Electronic Supplementary Information

Artificial Amidase with Modifiable Active Sites and Designable Substrate Selectivity for Aryl Amide Hydrolysis

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Table of Contents

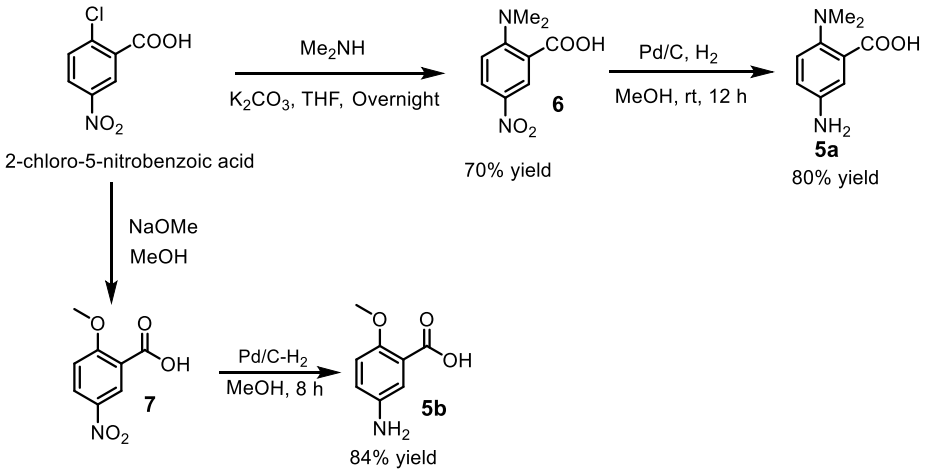
Materials and Methods

All organic solvents and reagents were of ACS-certified grade or higher grade and were purchased from Fisher Scientific and dried using standard procedures. Ultrapure water (18.2 MU; Millipore Co., USA) was used in the preparation of all buffers and nanoparticles. Flash column chromatography was performed on SiliFlash P60 silica gel (40-63 µm, 60 Å). All reactions were performed using standard Schlenk techniques. NMR spectra (^{1}H and ^{13}C NMR) were recorded on a Bruker DRX-400, a Bruker AV III 600, or a Varian VXR-400 spectrometer. Chemicals shifts are reported in ppm relative to residual solvent peaks ($CDCl_3$ = 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR, CD_3OD = 3.31 ppm for ^{1}H NMR and 49.00 for ^{13}C NMR). Coupling constants are reported in hertz. ESI-mass spectrometry was recorded on an Agilent QTOF 6540 mass spectrometer with a QTOF detector. Dynamic light scattering (DLS) was performed on a Malvern Zetasizer Nano ZS. UV-vis spectra were recorded on a Cary 100 Bio UV-visible spectrophotometer. LC-MS analysis was performed with a Thermo Scientific HPLC-LC column (4.6 mm, 150 mm) coupled to an Agilent 1200 Series Binary VWD system with an Agilent 6540 UHD Accurate Mass Q-TOF mass spectrometry detector.

Synthesis & Characterization

Syntheses of compounds **5a**[1,2] and **5b**[3,4] followed previously reported procedures.

Scheme S1. Syntheses of functional molecules used in the study

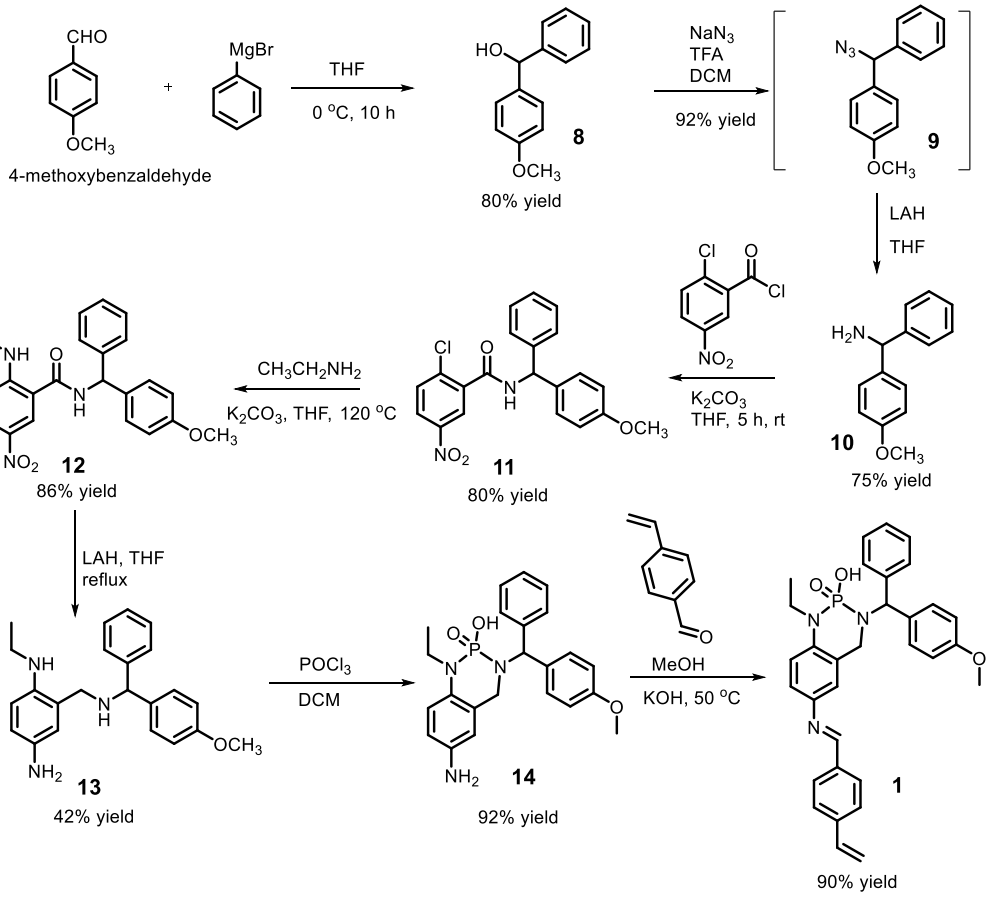


Synthesis of compound 6. 2-Chloro-5-nitrobenzoic acid (0.660 g, 3.3 mmol) was added to a suspension of potassium carbonate (0.621 g, 4.5 mmol) in anhydrous methanol (20 mL) containing dimethylamine (0.33 mL, 5 mmol). After the reaction mixture was heated to reflux overnight under nitrogen, it was cooled to room temperature and diluted with 1 N aqueous HCl (50 mL). The mixture was extracted with ethyl acetate (3 × 30 mL). The combined organic phase was washed with brine (30 mL), dried over $MgSO_4$, and concentrated by rotary evaporation. The residue was purified by column chromatography over silica gel using 6:4 hexane/ethyl acetate as the eluent to afford a yellowish powder (0.485 g, 70% yield). ^{1}H NMR (600 MHz, CD_3OD) δ 8.37 (d, J = 2.7

Hz, 1H), 8.07 (dd, J = 9.0, 2.8 Hz, 1H), 7.07 (d, J = 9.1 Hz, 1H), 2.90 (s, 6H). ^{13}C{1H} NMR (151 MHz, CD_3OD) δ 157.15, 141.10, 133.45, 124.13, 116.72, 42.73. HRMS (ESI$^+$/QTOF) Calcd for $C_9H_{10}N_2O_4$ m/z: $[M+H]^+$ 211.1969; Found m/z 211.1979.

Synthesis of compound 8. A solution of 4-methoxybenzaldehyde (0.272 g, 2 mmol) in anhydrous THF (3 mL) was added to a flame-dried flask under nitrogen. After the solution was cooled to 0 °C, phenyl magnesium bromide (1.0 M solution in THF, 3 mL) was added dropwise over 10 min, and stirring was continued for 3 h. After the disappearance of the aldehyde by TLC, the reaction mixture was quenched with saturated ammonium chloride (5 mL). The crude reaction mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic phase was dried over Na_2SO_4 and concentrated by rotary evaporation. The residue was purified by column chromatography over silica gel using 10:1 hexane/ethyl acetate as the eluent to afford a white powder (0.217 g, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.37 (m, 4H), 7.34 – 7.28 (m, 3H), 6.95 – 6.88 (m, 2H), 5.77 (d, J = 3.0 Hz, 1H), 3.81 (s, 3H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 158.52, 145.21, 127.86, 126.37, 125.65, 112.37, 91.24, 68.28, 55.82. HRMS (ESI$^+$/QTOF) Calcd for $C_{14}H_{14}O_2$ m/z: $[M+H]^+$ 215.1073; Found m/z 215.1070.

Scheme S2. Synthesis of Template 1a



Synthesis of compound 10. A solution of compound **8** (0.428 g, 2 mmol) in anhydrous dichloromethane (5 mL) was treated with NaN_3 (0.325 g, 5 mmol) at room temperature and then cooled to −5 °C under nitrogen. A solution of trifluoroacetic acid (2.29 mL, 30 mmol) in

dichloromethane (6 mL) was added dropwise and the mixture was stirred at −5 °C for 15 min and then at 0 °C for another 12 h. Upon the completion of the reaction (indicated by TLC), water (10 mL) was added slowly to quench the reaction, followed by slow addition of a 14% ammonia solution (10 mL). After vigorously stirred for 30 min, the reaction mixture was allowed to warm to room temperature and extracted with dichloromethane (3 × 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated by vacuo to provide the crude azide intermediate **9**. A solution of the crude azide in ether (5 mL) was added dropwise to a suspension of lithium aluminum hydride (0.222 g, 6 mmol) in anhydrous ether (5 mL) at 0 °C under nitrogen. The reaction mixture was stirred at room temperature for 3 h and then quenched with 1 N NaOH solution (pH > 10). The insoluble solid was removed by filtration, and the filtrate was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4, concentrated by rotary evaporation, and purified through silica gel chromatography to obtain a white powder (0.319 g, 75% yield). ^{1}H NMR (600 MHz, $CDCl_3$) 1H NMR (400 MHz, CDCl3) δ 7.41 – 7.12 (m, 7H), 7.07 – 6.67 (m, 2H), 5.19 (s, 1H), 3.82 (s, 3H), 1.98 (s, 2H). ^{13}C{1H} NMR (100 MHz, CDCl3) δ 158.60, 145.80, 137.77, 128.52, 128.02, 126.84, 114.07, 113.89, 59.13, 55.29. HRMS (ESI+/QTOF) Calcd for $C_{14}H_{15}NO$ m/z: 214.1233; Found m/z 214.1230.

