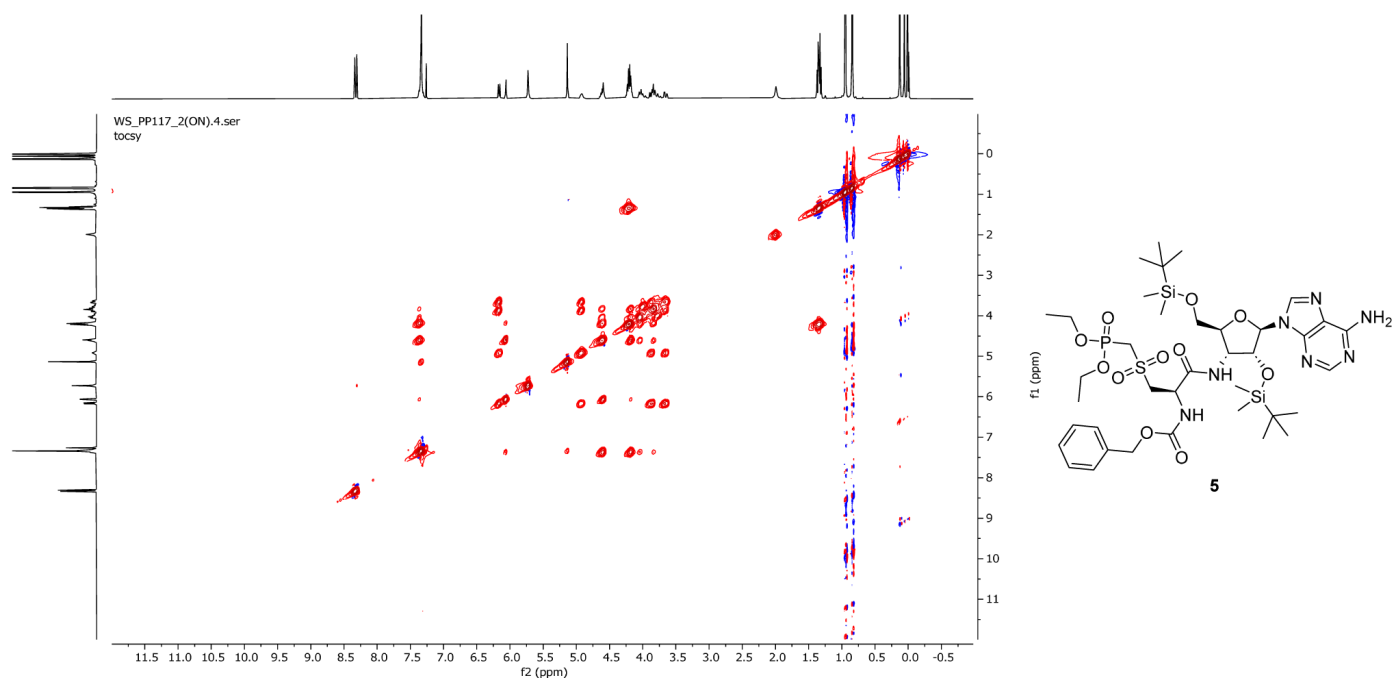


Fig. S16 Total correlation spectrum of compound 5 (400 MHz, CDCl₃), where ppm = parts per million

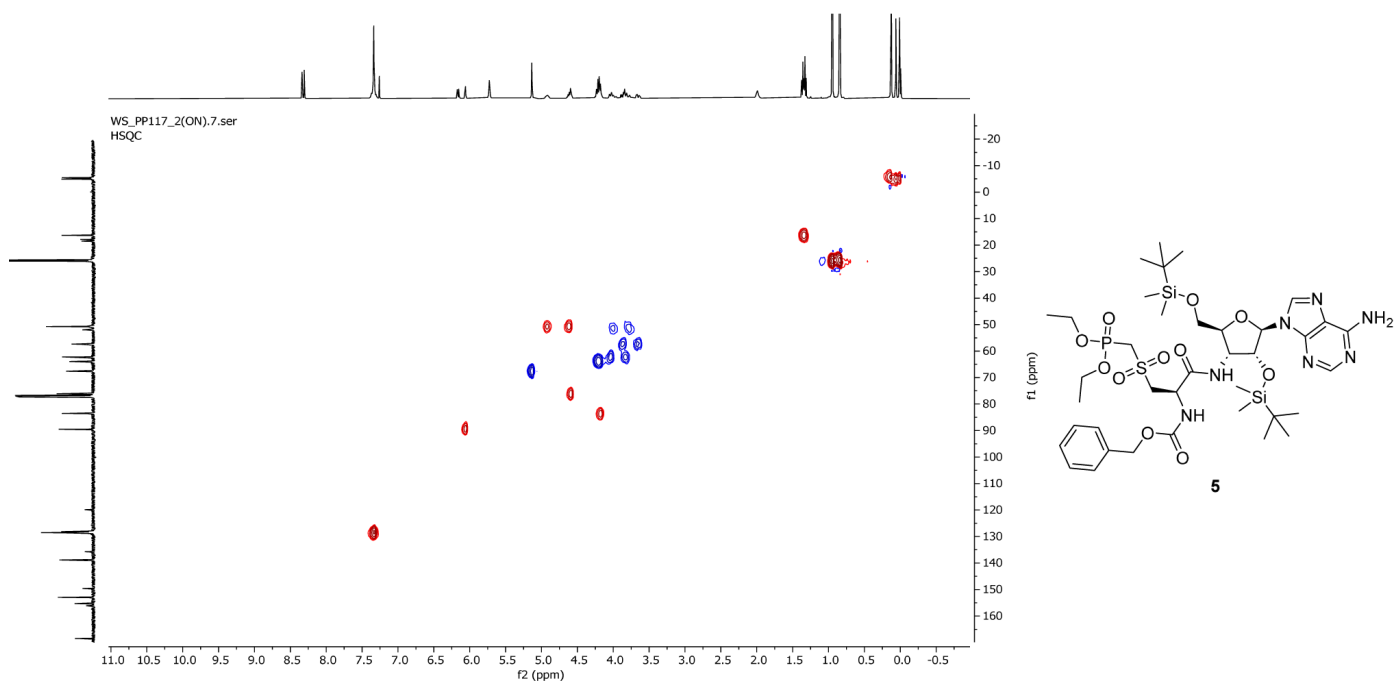


Fig. S17 Nuclear Overhauser effect spectrum of compound 5 (400 MHz, CDCl_3), where ppm = parts per million

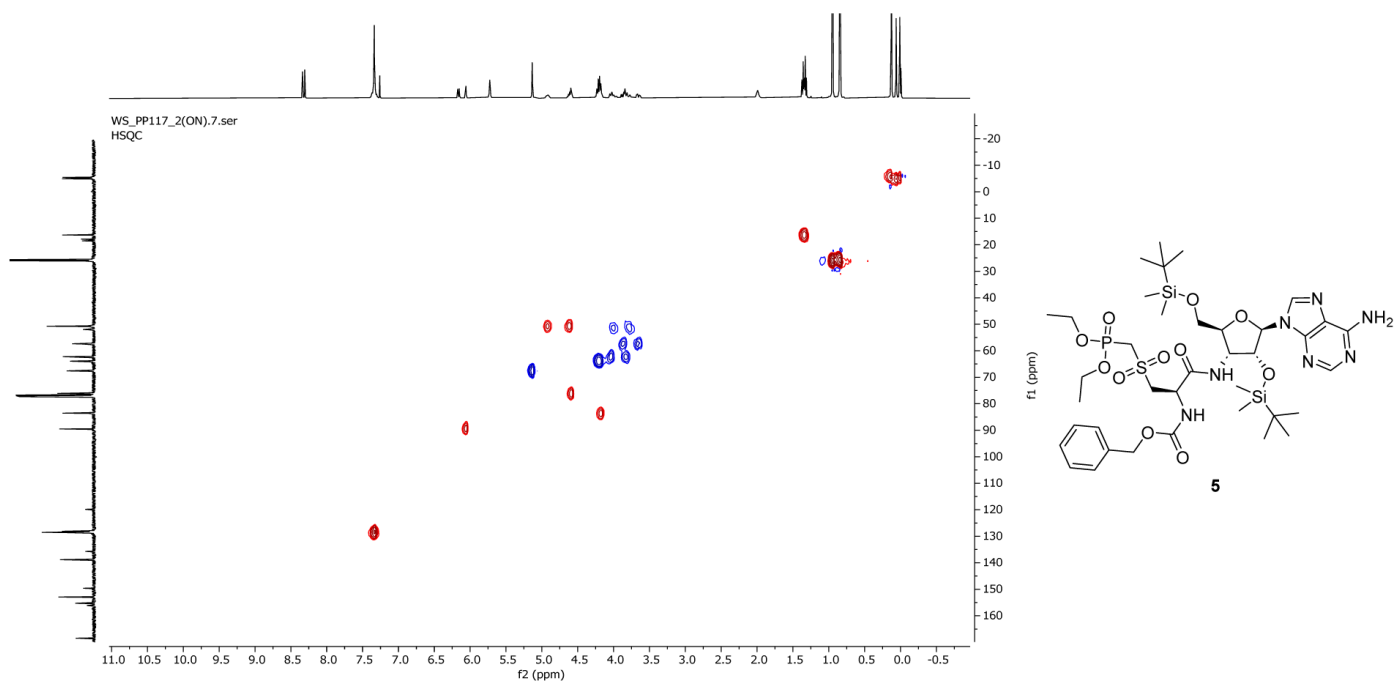


Fig. S18 HSQC-edited spectrum of compound 5 (400 MHz, CDCl_3), where ppm = parts per million