Synthesis of compound 11. 2-Chloro-5-nitrobenzoyl chloride (0.327 g, 1.5 mmol) was added to a mixture of compound **10** (0.273 g, 1 mmol) and K_2CO_3 (0.552 g, 4 mmol) in dry THF (10 mL) at 0 °C. After the mixture was stirred at 0 °C for 15 min and warmed up to room temperature over 8 h, water was added, followed by dichloromethane. The organic phase was washed with a 5% aqueous HCl solution (2 × 5 mL) and brine (2 × 5 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation to afford a yellow powder (0.475 g, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, J = 2.7 Hz, 1H), 8.55 (d, J = 2.7 Hz, 1H), 8.40 – 8.21 (m, 2H), 7.78 – 7.60 (m, 2H), 7.37 (dd, J = 3.5, 1.8 Hz, 2H), 7.35 – 7.31 (m, 2H), 7.25 (d, J = 7.1 Hz, 2H), 6.96 – 6.84 (m, 2H), 6.42 (d, J = 7.7 Hz, 1H), 3.80 (s, 3H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 163.28, 159.19, 146.61, 140.76, 137.53, 136.21, 133.17, 132.75, 131.47, 128.80 (d, *J* = 11.6 Hz), 128.58, 127.77, 127.32, 125.78, 57.66, 55.33. HRMS (ESI^+/QTOF) Calcd for $C_{21}H_{17}ClN_2O_4$ m/z: $[M+H]^+$ 397.0956; Found m/z 397.0950.

Synthesis of compound 12. Compound **11** (0.198 g, 0.5 mmol), ethylamine (0.2 mL, 3 mmol), K_2CO_3 (0.207 g, 1.5 mmol), and anhydrous THF (5 mL) were charged to a Schlenk tube. The sealed tube was heated to 120 °C overnight. After evaporation to dryness, the residue was combined with a 1 N HCl solution. The mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation. Purification by flash column chromatography (silica gel; using hexane/ethyl acetate = 10/1, v/v) provided the final product as a yellow powder (0.158 g, 86% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.41 (d, *J* = 2.6 Hz, 1H), 8.19 (ddd, *J* = 9.4, 2.6, 0.6 Hz, 1H), 7.42 – 7.31 (m, 5H), 7.28 – 7.19 (m, 2H), 6.99 – 6.88 (m, 2H), 6.71 (dd, *J* = 37.9, 8.3 Hz, 2H), 6.33 (d, *J* = 7.1 Hz, 1H), 3.83 (s, 3H), 3.25 (td, *J* = 7.2, 5.3 Hz, 2H), 1.33 – 1.31 (m, 3H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 167.24, 159.21, 154.43, 141.11, 135.09, 133.02, 128.91, 128.87, 128.77, 127.71, 127.28, 124.61, 114.31, 112.44, 110.78, 57.17, 55.34, 43.24, 14.11. HRMS (ESI^+/QTOF) Calcd for $C_{23}H_{23}N_3O_4$ m/z: $[M+H]^+$ 406.1768; Found m/z 406.1736.

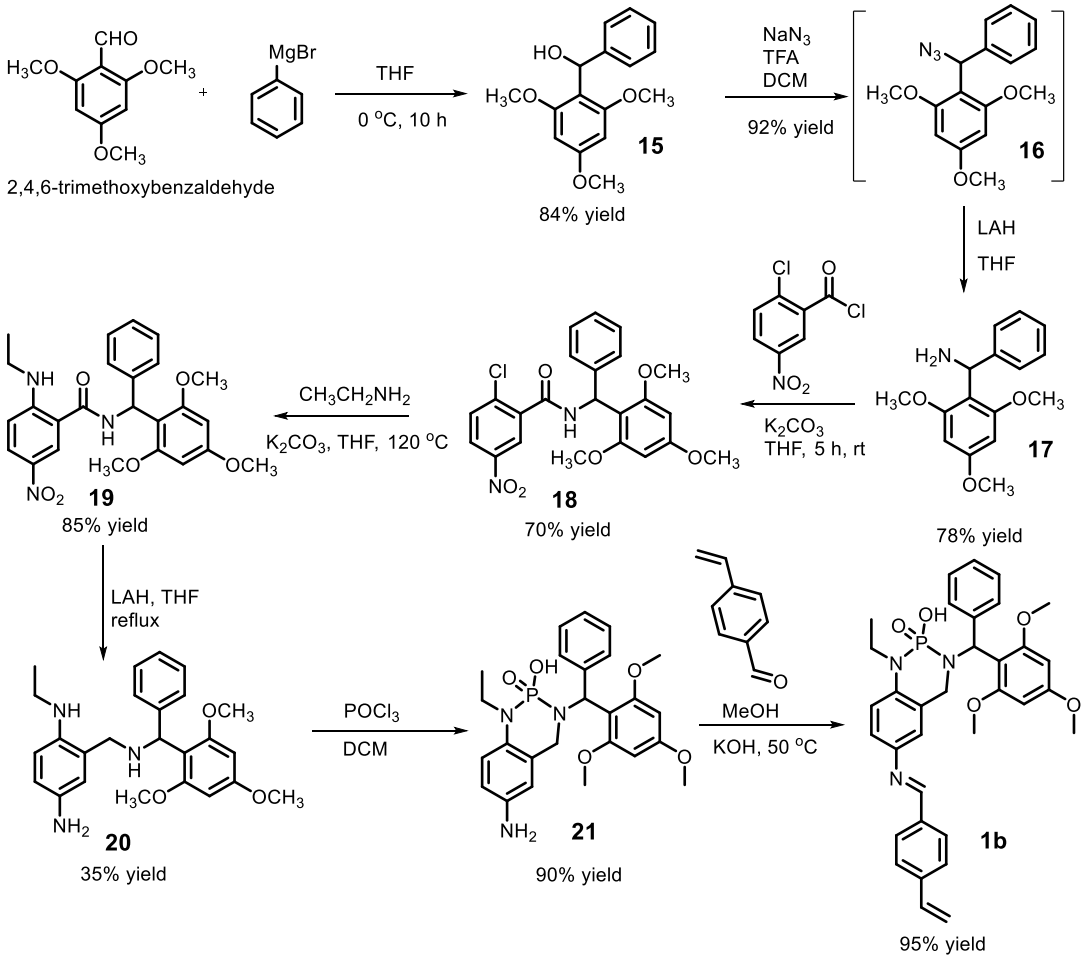
Synthesis of compound 13. Lithium aluminum hydride (0.195 g, 6 mmol) was added slowly to a stirred solution of compound **12** (0.203 g, 0.5 mmol) in anhydrous THF (5 mL) at 0 °C under

nitrogen. The reaction mixture was stirred for 10 h under reflux and then cooled to room temperature, followed by the addition of a saturated Na_2SO_4 solution. The mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation to afford a white powder (0.075 g, 42% yield). ^{1}H NMR (600 MHz, CDCl3) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 2H), 7.26 (d, *J* = 1.7 Hz, 1H), 7.25 (d, *J* = 1.8 Hz, 1H), 7.20 – 7.14 (m, 2H), 6.87 – 6.82 (m, 2H), 6.79 (d, *J* = 2.9 Hz, 2H), 6.74 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.58 (d, *J* = 8.7 Hz, 2H), 6.27 (d, *J* = 7.3 Hz, 1H), 5.26 (s, 1H), 3.76 (s, 3H), 3.74 (d, *J* = 0.9 Hz, 2H), 3.06 (dd, *J* = 7.9, 6.3 Hz, 2H), 1.18 (d, *J* = 7.1 Hz, 3H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 159.16, 154.38, 141.06, 135.05, 132.97, 128.86, 128.82, 128.73, 127.67, 127.24, 124.56, 114.26, 112.40, 110.73, 57.13, 55.29, 43.20, 31.75, 14.06. HRMS (ESI$^+$/QTOF) Calcd for $C_{23}H_{27}N_3O$ m/z: $[M+H]^+$ 362.2233; Found m/z 362.2230.

Synthesis of compound 14. Compound **13** (0.180 g, 0.5 mmol) was dissolved in dry dichloromethane (5 mL) at 0 °C, followed by slow addition of Et_3N (13 µL, 0.1 mmol) and $POCl_3$ (46 µL, 0.5 mmol). The reaction mixture was stirred for 10 h at room temperature, followed by the addition of saturated Na_2SO_4 solution. The mixture was extracted with dichloromethane (2 × 10 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation to afford a white powder (0.195 g, 92% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 2H), 7.26 (d, *J* = 1.7 Hz, 1H), 7.25 (d, *J* = 1.8 Hz, 1H), 7.16 (d, *J* = 8.6 Hz, 2H), 6.86 – 6.81 (m, 2H), 6.80 (s, 1H), 6.74 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.58 (d, *J* = 8.7 Hz, 1H), 6.27 (d, *J* = 7.3 Hz, 1H), 5.26 (s, 1H), 3.76 (s, 3H), 3.74 (d, *J* = 0.9 Hz, 2H), 3.06 (t, *J* = 7.9, 6.3 Hz, 2H), 1.18 (t, *J* = 7.1 Hz, 3H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 159.17, 154.28, 141.15, 135.17, 133.04, 128.90, 128.84, 128.79, 127.68, 127.30, 124.73, 114.27, 112.52, 110.69, 67.95, 57.22, 55.32, 37.79, 14.12. HRMS (ESI$^+$/QTOF) Calcd for $C_{23}H_{26}N_3O_3P$ m/z: $[M+H]^+$ 424.1791; Found m/z 424.1780.

Synthesis of compound 1. Compound **14** (0.084 g, 0.2 mmol) and 4-vinyl benzaldehyde (0.026 g, 0.2 mmol) were dissolved in dry MeOH (5 mL), followed by the addition of a catalytic amount of KOH (0.005 g, 0.01 mmol). The reaction mixture was stirred for 8 h at 50 °C. After completion of the reaction, the mixture was concentrated by rotary evaporation to dryness to afford a white powder (0.113 g) that was used directly in the preparation of the nanoparticle catalysts without further purification. ^{1}H NMR (600 MHz, CD_3OD) δ 8.57 (s, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.56 – 7.31 (m, 8H), 7.33-7.20 (m, 4H), 6.77 (dd, *J* = 8.0, 11.0 Hz, 5H), 5.91 – 5.76 (m, 1H), 5.27 (d, *J* = 7.5 Hz, 1H), 3.93 (s, 2H), 3.80 (s, 1H), 3.22 (t, *J* = 7.5 Hz, 2H), 1.39 (s, 3H). HRMS (ESI$^+$/QTOF) Calcd for $C_{32}H_{32}N_3O_3P$ m/z: $[M+H]^+$ 538.2260; Found m/z 538.2250.

Scheme S3. Synthesis of Template 1b



Synthesis of compound 15. A solution of 2,4,6-trimethoxybenzaldehyde (0.392 g, 2 mmol) in anhydrous THF (3 mL) was added to a flame-dried flask under nitrogen. After the solution was cooled to 0 °C, phenyl magnesium bromide (1.0 M solution in THF, 3 mL) was added dropwise over 10 min, and stirring was continued for 3 h. After the disappearance of the aldehyde by TLC, the reaction mixture was quenched with saturated ammonium chloride (5 mL). The crude reaction mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic phase was dried over Na_2SO_4 and concentrated by rotary evaporation. The residue was purified by column chromatography over silica gel using 10:1 hexane/ethyl acetate as the eluent to afford a white powder (0.460 g, 84% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.35 – 7.28 (m, 2H), 7.27 – 7.18 (m, 1H), 6.28 (d, *J* = 11.6 Hz, 1H), 6.20 (s, 2H), 3.85 (s, 3H), 3.80 (s, 6H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 160.71, 158.52, 145.21, 127.86, 126.37, 125.65, 112.37, 91.24, 68.28, 55.82, 55.38. HRMS (ESI$^+$/QTOF) Calcd for $C_{16}H_{18}O_4$ m/z: $[M+H]^+$ 275.1284; Found m/z 275.1280.

Synthesis of compound 17. A solution of compound **15** (0.548 g, 2 mmol) in anhydrous dichloromethane (5 mL) was treated with NaN_3 (0.325 g, 5 mmol) at room temperature and then cooled to −5 °C under nitrogen. A solution of trifluoroacetic acid (2.29 mL, 30 mmol) in dichloromethane (6 mL) was added dropwise and the mixture was stirred at −5 °C for 15 min and

then at 0 °C for another 12 h. Upon the completion of the reaction (indicated by TLC), water (10 mL) was added slowly to quench the reaction, followed by slow addition of a 14% ammonia solution (10 mL). After vigorously stirred for 30 min, the reaction mixture was allowed to warm to room temperature and extracted with dichloromethane (3 × 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated by vacuo to provide the crude azide intermediate **16**. A solution of the crude azide in ether (5 mL) was added dropwise to a suspension of lithium aluminum hydride (0.222 g, 6 mmol) in anhydrous ether (5 mL) at 0 °C under nitrogen. The reaction mixture was stirred at room temperature for 3 h and then quenched with 1 N NaOH solution (pH > 10). The insoluble solid was removed by filtration, and the filtrate was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4, concentrated by rotary evaporation, and purified through silica gel chromatography to obtain a white powder (0.425 g, 78% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 5.4 Hz, 3H), 7.36 – 7.29 (m, 2H), 6.19 (d, *J* = 19.2 Hz, 2H), 4.69 (s, 1H), 3.89 – 3.77 (m, 9H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 155.04, 152.76, 152.25, 148.22, 141.06, 128.52, 128.13, 127.85, 127.55, 126.96, 126.81, 118.62, 91.41, 65.19, 55.85, 55.54, 52.16. HRMS (ESI$^+$/QTOF) Calcd for $C_{16}H_{19}NO_3$ m/z: $[M+H]^+$ 274.1438; Found m/z 274.1494.

Synthesis of compound 18. 2-Chloro-5-nitrobenzoyl chloride (0.327 g, 1.5 mmol) was added to a mixture of compound **17** (0.273 g, 1 mmol) and K_2CO_3 (0.552 g, 4 mmol) in dry THF (10 mL) at 0 °C. After the mixture was stirred at 0 °C for 15 min and warmed up to room temperature over 8 h, water was added, followed by dichloromethane. The organic phase was washed with a 5% aqueous HCl solution (2 × 5 mL) and brine (2 × 5 mL), dried over Na_2SO_4, filtered, and concentrated by rotary evaporation to afford a yellow powder (0.319 g, 70% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 2.7 Hz, 1H), 7.95 (dd, *J* = 8.8, 2.8 Hz, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.28 – 7.22 (m, 3H), 5.82 (s, 2H), 4.95 (s, 1H), 3.70 (s, 9H). ^{13}C{1H} NMR (151 MHz, $CDCl_3$) δ 167.20, 160.87, 156.71, 145.04, 138.65, 137.30, 136.80, 130.64, 129.74, 127.68, 127.25, 124.14, 123.35, 111.27, 89.97, 55.32, 55.26, 51.15. HRMS (ESI$^+$/QTOF) Calcd for $C_{23}H_{21}ClN_2O_6$ m/z: $[M+H]^+$ 457.1161; Found m/z 457.1160.

Synthesis of compound 19. Compound **18** (0.228 g, 0.5 mmol), ethylamine (0.2 mL, 3 mmol), K_2CO_3 (0.207 g, 1.5 mmol), and anhydrous THF (5 mL) were charged to a Schlenk tube. The sealed tube was heated to 120 °C overnight. After evaporation to dryness, the residue was combined with a 1 N HCl solution. The mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation. Purification by flash column chromatography (silica gel; using hexane/ethyl acetate = 10/1, v/v) provided the final product as a yellow powder (0.196 g, 85% yield). ^{1}H NMR (600 MHz, CD_3OD) δ 8.05 – 7.83 (m, 2H), 7.36 – 7.17 (m, 5H), 6.95 (s, 1H), 6.62 (d, *J* = 9.3 Hz, 1H), 6.01 (s, 2H), 3.66 (d, *J* = 16.5 Hz, 9H), 3.24 (td, *J* = 4.9, 1.2 Hz, 2H), 1.31 (d, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (151 MHz, CD_3OD) δ 171.42, 161.00, 156.24, 151.67, 136.91, 134.88, 129.29, 127.34, 126.94, 126.68, 124.94, 124.74, 117.75, 112.65, 109.07, 90.17, 54.80, 54.46, 50.95, 37.25, 13.26. HRMS (ESI$^+$/QTOF) Calcd for $C_{25}H_{27}N_3O_6$ m/z: $[M+H]^+$ 466.1173; Found m/z 463.1170.

Synthesis of compound 20. Lithium aluminum hydride (0.195 g, 6 mmol) was added slowly to a stirred solution of compound **19** (0.231 g, 0.5 mmol) in anhydrous THF (5 mL) at 0 °C under nitrogen. The reaction mixture was stirred for 10 h under reflux and then cooled to room temperature, followed by the addition of a saturated Na_2SO_4 solution. The mixture was extracted

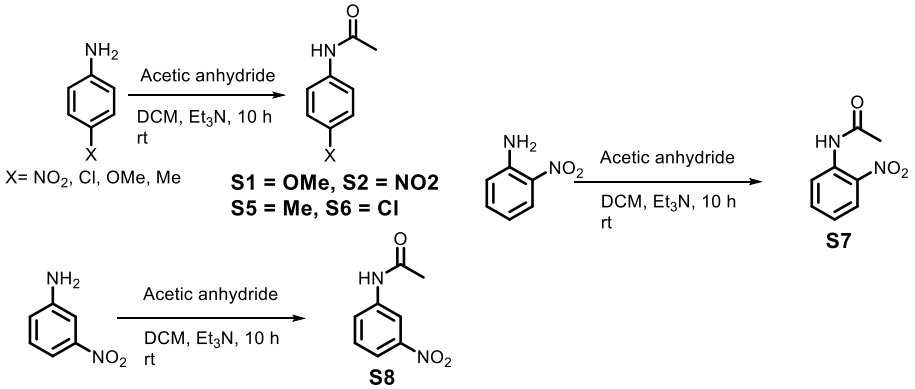
with ethyl acetate (3 × 20 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation to afford a white powder (0.078 g, 35% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 1H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.21 – 7.19 (m, 1H), 6.85 (dd, *J* = 9.5, 7.1 Hz, 3H), 6.60 – 6.56 (m, 1H), 6.30 (s, 1H), 3.77 (t, *J* = 5.3 Hz, 9H), 3.62 (s, 2H), 3.09 (t, *J* = 8.0 Hz, 2H), 1.38 – 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (151 MHz, CD_3OD) δ 160.38, 155.62, 151.05, 136.29, 134.26, 128.67, 126.72, 126.06, 124.31, 124.12, 117.13, 112.03, 108.44, 89.55, 54.18, 53.83, 50.33, 36.62, 12.64. HRMS (ESI$^+$/QTOF) Calcd for $C_{25}H_{31}N_3O_3$ m/z: $[M+Na]^+$ 444.2258; Found m/z 444.2231.

Synthesis of compound 21. Compound **20** (0.213 g, 0.5 mmol) was dissolved in dry dichloromethane (5 mL) at 0 °C, followed by slow addition of Et_3N (13 µL, 0.1 mmol) and $POCl_3$ (46 µL, 0.5 mmol). The reaction mixture was stirred for 10 h at room temperature, followed by the addition of saturated Na_2SO_4 solution. The mixture was extracted with dichloromethane (2 × 10 mL). The combined organic layer was dried over $MgSO_4$, filtered, and concentrated by rotary evaporation to afford a white powder (0.216 g, 90% yield). ^{1}H NMR (600 MHz, CD_3OD) δ 7.56 (s, 1H), 7.38 – 7.31 (m, 1H), 7.30 – 7.25 (m, 2H), 7.24 – 7.17 (m, 3H), 6.96 (s, 1H), 6.52 (d, *J* = 9.3 Hz, 1H), 5.91 (s, 2H), 4.62 (s, 1H), 3.72 (s, 2H), 3.69 (s, 3H), 3.60 (s, 6H), 3.29 (d, *J* = 7.2 Hz, 2H), 1.32 (d, *J* = 7.2 Hz, 3H). ^{13}C{1H} NMR (151 MHz, CD_3OD) δ 160.25, 155.73, 151.38, 136.40, 136.31, 134.56, 128.94, 127.77, 127.14, 126.74, 126.71, 126.69, 126.36, 125.09, 124.81, 117.15, 112.59, 108.69, 89.93, 54.84, 54.57, 51.03, 47.82, 47.67, 47.53, 37.10, 33.72, 13.50. HRMS (ESI$^+$/QTOF) Calcd for $C_{25}H_{30}N_3O_5P$ m/z: [M+] 483.1918; Found m/z 483.1956.