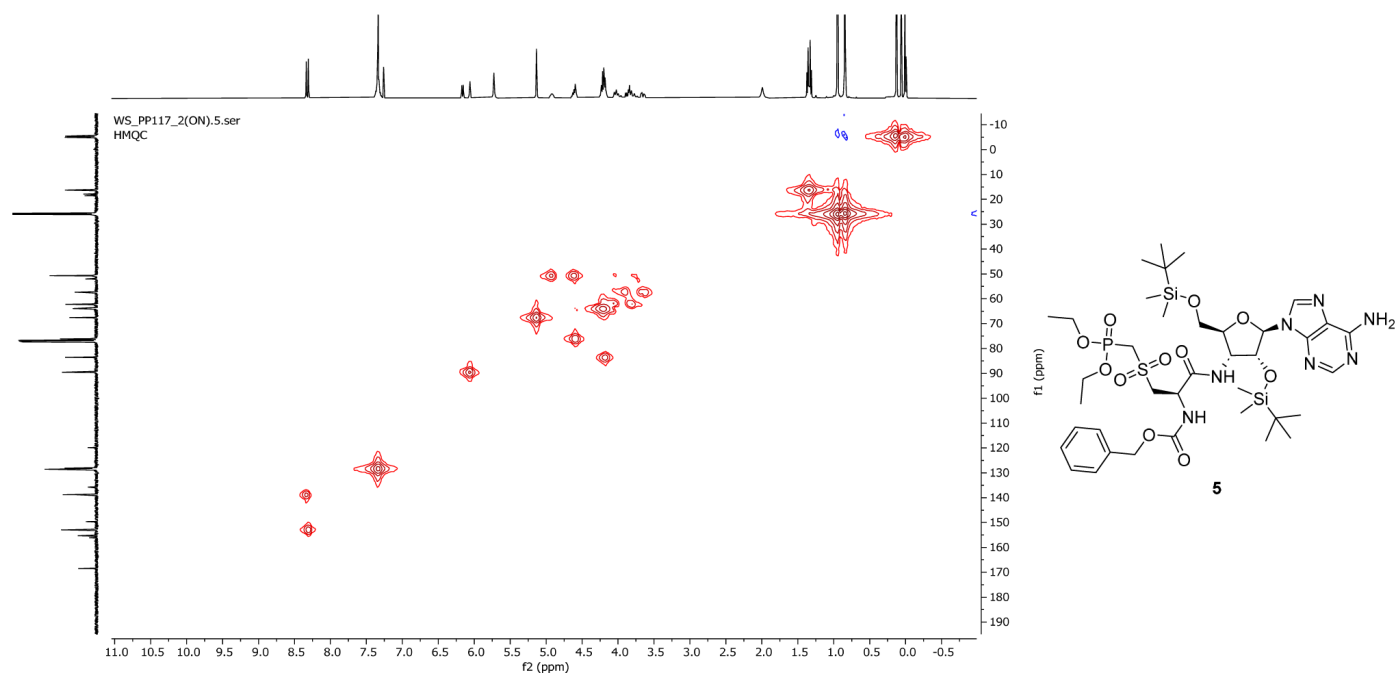


Fig. S19 HMBC spectrum of compound 5 (400 MHz, CDCl_3), where ppm = parts per million

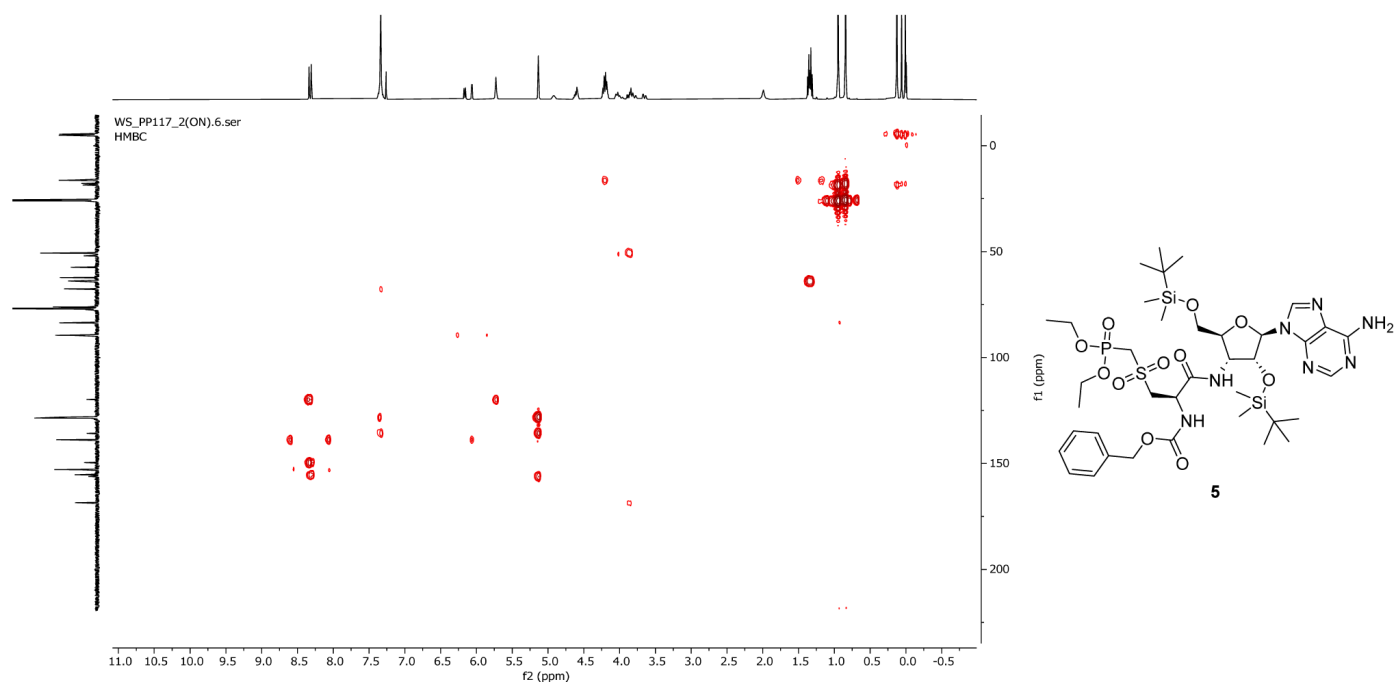


Fig. S20 HMBC spectrum of compound 5 (400 MHz, CDCl_3), where ppm = parts per million

Mass Spectrum SmartFormula Report

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 Sample Name WS_code57-1_EtPhosCbz
 Comment

Acquisition Date 08-Nov-21 11:34:08 AM

Operator BDAL@DE
 Instrument micrOTOF-Q III 8228888.20478

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source

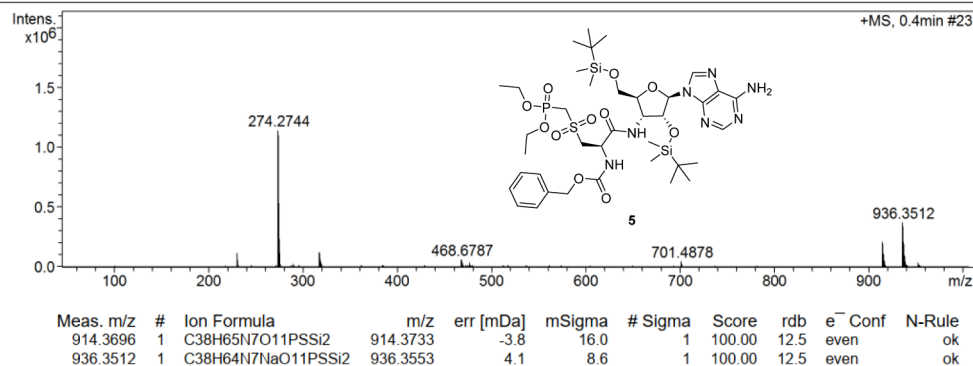


Fig. S21 High-resolution mass spectrum (HRMS) of compound 5

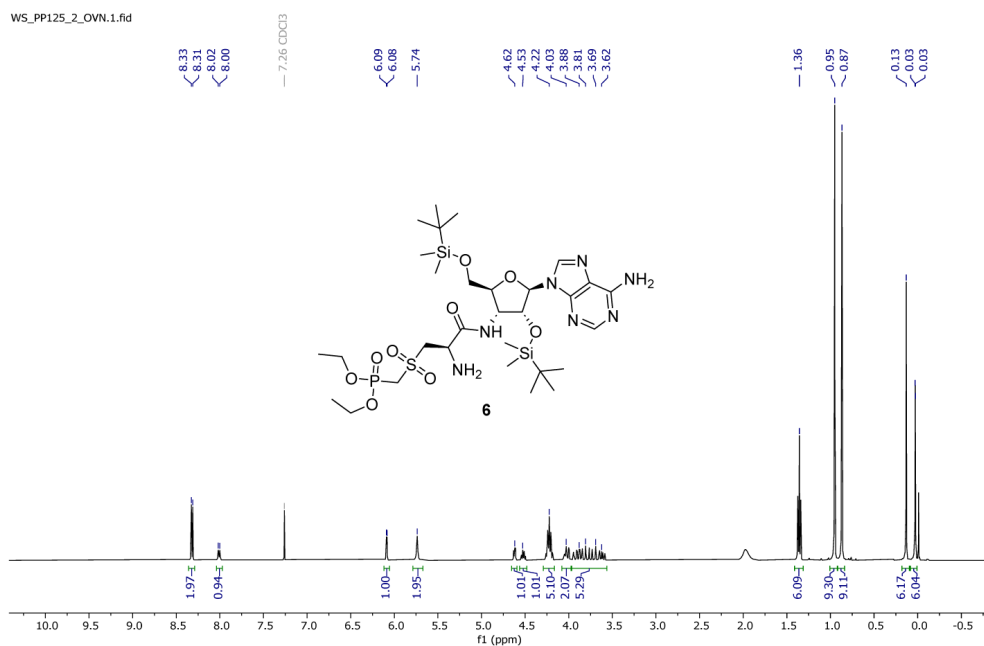


Fig. S22 ¹H NMR spectrum of compound 6 (400 MHz, CDCl₃), where ppm = parts per million