Synthesis of compound 1b. Compound **21** (0.096 g, 0.2 mmol) and 4-vinyl benzaldehyde (0.026 g, 0.2 mmol) were dissolved in dry MeOH (5 mL), followed by the addition of a catalytic amount of KOH (0.005 g, 0.01 mmol). The reaction mixture was stirred for 8 h at 50 °C. After completion of the reaction, the mixture was concentrated by rotary evaporation to dryness to afford a white powder (0.113 g) that was used directly in the preparation of the nanoparticle catalysts without further purification. ^{1}H NMR (600 MHz, CD_3OD) δ 8.57 (s, 1H), 7.71 (s, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.43 – 7.39 (m, 4H), 7.36 (m, 3H), 7.19 (d, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 7.3 Hz, 1H), 6.74 (t, *J* = 8.9 Hz, 2H), 6.47 (d, *J* = 7.9 Hz, 1H), 5.77 (d, *J* = 17.6 Hz, 1H), 5.21 (d, *J* = 10.7 Hz, 2H), 3.64 (s, 2H), 3.55 (d, *J* = 3.4 Hz, 9H), 3.08 (s, 2H), 1.50 – 1.33 (m, 3H). HRMS (ESI$^+$/QTOF) Calcd for $C_{34}H_{36}N_3O_5P$ m/z: $[M+H]^+$ 598.2465; Found m/z 598.2081.

Scheme S4. Synthesis of substrates

Syntheses of compounds **S3-S11** followed previously reported procedures.[5-7]



Typical procedure for the preparation of NP catalysts

To a micellar solution of surfactant **2** (9.3 mg, 0.02 mmol) in H_2O (2.0 mL) was added divinylbenzene (DVB) (2.8 μL, 0.015 mmol), template **1** in DMSO (10 μL of a 0.04 M solution, 0.0004 mmol), and 2,2-dimethoxy-2-phenylacetophenone (DMPA) in DMSO (10 μL of a 12.8 mg/mL solution, 0.0005 mmol). The mixture was sonicated for 10 min before cross-linker **3** (4.1 mg, 0.024 mmol), $CuCl_2$ in H_2O (10 μL of 6.7 mg/mL solution, 0.0005 mmol), and sodium ascorbate in H_2O (10 μL of 99 mg/mL solution, 0.005 mmol) were added and the reaction mixture was stirred slowly at room temperature for 12 h. Compound **4** (10.6 mg, 0.04 mmol), $CuCl_2$ in H_2O (10 μL of a 6.7 mg/mL solution, 0.0005 mmol), and sodium ascorbate in H_2O (10 μL of a 99 mg/mL solution, 0.005 mmol) were then added and the solution stirred for another 6 h at room temperature. The reaction mixture was transferred to a glass vial, purged with nitrogen for 15 min, sealed with a rubber stopper, and irradiated in a Rayonet reactor for 12 h. The progress of the reaction was monitored by ^{1}H NMR spectroscopy (Figure S7) and dynamic light scattering (DLS, Figures S8–10). The reaction mixture was poured into acetone (8 mL). The precipitate was collected by centrifugation and was washed with a mixture of 5 mL of acetone and 1 mL water (three times each), followed by methanol/acetic acid (5 mL/0.1 mL) three times. The solid was then rinsed with 5 mL of acetone (2 times) and was dried in air to afford off-white **NP1a**. Typical yields were >80%.[8]

The above obtained **NP1a** was sonicated in 2.0 mL of 6 N HCl aqueous solution for 20 min. The resulting solution was stirred at 95 °C for 2 h. After cooled down to room temperature, the reaction mixture was poured into acetone (8 mL). The precipitate formed was collected by centrifugation and washed with a mixture of acetone/water/methanol (5 mL/1 mL/1 mL) three times and acetone (5 mL) twice. The off-white product was dried in air to afford **NP**.[9, 10] The resulting **NP** (5 mg, 0.0001 mmol) was dissolved in 0.5 mL of dry DMF and was sonicated for 20 min. An aliquot of a stock solution of compound **5a**–**d** (10 μL of 0.1 M stock solution in DMSO, 0.001 mmol) was added. After the reaction mixture was stirred for 6 h at 50 °C, borane-pyridine complex (10 μL of 0.1 M in dry DMF, 0.001 mmol) was added. The reaction mixture was stirred at 50 °C overnight, cooled to room temperature, and poured into acetone (8 mL). The precipitate formed was collected by centrifugation and washed three times with a mixture of 5 mL of acetone and 1 mL of methanol, three times with methanol/HCl (5 mL/0.1 mL, 1 M), and twice with acetone (5 mL). The resulting solid was air-dried to give the final **NP(1)$_{5a–d}$** as an off-white powder. Typical yields were >75%.[9,10]

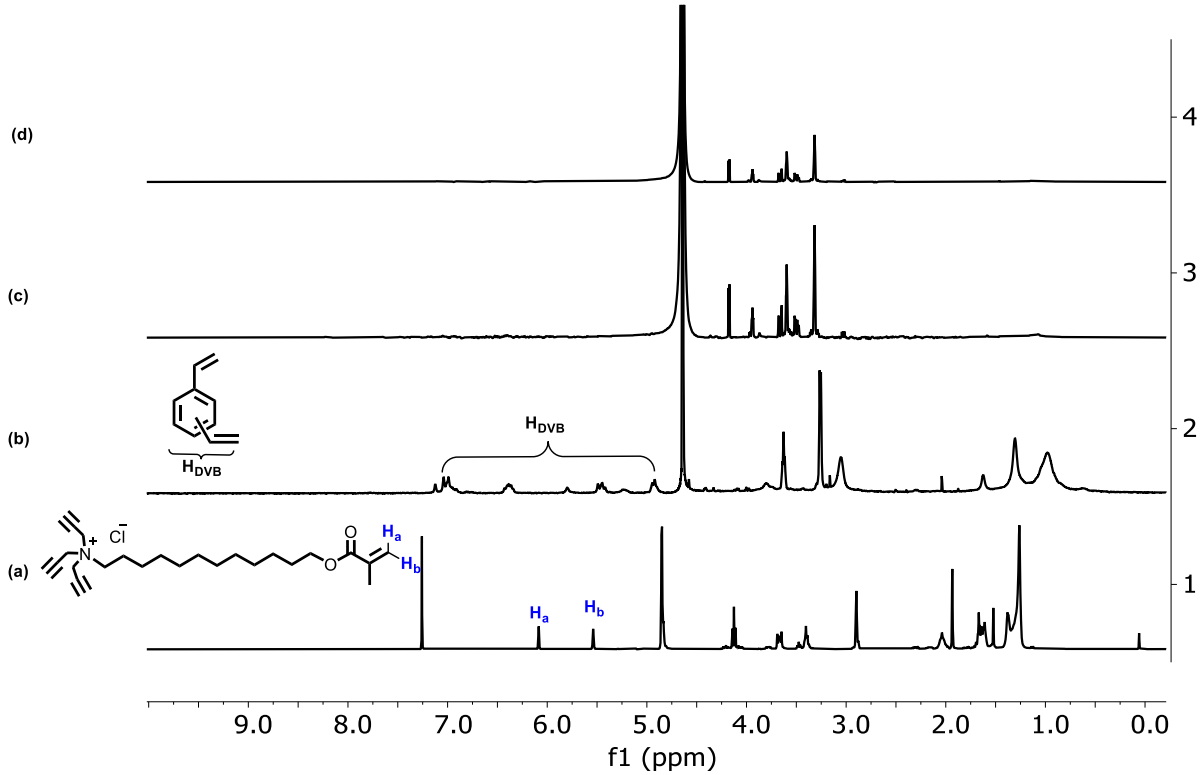


Figure S1. Stacked ^{1}H NMR spectra of (a) surfactant **2** in $CDCl_3$, (b) typical surface-cross-linked micelle (SCM) after diazide **3** cross-linking in D_2O, (c) typical SCM functionalized with ligand **4** in D_2O, and (d) typical **NP(1a)$_{5a}$** after washing and re-dissolving in D_2O.

Dynamic Light Scattering

The particle size of MINP was determined on a Malvern Zetasizer Nano ZS using the Zetasizer software according to the Stokes-Einstein equation (1). The volume of a spherical nanoparticle (V_{D_h}) was calculated from equation (2). Assuming a density of 1.37 g/cm^3 (the density of protein), the molecular weight of the particle can be calculated using equation (3).[11] A nanoparticle with a hydrodynamic diameter of 4.87 nm has a calculated molecular weight of 50 kDa, which was used in making MINP solution for ITC titration.

$$D_h = \frac{k_B T}{6\pi\eta D_t} \qquad (1)$$

in which D_h is the hydrodynamic diameter, D_t the translational diffusion coefficient measured by dynamic light scattering, T the temperature, k_B the Boltzmann's constant, and η is dynamic viscosity of water (0.890 cP at 298 K).

$$V_{D_h} = \frac{4\pi}{3}\left(\frac{D_h}{2}\right)^3 \qquad (2)$$

$$\text{Mw in dalton} = \left(\frac{D_h}{0.132}\right)^3 \qquad (3)$$

in which D_h is the hydrodynamic diameter in nm.

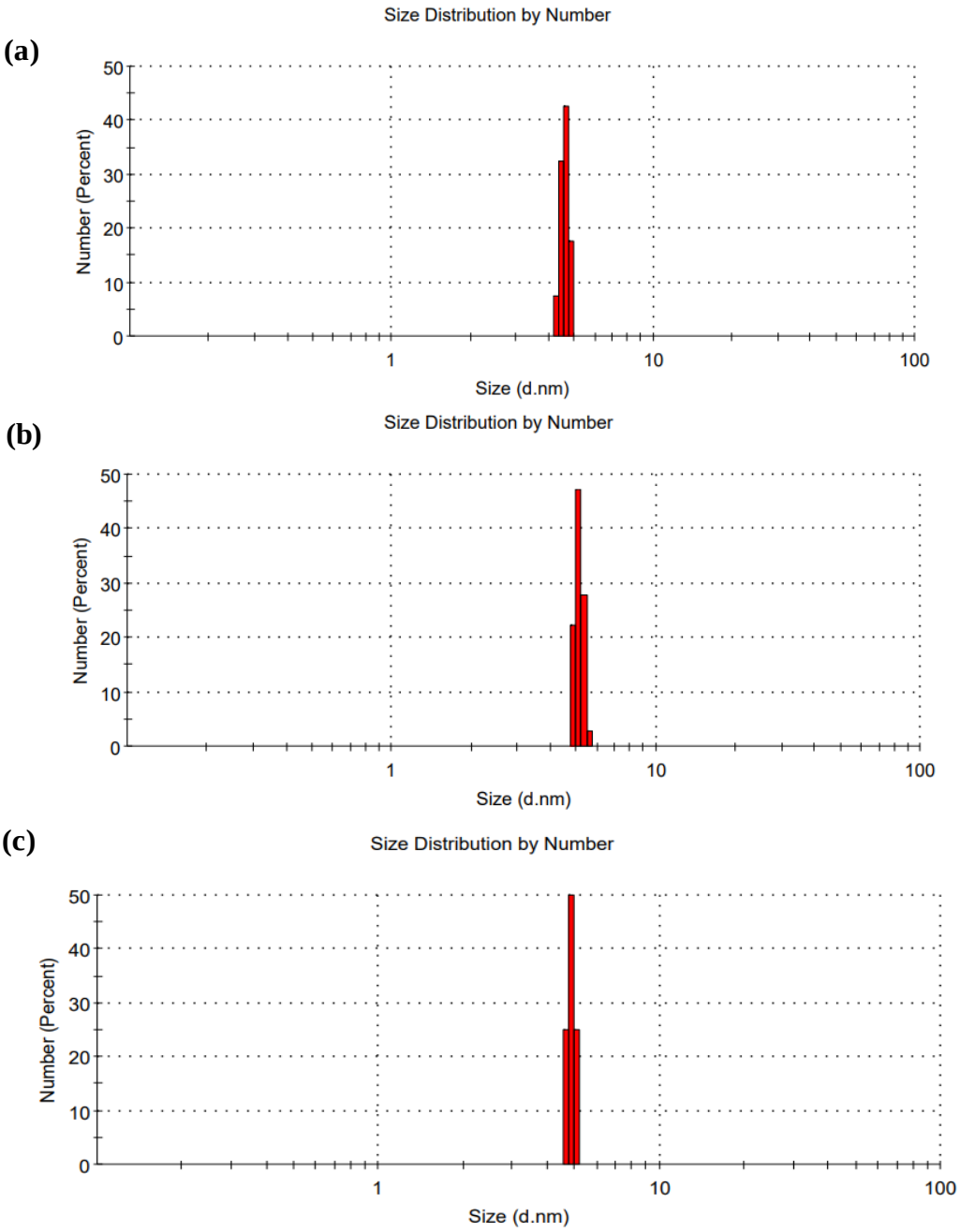


Figure S2. (a) Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for typical surface-cross-linked micelle (SCM) after diazide **3** cross-linking (Scheme 1, step a). D = 4.56 ± 0.11 nm. (b) Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for SCM functionalized with ligand **4** (Scheme 1, step b). D = 5.10 ± 0.10 nm. (c) Distribution of the hydrodynamic diameters of the nanoparticles in water as determined by DLS for **NP(1a)**$_{5a}$. D = 4.97 ± 0.18 nm.

Reactivity of 5a toward Substrates

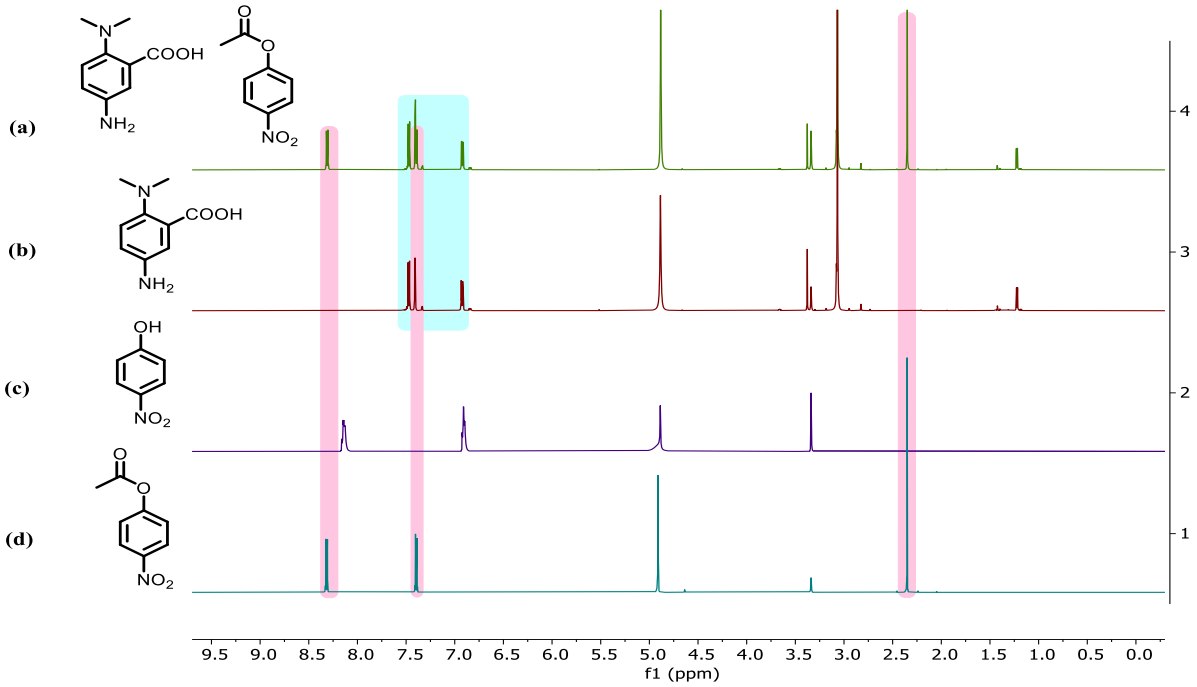


Figure S3. ^{1}H NMR spectra of (a) a 1:1 mixture of **5a** and *p*-nitrophenyl acetate (0.20 M) in CD_3OD after 24 h at room temperature, (b) compound **5a** in CD_3OD, (c) *p*-nitrophenol in CD_3OD and (d) compound *p*-nitrophenyl acetate (S1) in CD_3OD.

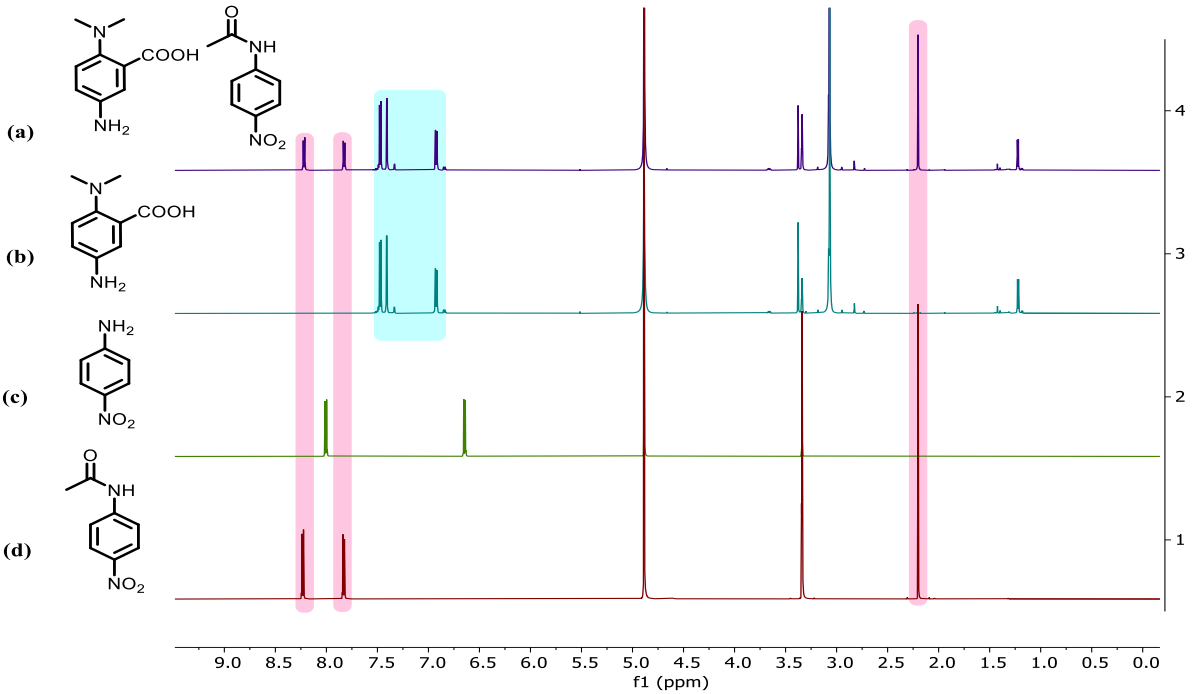


Figure S4. ^{1}H NMR spectra of (a) a 1:1 mixture of **5a** and **S1** (0.20 M) in CD_3OD after 24 h at room temperature, (b) compound **5a** in CD_3OD, (c) *p*-nitroaniline in CD_3OD and (d) compound **S1** in CD_3OD.