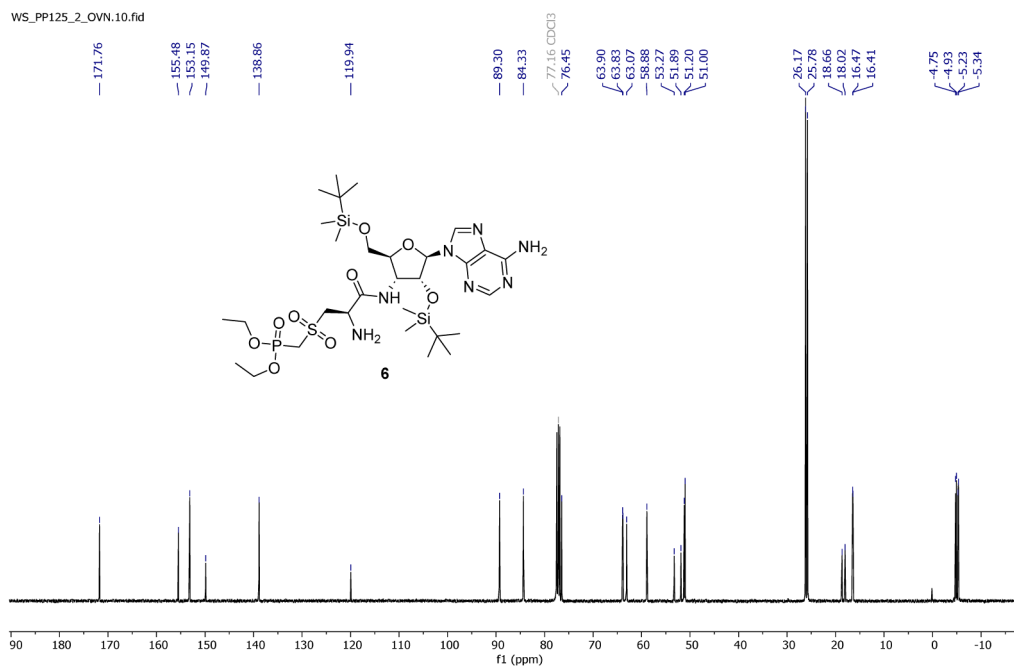


Fig. S23 ¹³C NMR spectrum of compound 6 (100 MHz, CDCl₃), where ppm = parts per million

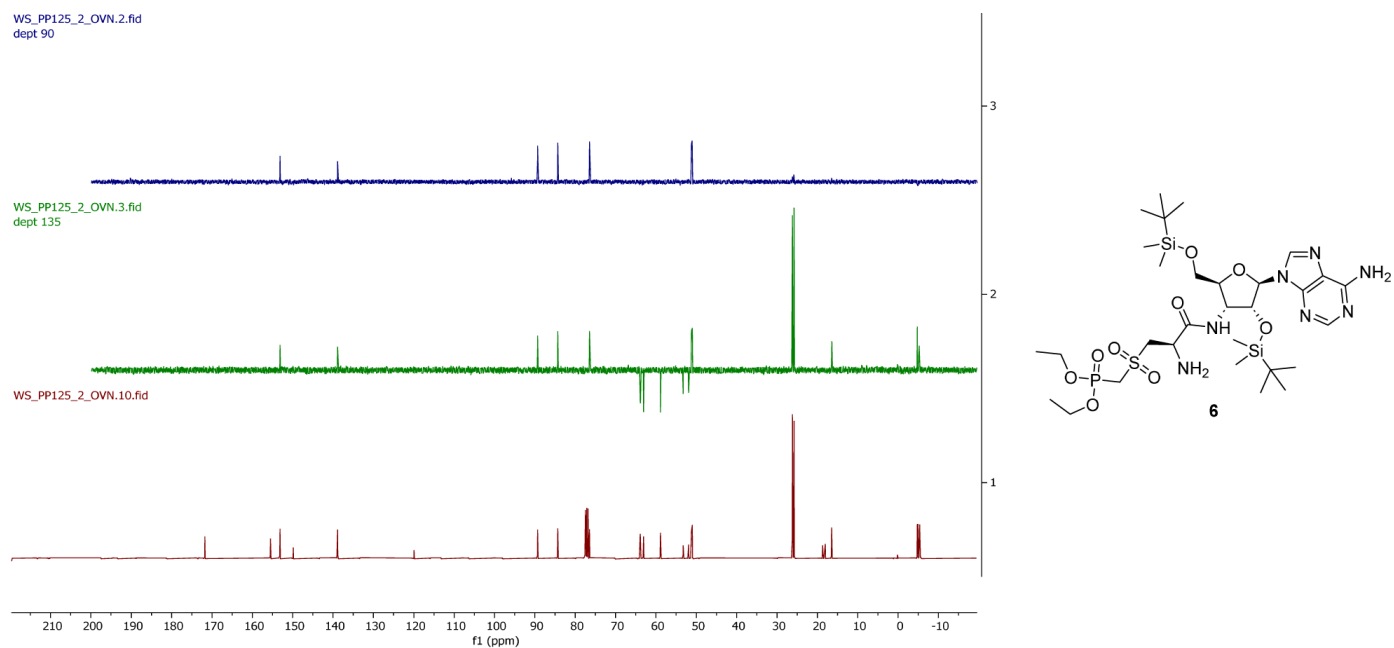


Fig. S24 DEPT spectra of compound 6 (100 MHz, CDCl₃), where ppm = parts per million

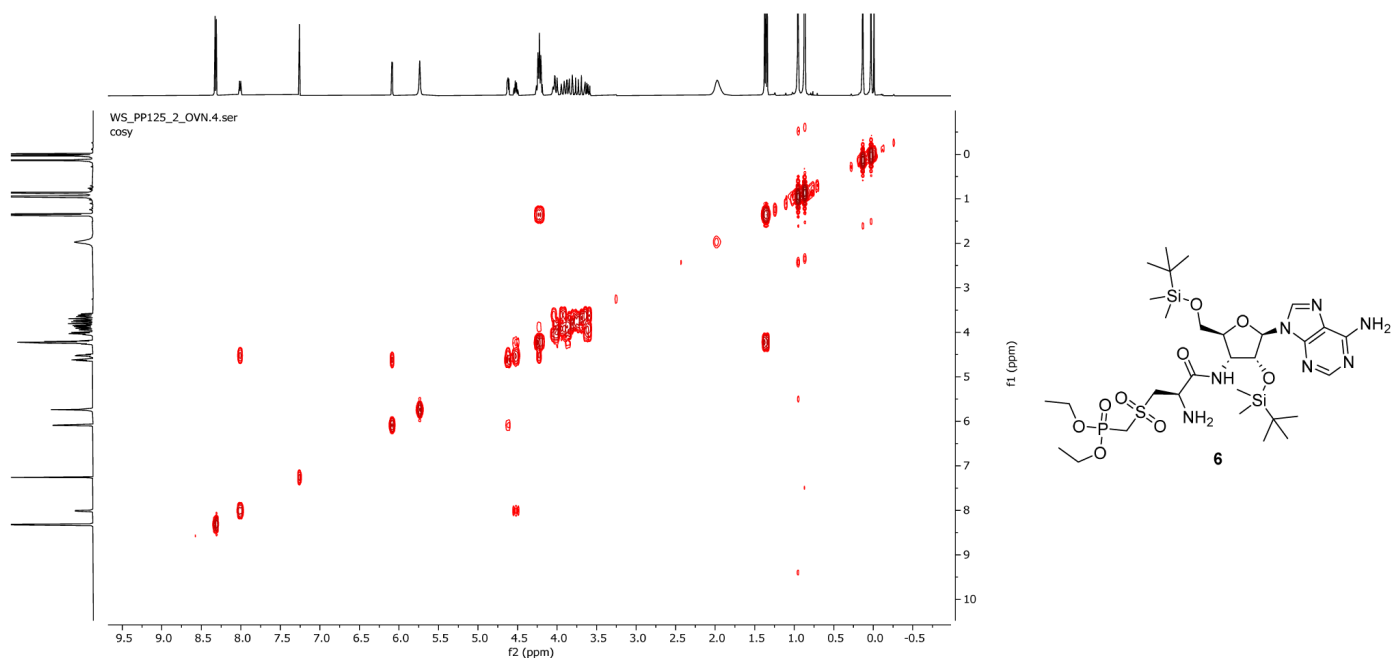


Fig. S25 COSY spectrum of compound 6 (400 MHz, CDCl₃), where ppm = parts per million