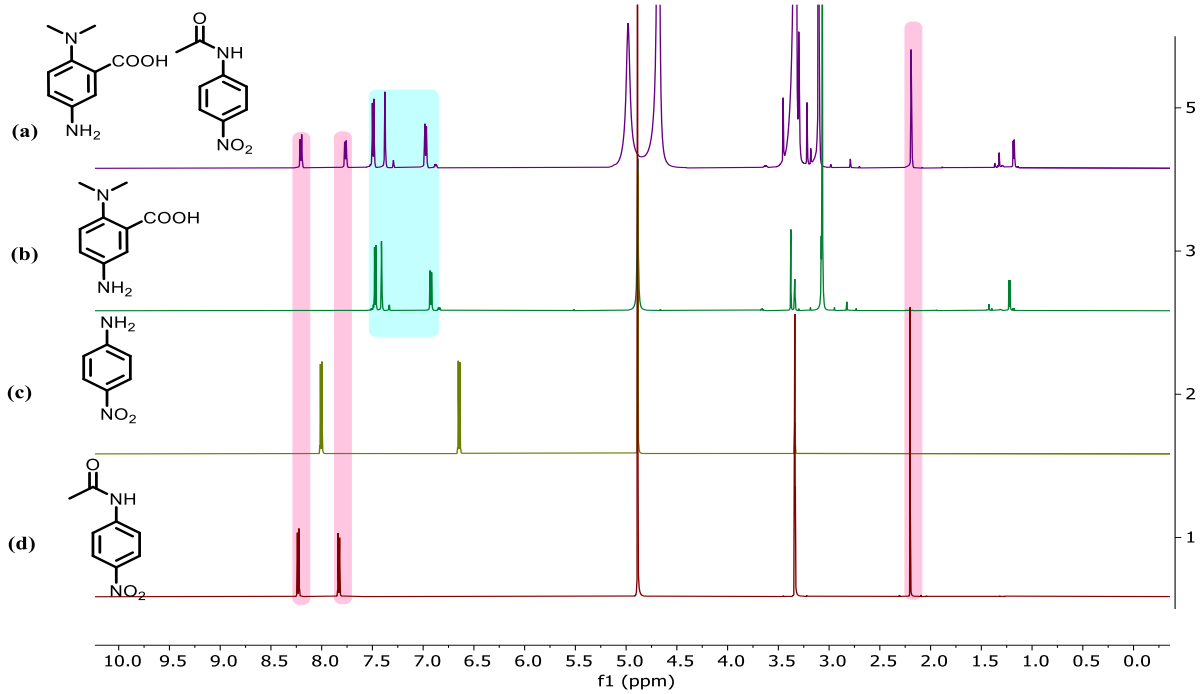


Figure S5. ^{1}H NMR spectra of (a) a 1:1 mixture of **5a** and **S1** (0.20 M) in D_2O after 24 h at room temperature, (b) compound **5a** in CD_3OD, (c) *p*-nitroaniline in CD_3OD and (d) compound **S1** in CD_3OD.

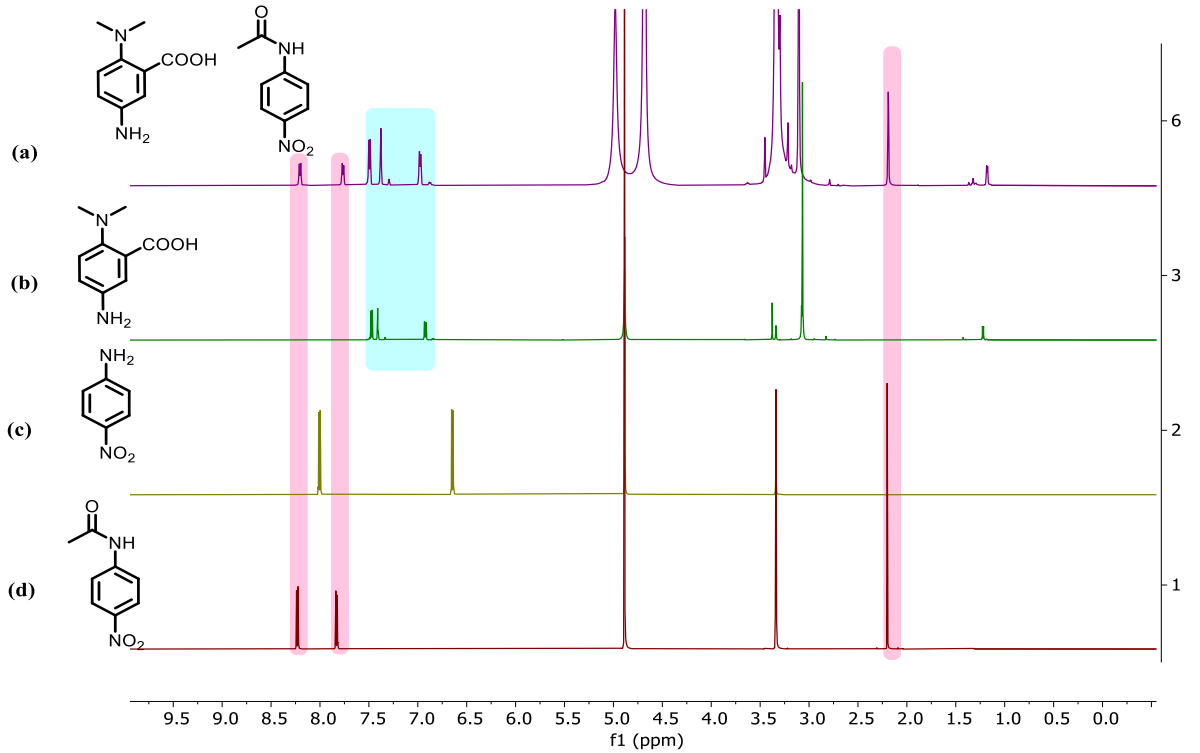


Figure S6. ^{1}H NMR spectra of (a) a 1:1 mixture of **5a** and **S1** (0.20 M) in D_2O after 24 h at 40 °C, (b) compound **5a** in CD_3OD, (c) *p*-nitroaniline in CD_3OD and (d) compound **S1** in CD_3OD.

Kinetic Measurements

Stock solutions (10 mM) of aryl esters in methanol were prepared and used freshly. Stock solutions of the appropriate catalytic NPs (100 μM) in a 25 mM HEPES buffer (pH 7.0.) were prepared. For the kinetic experiment, a typical procedure is as follows: An aliquot of 300 μL of the above NP stock solution was combined with 1690 μL of the same buffer in a cuvette. The cuvette was placed in a UV-vis spectrometer and equilibrated to 40.0 °C. After 5 min, an aliquot of 10 μL of the ester stock solution was added. The amount of the product formed was calculated from a calibration curve obtained from the corresponding phenols.

Hammett σ–ρ correlation

The hydrolysis of para-substituted-phenyl acetates was performed at 25 °C following the typical procedure as described above.[12]

Table S1. **Hammett σ–ρ correlation in the hydrolysis of *para*-substituted-phenyl acetates catalyzed by NP(1b)$_{5a}$.**

entry	substrates	σ	k ($\times 10^{-4}$ s^{-1})[a]
1	*p*-NO_2	1	40 ± 8.5
2	*p*-CH_3CO	0.52	5.2 ± 2.0
3	*p*-Cl	0.23	2 ± 1.0
4	*p*-CHO	0.22	3 ± 1.5
5	*H*	0.00	1.5 ± 1.0
6	*p*-CH_3	0.17	0.8 ± 0.5

[a] Reaction rates were measured in HEPES buffer (at pH 7.0) at 25 °C and [substrate] = 50 μM. [catalyst- NP(1b)$_{5a}$] = 10 μM.

Catalytic Turnover Number (TON)

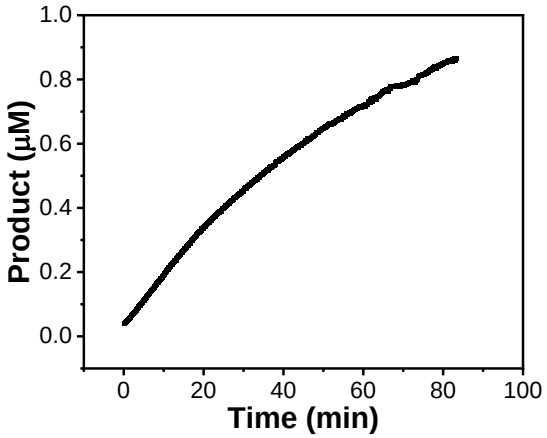


Figure S7. Amount of *p*-nitrophenoxide formed as a function of time in a 25 mM HEPES buffer at 40 °C and pH 7.0. [substrate] = 100 μM. [**NP(1b)$_{5a}$** catalyst] = 0.1 μM. TON = 949.

Table S2. Solvent isotope effect

entry	catalyst	system	k (× 10^{-4} s^{-1})[a]	k_{H2O}/k_{D2O}
1	**NP(1b)$_{5a}$**	D_2O	66 ± 0.5	1.06
2	**NP(1b)$_{5a}$**	H_2O	70 ± 1.5	

[a] Reaction rates were measured in HEPES buffer (at different pH) at 40 °C and [substrate] = 50 μM. [catalyst-MINP] = 10 μM. The pD values were determined by adding 0.4 to the pH meter reading.

LC-MS Characterization of Hydrolysis Products

In a typical procedure, a reaction mixture containing *p*-substituted phenylacetamide (50 μM) and the catalyst (10 μM) in 1.0 mL of buffer was incubated at the indicated temperature for 20 h. After cooled to room temperature, the reaction mixture was centrifuged at 20,000 RPM for 10 min to remove the nanoparticle catalyst before LC-MS analysis. Analysis of reaction mixture after hydrolysis was performed by LC-MS analysis using an Agilent 1200 Series Binary VWD system with an Agilent 6540 UHD Accurate Mass Q-TOF mass detector. Separation of the products was performed on a Thermo Scientific C18-LC column (4.6 mm, 150 mm) at 40 °C. For quantitative analysis, injection volumes were adjusted for the signal intensity to stay within the linear range of the calibration curve. All samples were centrifuged at 20,000 RPM before analysis to remove the nano particles (to avoid column blockage over extended usage). Comparison with non-centrifuged samples showed no change in substrate concentration during the centrifugation step. The mobile phase was a mixture of acetonitrile and water, with 0.1% formic acid. Product peaks were identified by a high-resolution mass detector in the positive ion mode.

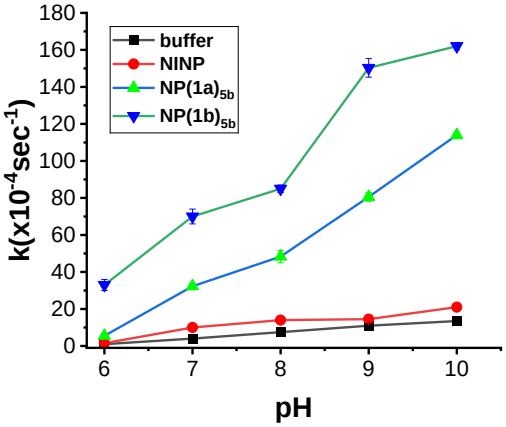


Figure S8. (a, b) pH profile for the hydrolysis of *p*-nitrophenyl acetate under different pH conditions. NINP is the nonimprinted nanoparticle prepared without the template and is used as the control. All the reactions were performed in HEPES buffer at 40 °C with [substrate] = 50 μM and [NP(1a-b)$_{5b}$] = [NINP] = 10 μM.

Calibration for substrates

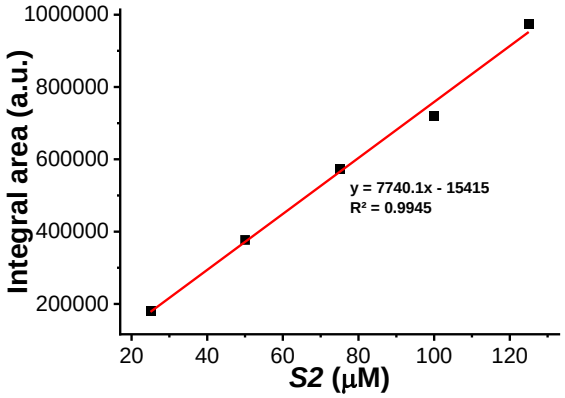


Figure S9. Calibration curve of compound **S2** generated from authentic samples by LC-MS.

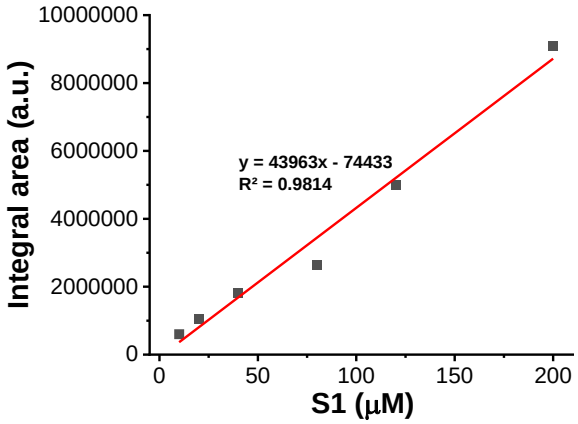


Figure S10. Calibration curve of compound **S1** generated from authentic samples by LC-MS.

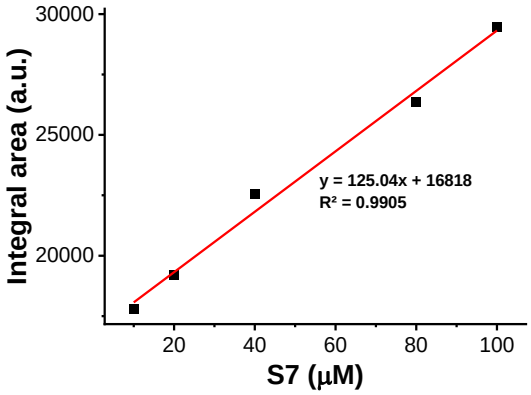


Figure S11. Calibration curve of compound **S7** generated from authentic samples by LC-MS.

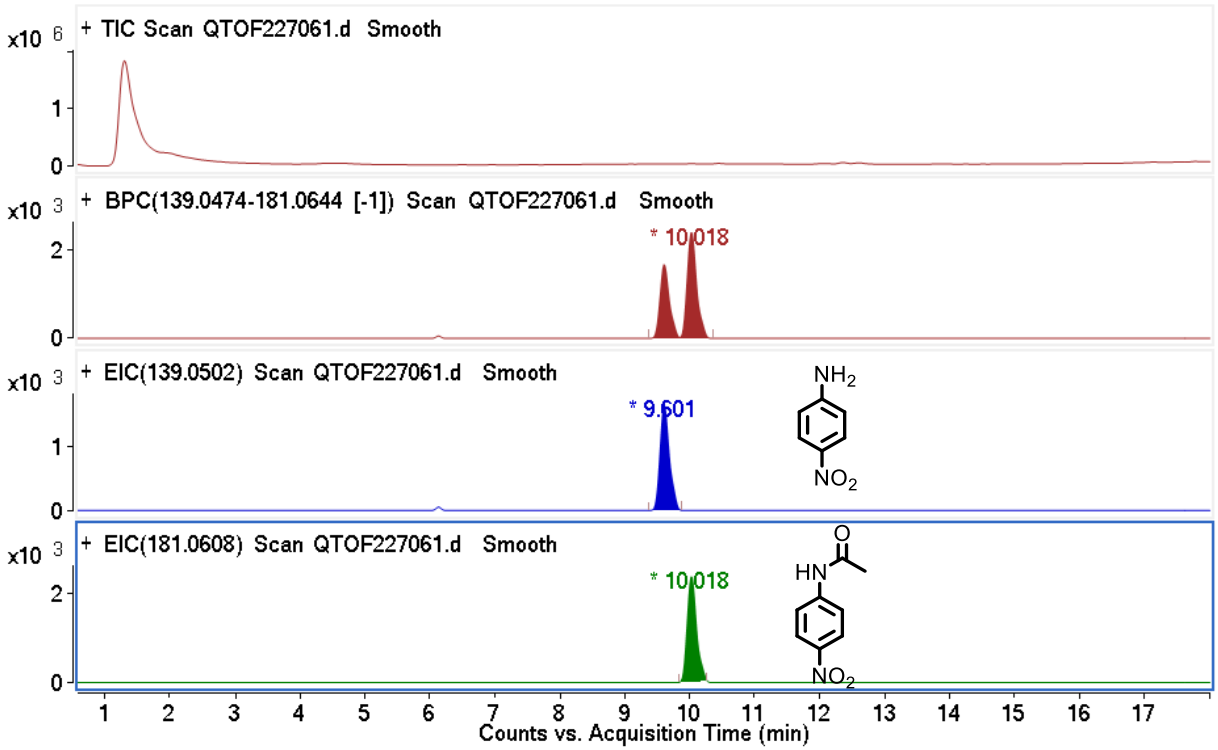


Figure S12. A representative LC-MS trace for the reaction mixture of substrate **S2** hydrolysis catalyzed by **NP(1b)**$_{5b}$ at 40 °C for 24 h. Extracted ion chromatography (EIC) spectra indicate that *p*-nitroaniline (blue) was observed at 9.6 min and substrate **S2** (green) at 10.0 min. The experiments were repeated three times and gave similar results.

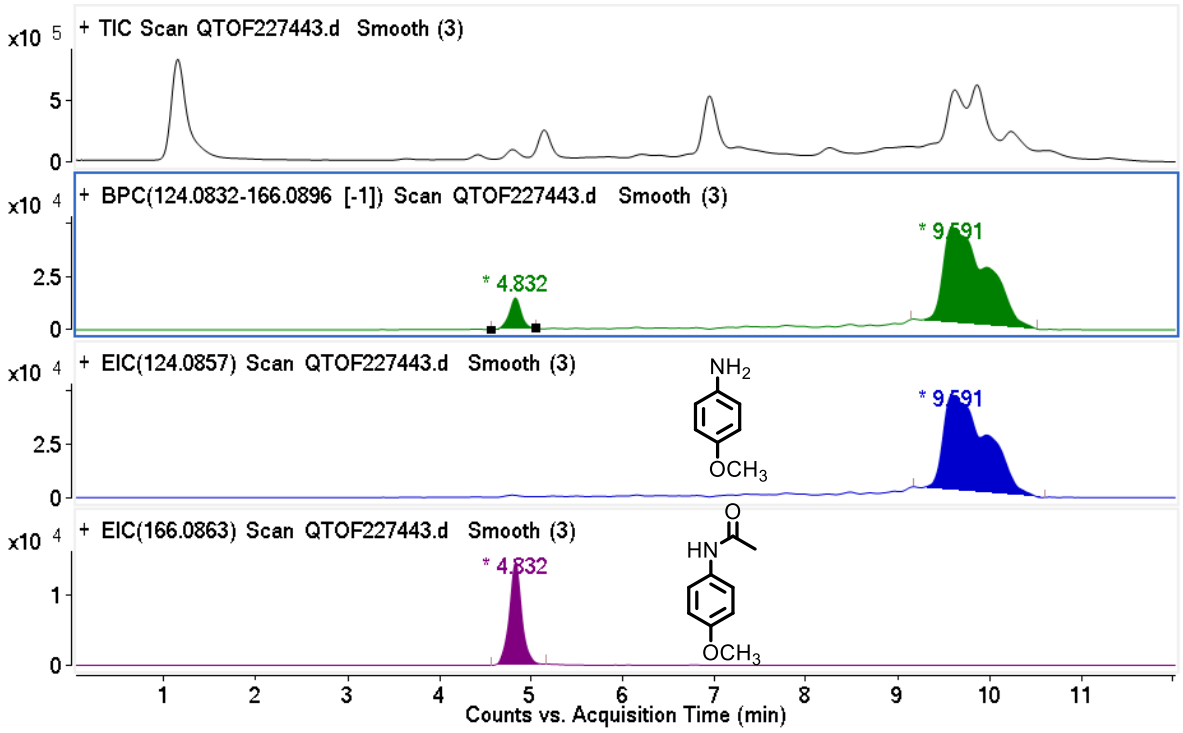


Figure S13. A representative LC-MS trace for the reaction mixture of substrate **S1** hydrolysis catalyzed by NP(**1b**)$_{5a}$ at 40 °C for 24 h. Extracted ion chromatography (EIC) spectra indicate that *p*-nitroaniline (blue) was observed at 9.5 min and substrate **S1** (purple) at 4.8 min. The experiments were repeated three times and gave similar results.