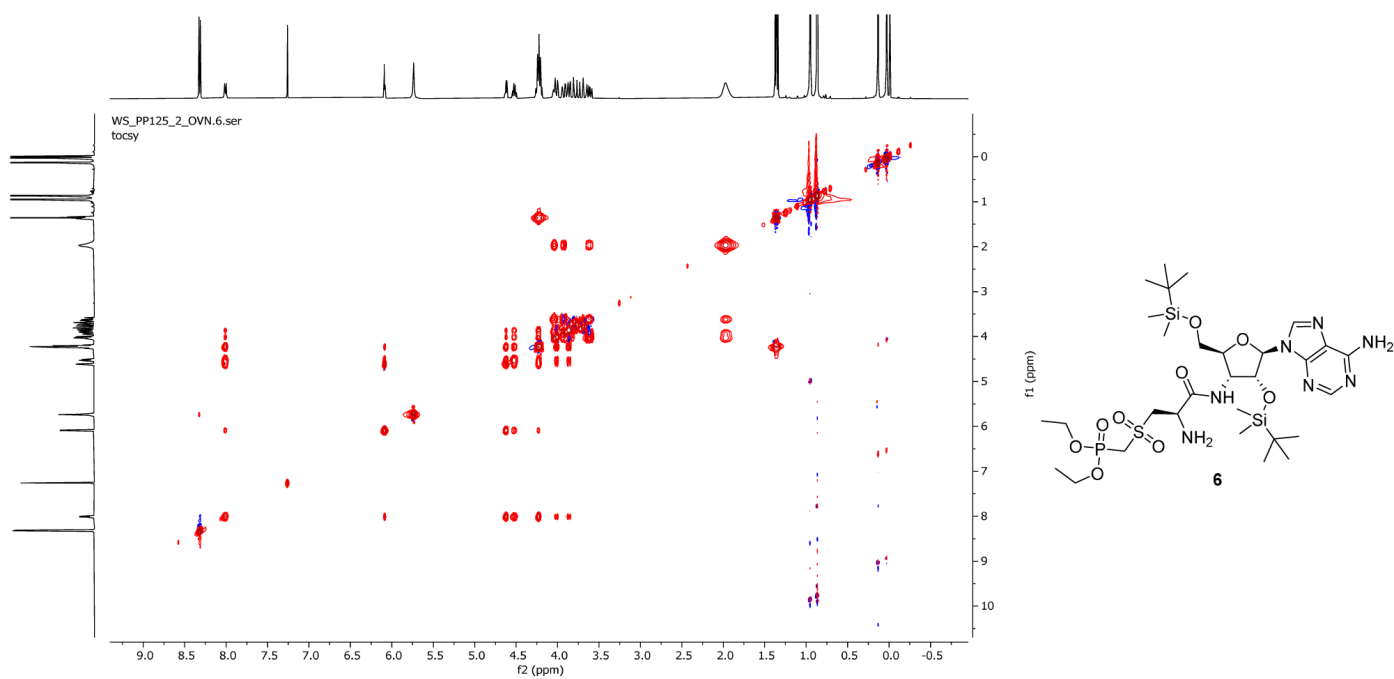


Fig. S26 TOCSY spectrum of compound 6 (400 MHz, CDCl₃), where ppm = parts per million

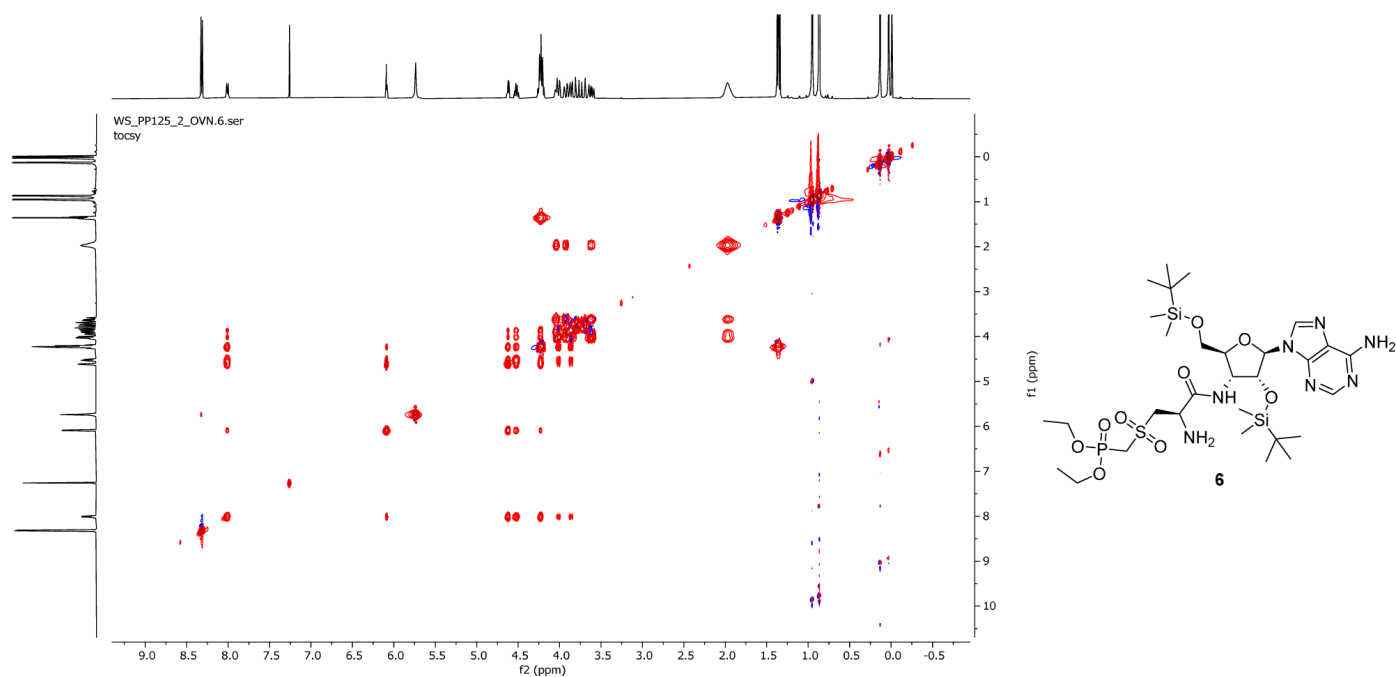


Fig. S27 NOESY spectrum of compound 6 (400 MHz, CDCl₃), where ppm = parts per million

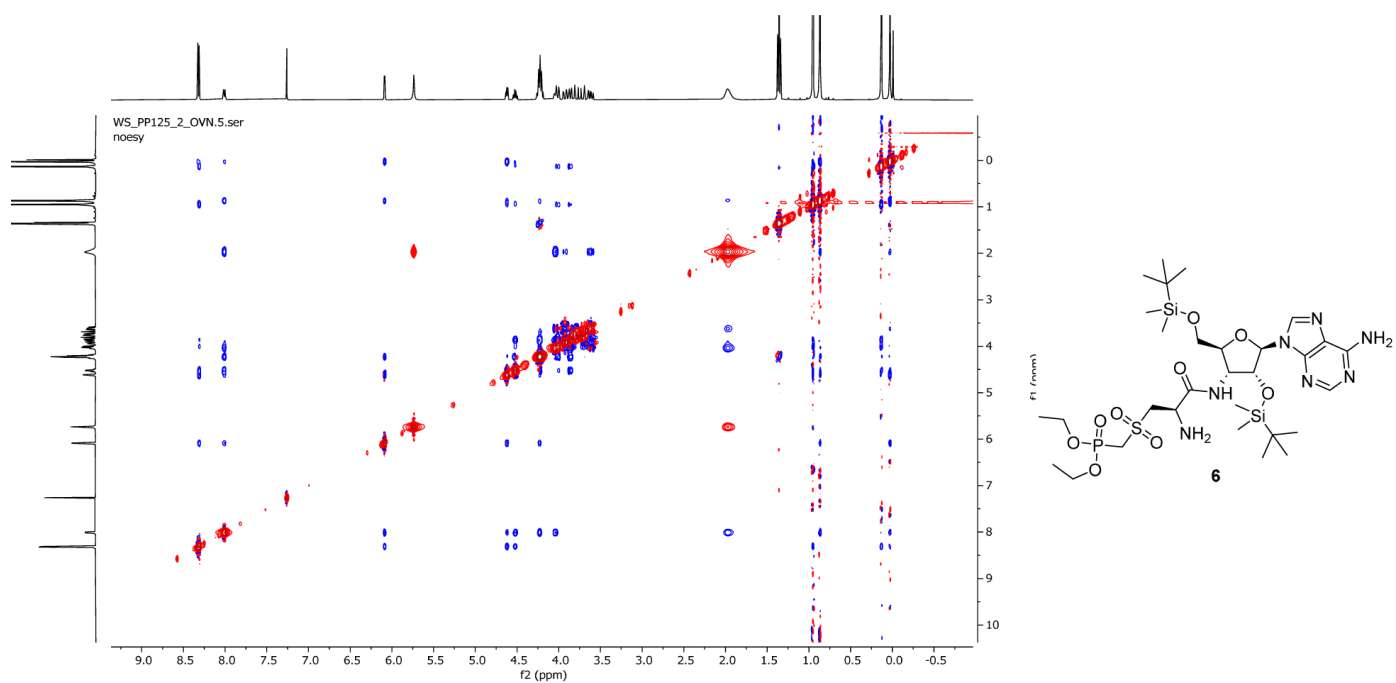


Fig. S28 HSQC-edited spectrum of compound 6 (400 MHz, CDCl₃), where ppm = parts per million

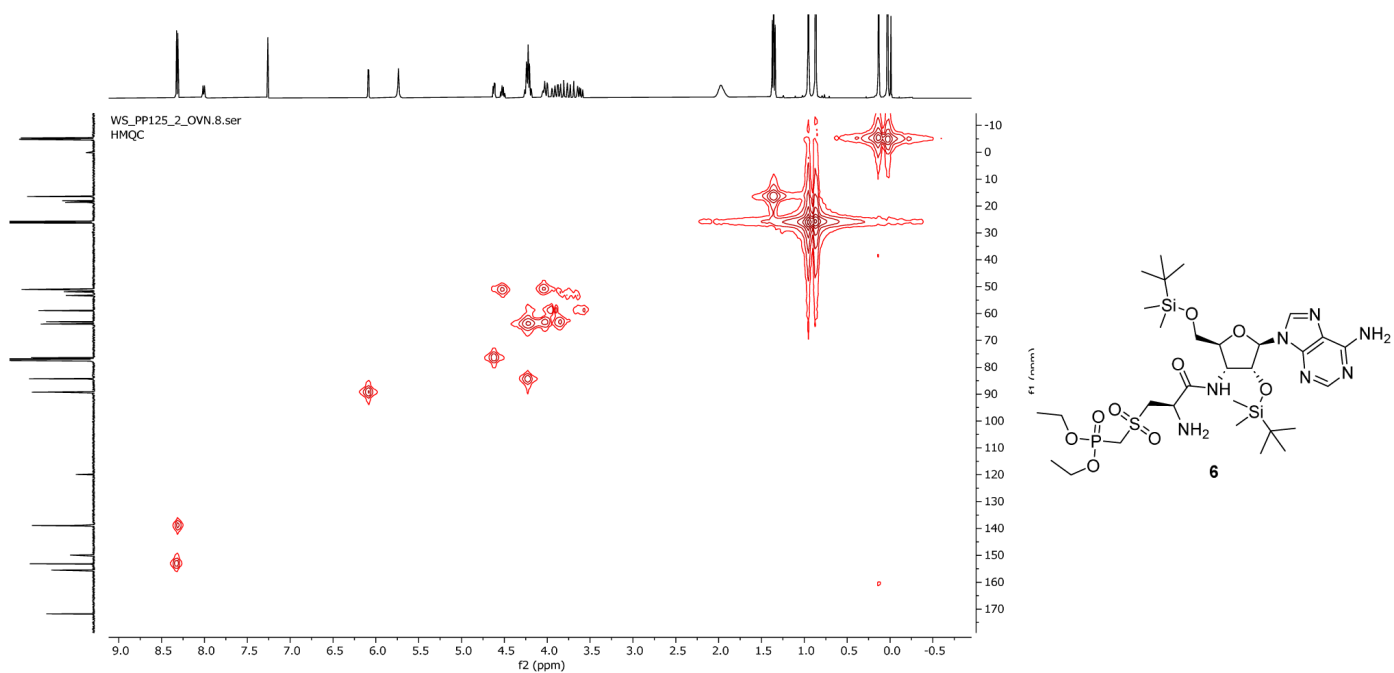


Fig. S29 HMBC spectrum of compound 6 (400 MHz, CDCl_3), where ppm = parts per million

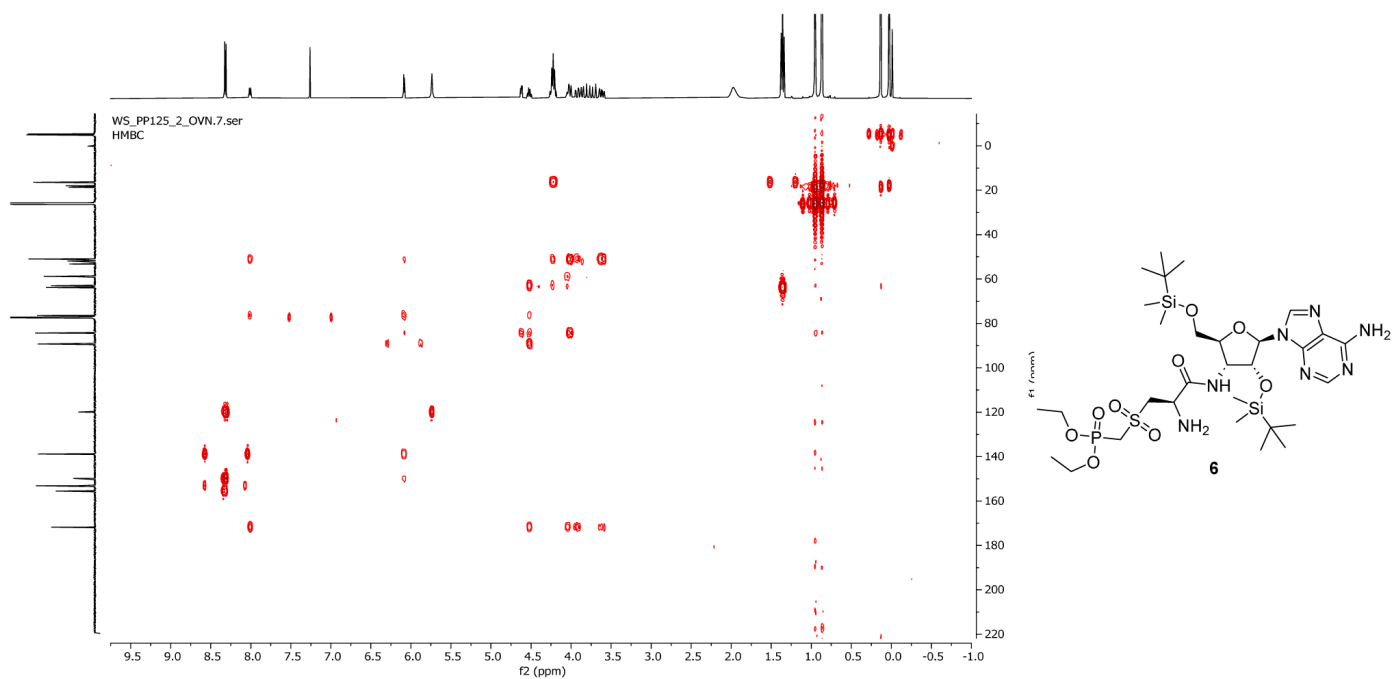


Fig. S30 HMBC spectrum of compound 6 (400 MHz, CDCl_3), where ppm = parts per million

Mass Spectrum SmartFormula Report

Analysis Info

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 Sample Name WS_code72_NH2
 Comment

Acquisition Date 02-Sep-21 2:17:15 PM

Operator BDAL@DE
 Instrument micrOTOF-Q III 8228888.20478

Acquisition Parameter

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Scan End	850 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Source

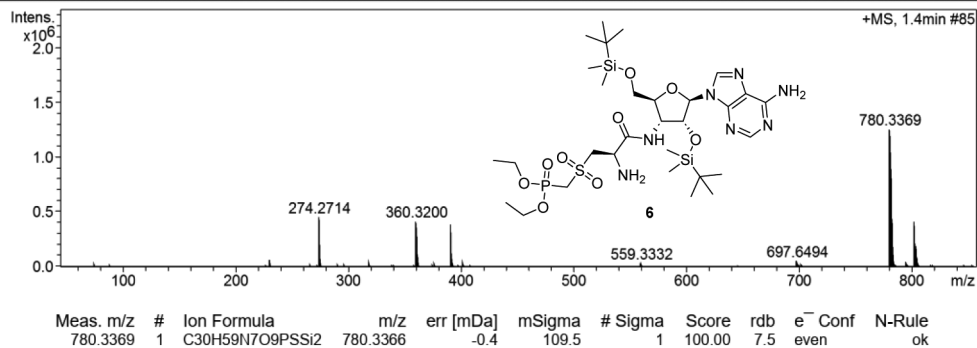
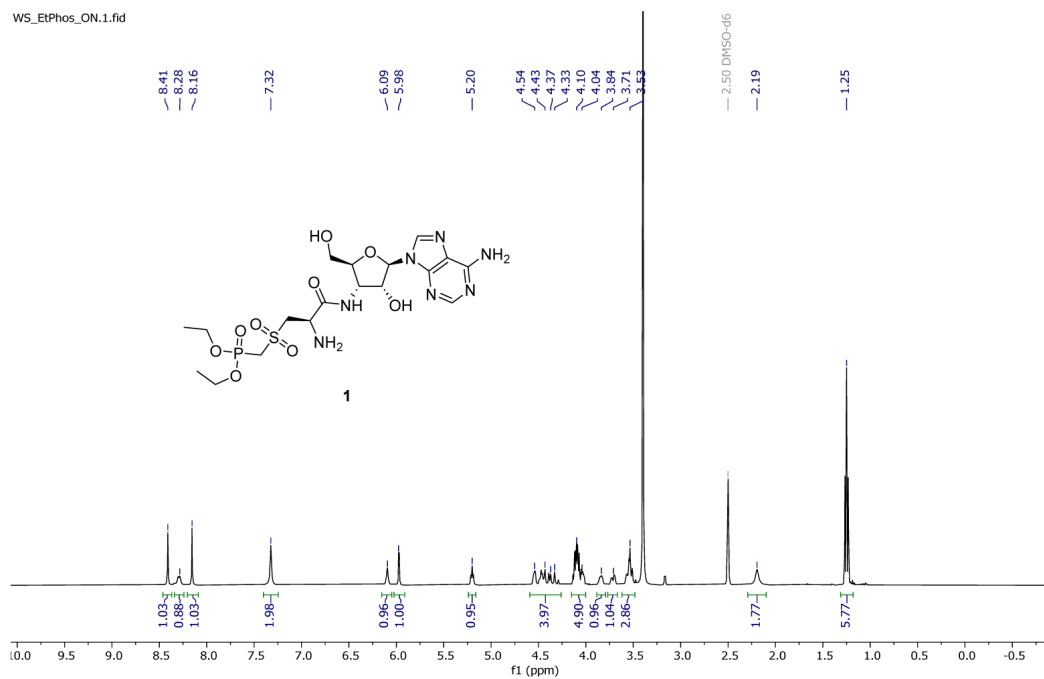


Fig. S31 High-resolution mass spectrum (HRMS) of compound 6

Fig. S32 ¹H NMR spectrum of compound 1 (400 MHz, DMSO-*d*₆), where ppm = parts per million

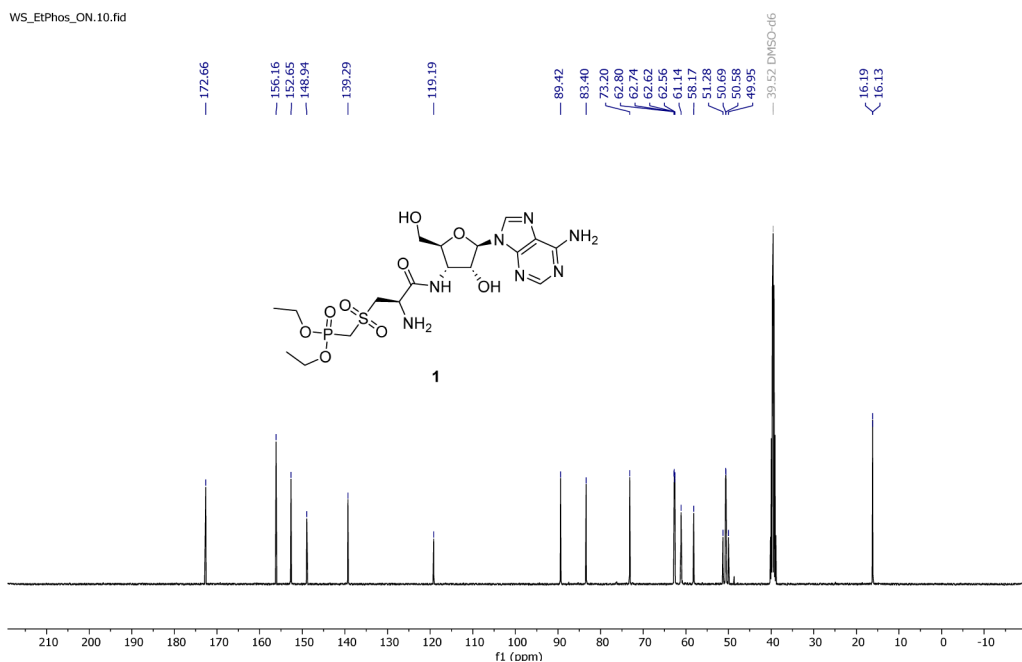


Fig. S33 ^{13}C NMR spectrum of compound 1 (100 MHz, $\text{DMSO-}d_6$), where ppm = parts per million

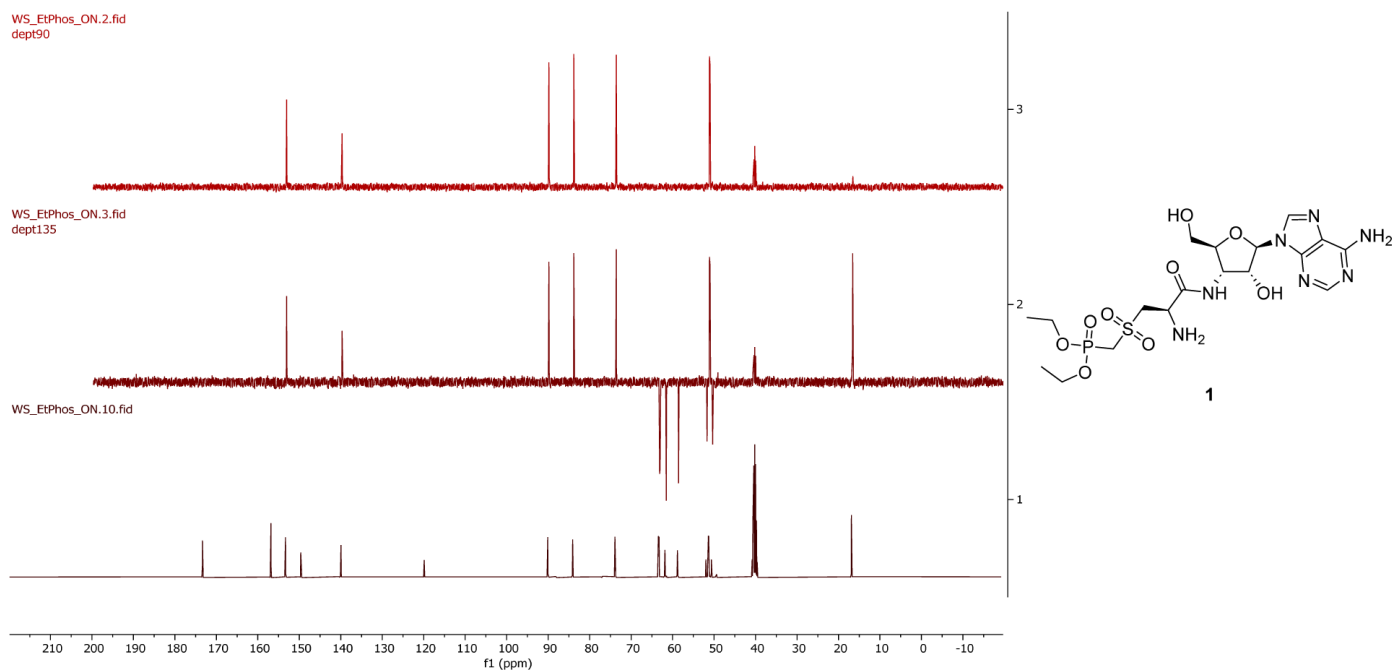


Fig. S34 DEPT spectra of compound 1 (100 MHz, $\text{DMSO-}d_6$), where ppm = parts per million

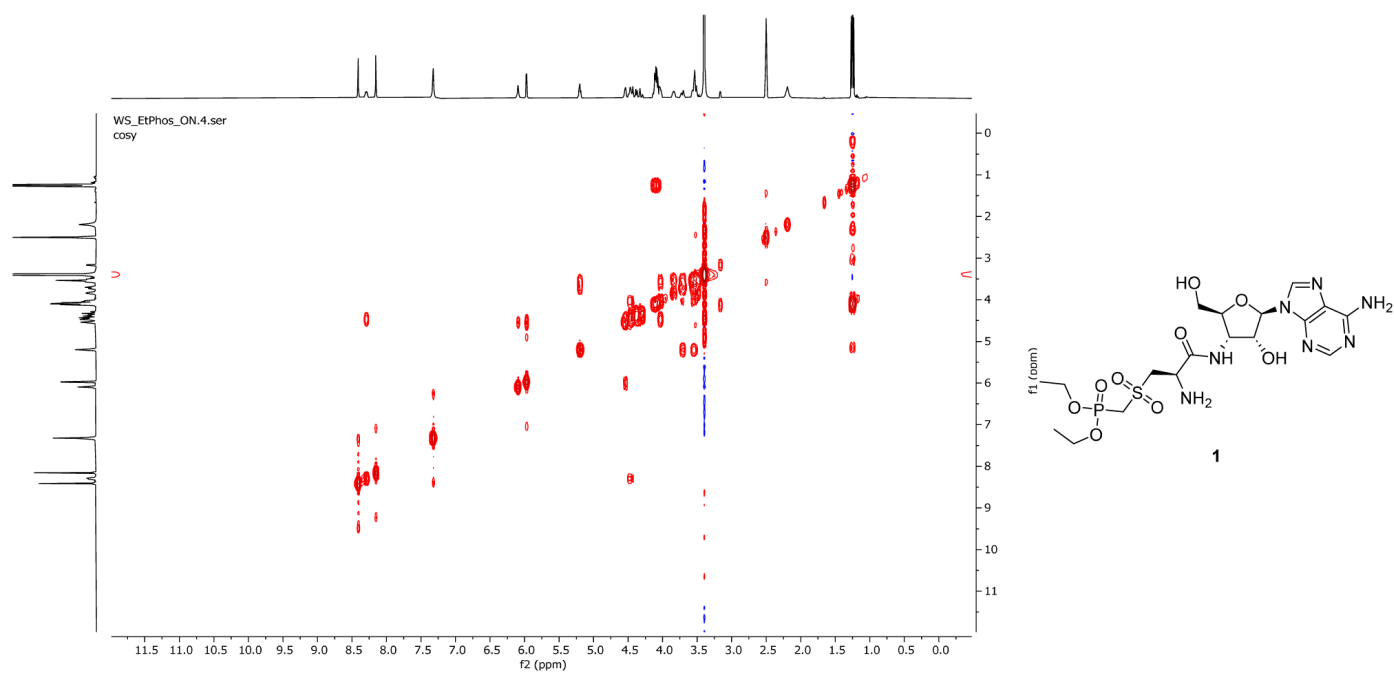


Fig. S35 COSY spectrum of compound 1 (400 MHz, DMSO- d_6), where ppm = parts per million

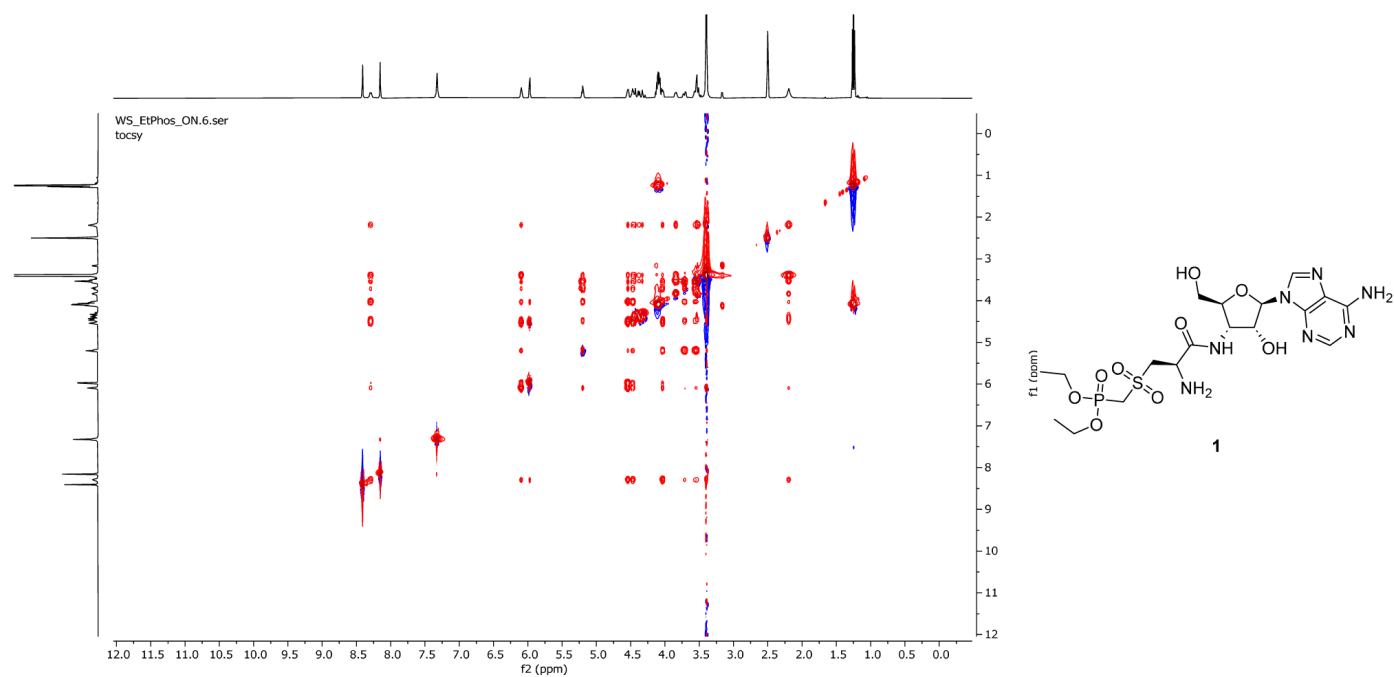


Fig. S36 TOCSY spectrum of compound 1 (400 MHz, DMSO- d_6), where ppm = parts per million

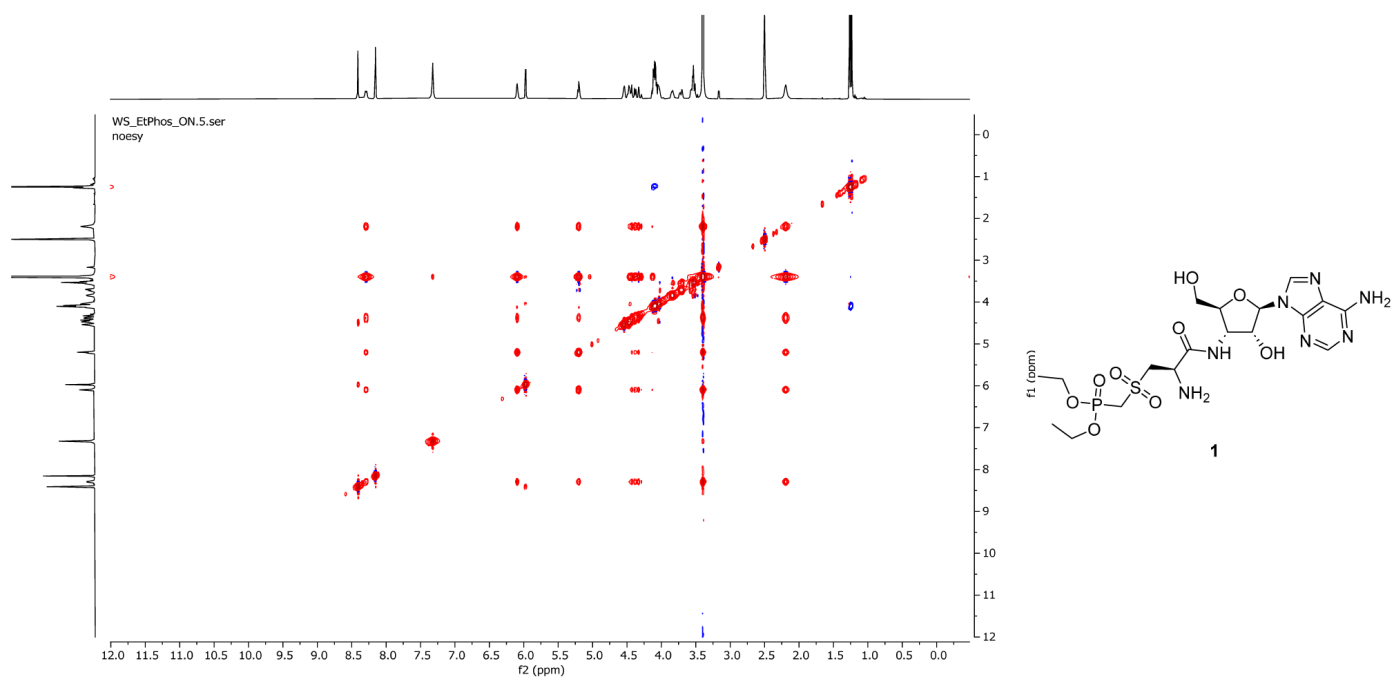


Fig. S37 NOESY spectrum of compound 1 (400 MHz, DMSO- d_6), where ppm = parts per million

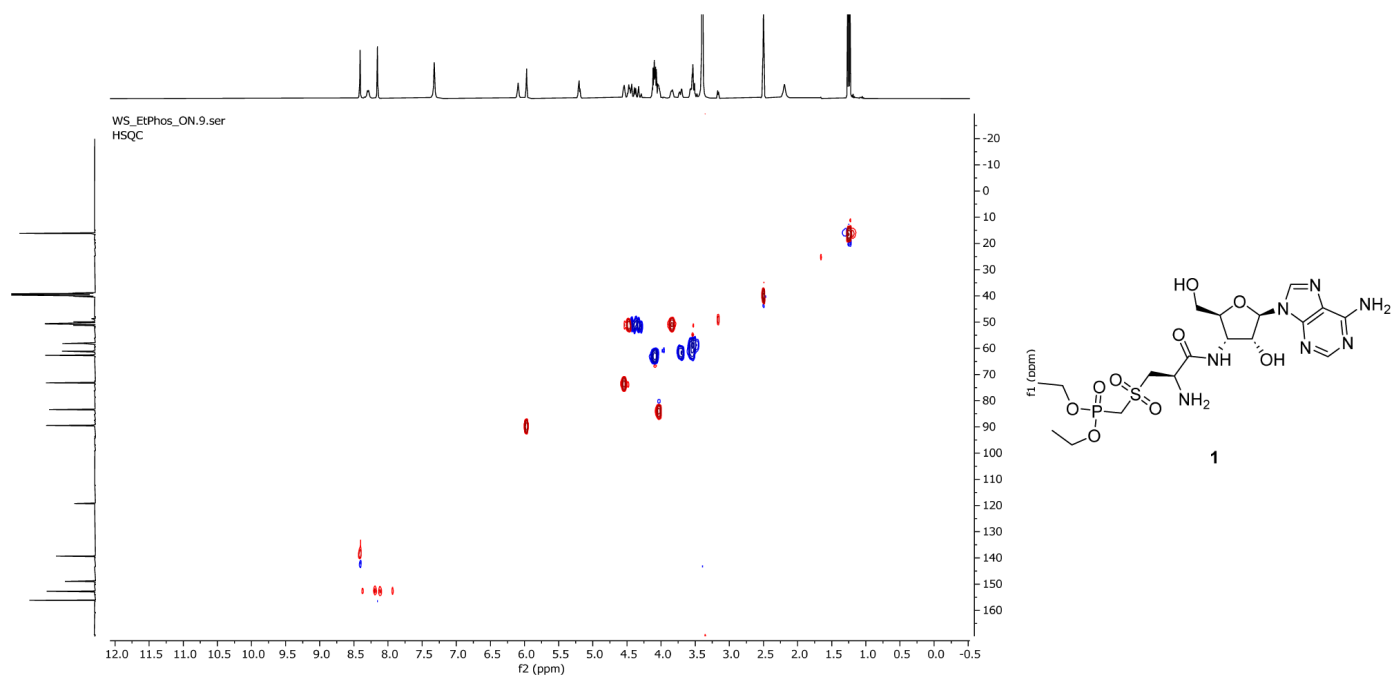


Fig. S38 HSQC-edited spectrum of compound 1 (400 MHz, DMSO- d_6), where ppm = parts per million

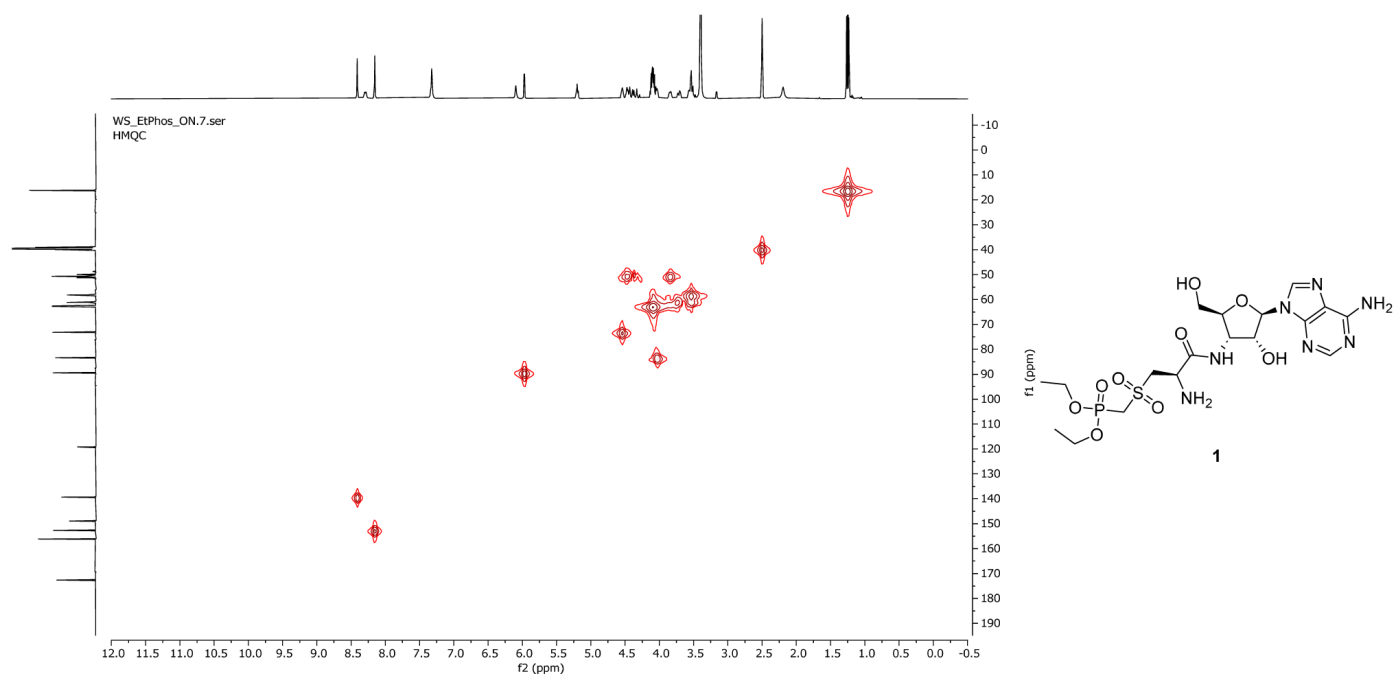


Fig. S39 HMQC spectrum of compound 1 (400 MHz, DMSO-*d*₆), where ppm = parts per million

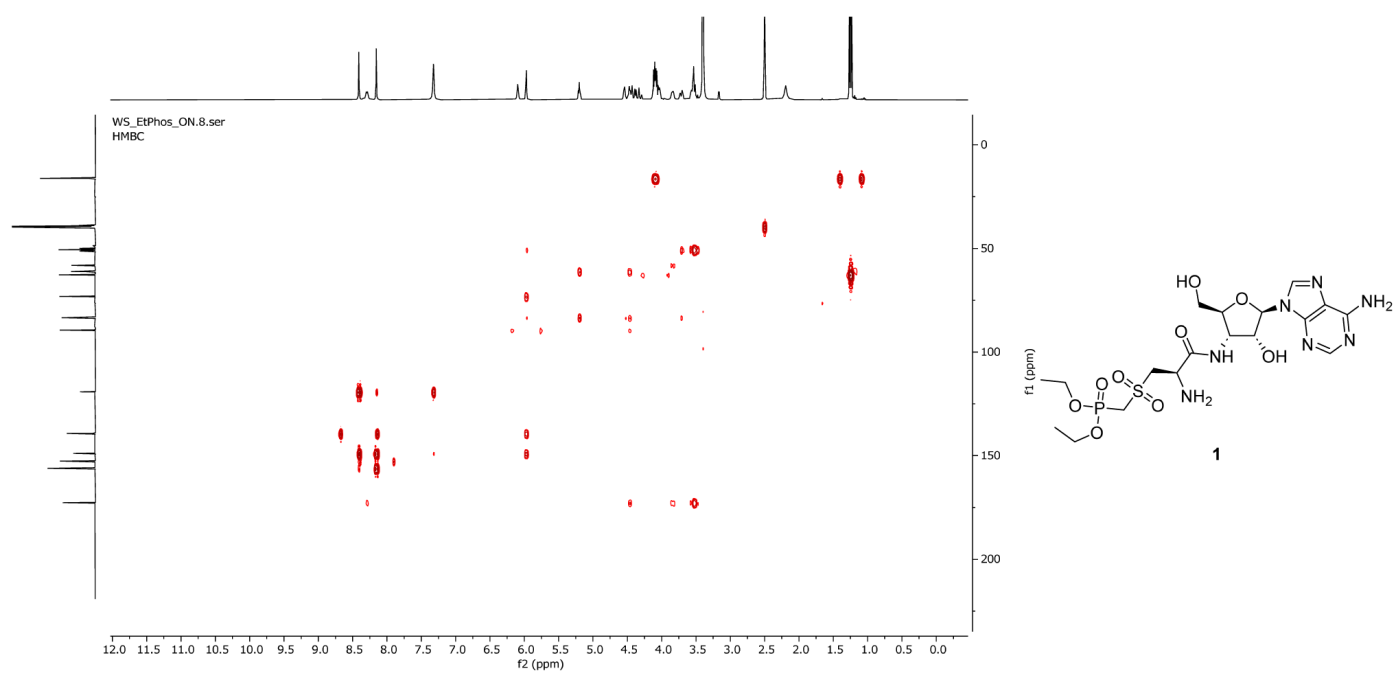


Fig. S40 HMBC spectrum of compound 1 (400 MHz, DMSO-*d*₆), where ppm = parts per million

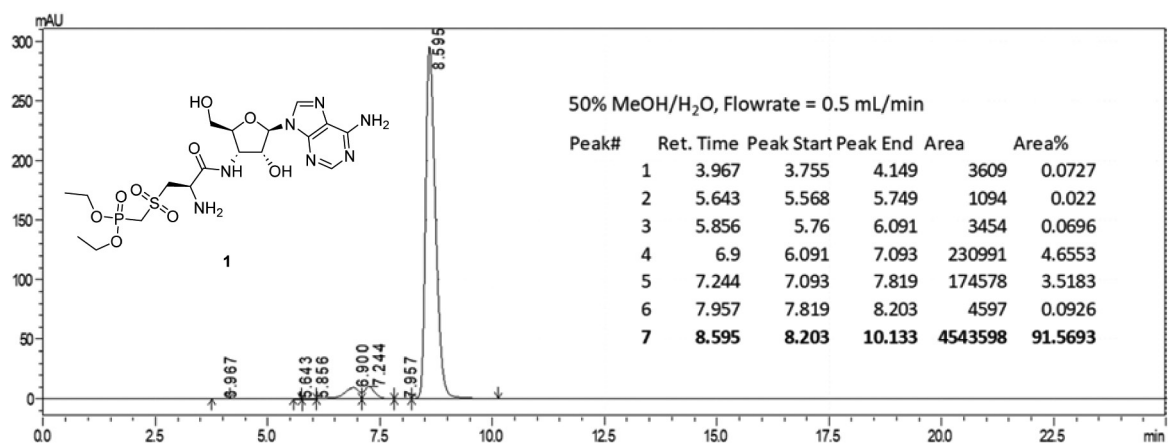


Fig. S41 High-resolution mass spectrum (HRMS) of compound 1

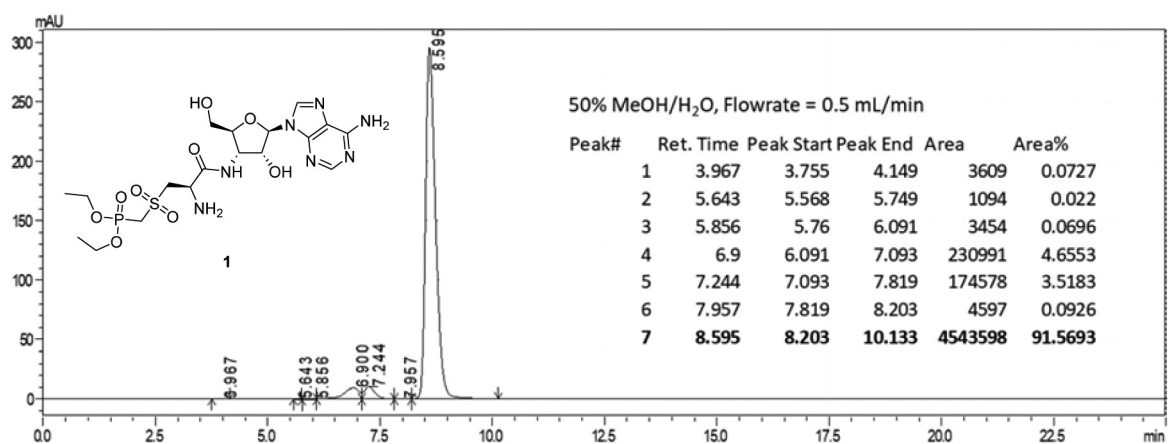


Fig. S42 HPLC trace chromatogram of compound 1

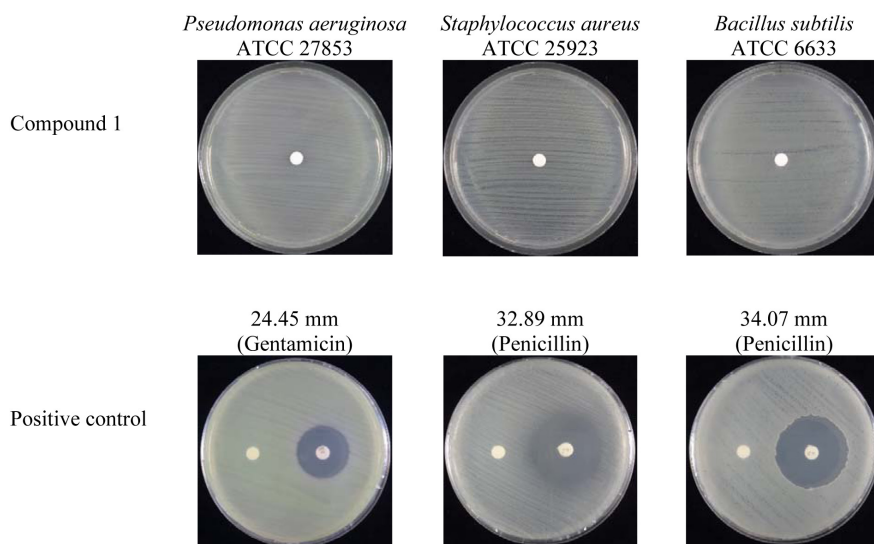


Fig. S43 Disc diffusion antibacterial results