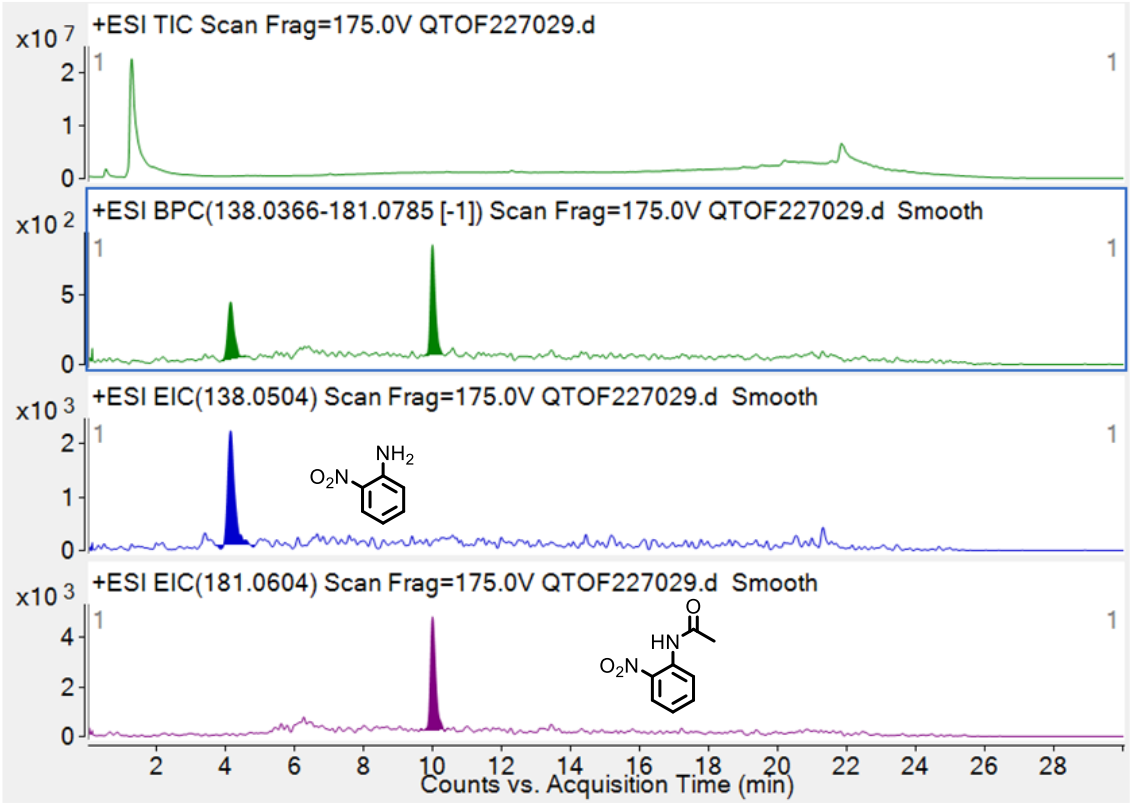


Figure S14. A representative LC-MS trace for the reaction mixture of substrate **S7** hydrolysis catalyzed by NP(**1b**)$_{5a}$ at 40 °C for 24 h. Extracted ion chromatography (EIC) spectra indicate that *p*-nitroaniline (blue) was observed at 4.18 min and substrate **S7** (purple) at 10.01 min. The experiments were repeated three times and gave similar results.

HPLC Characterization of Hydrolysis Products

In a typical procedure, a reaction mixture containing substituted phenylacetamide (50 µM) and the catalyst (10 µM) in 1.0 mL of buffer was incubated at indicated temperatures for 24 h. After cooled to room temperature, the reaction mixture was centrifuged at 20,000 RPM for 10 min to remove the nanoparticle catalyst before HPLC analysis. Analysis of reaction mixture after hydrolysis was performed by HPLC analysis using Waters HPLC system. Separation of the products was performed on a Xbridge analytical OBD C18 (5 µm, 30x250mm) column on a Waters HPLC system equipped with detection using a Waters 2998 Photodiode Array Detector. For quantitative analysis, injection volumes were adjusted for the signal intensity to stay within the linear range of the calibration curve. All samples were centrifuged at 20,000 RPM before analysis to remove the nano particles (to avoid column blockage over extended usage). Comparison with non-centrifuged samples showed no change in substrate concentration during the centrifugation step. The mobile phase was a mixture of acetonitrile and water, with 0.1% TFA.

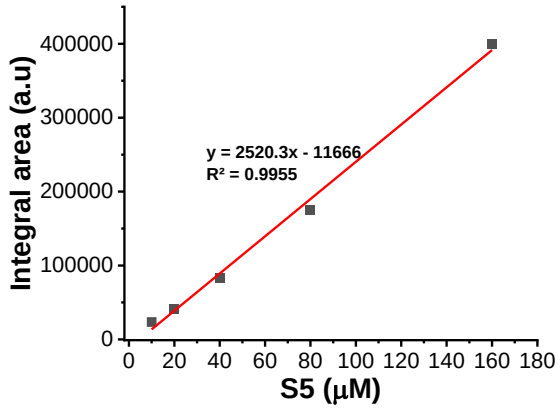


Figure S15. Calibration curve of compound **S5** generated from authentic samples by HPLC.

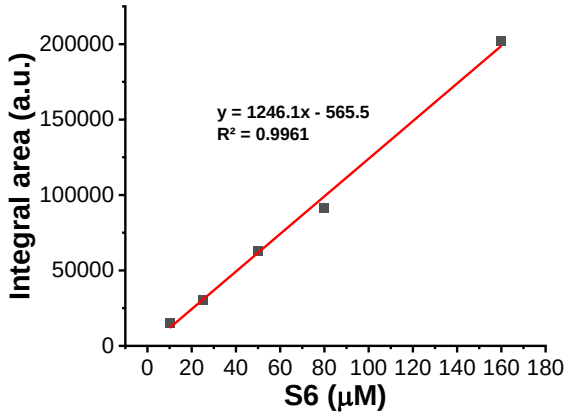


Figure S16. Calibration curve of compound **S6** generated from authentic samples by HPLC.

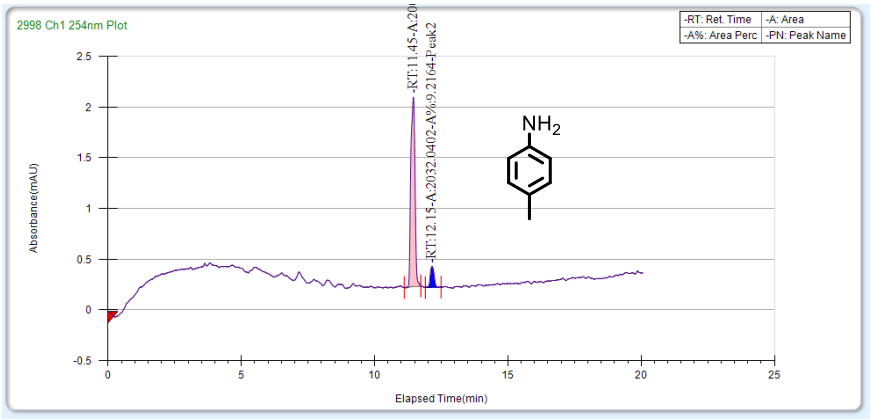


Figure S17. A representative HPLC trace for the reaction mixture of substrate **S5** hydrolysis catalyzed by NP(**1b**)$_{5a}$ at 40 °C for 24 h. HPLC spectra indicate that *p*-methylaniline (blue) was observed at 12.15 min and substrate **S5** (red) at 11.45 min. The experiments were repeated three times and gave similar results.

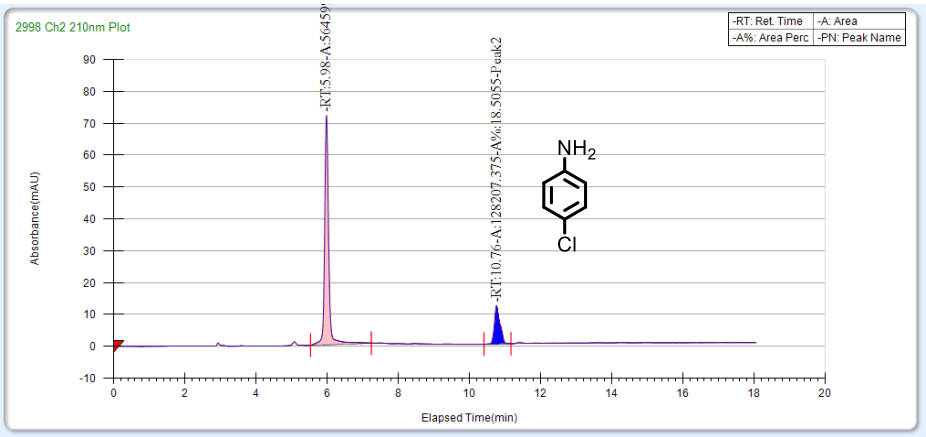


Figure S18. A representative HPLC trace for the reaction mixture of substrate **S6** hydrolysis catalyzed by NP(**1b**)$_{5a}$ at 40 °C for 24 h. HPLC spectra indicate that *p*-chloroaniline (blue) was observed at 10.76 min and substrate **S6** (red) at 5.98 min. The experiments were repeated three times and gave similar results.

Screening of various Nanoparticles (NPs)

In a typical procedure, a reaction mixture containing compound **S3** (50 µM) and the catalysts (10 µM) in 1.0 mL of buffer was incubated at 40 °C temperatures for 20 h. After cooled to room temperature, the reaction mixture was centrifuged at 20,000 RPM for 10 min to remove the nanoparticle catalyst before LC-MS analysis. All samples were centrifuged at 20,000 RPM before analysis to remove the nano particles (to avoid column blockage over extended usage). Comparison with non-centrifuged samples showed no change in substrate concentration during the centrifugation step. The mobile phase was a mixture of acetonitrile and water, with 0.1% formic acid. Product peaks were identified by a high-resolution mass detector in the positive ion mode.

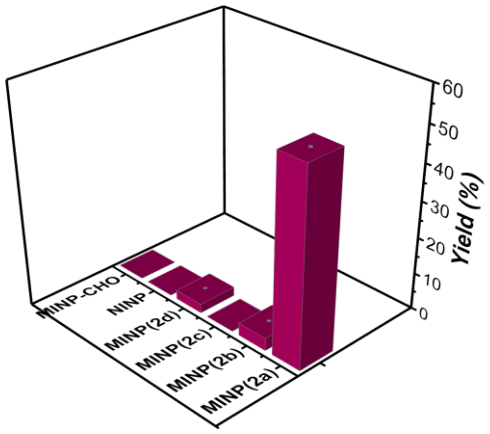


Figure S19. Selectivity of alcohol functionalized monomers of NP for amide hydrolysis of **S3** [10 µM catalyst- NP(**1b**)$_{5a}$ and substrate 50 µM] in 1 mL in HEPES buffer pH 7.4 at 40 °C for 24 h. The yields were determined by LC-MS analysis.

Michaelis-Menten Kinetics for PNPA Substrate

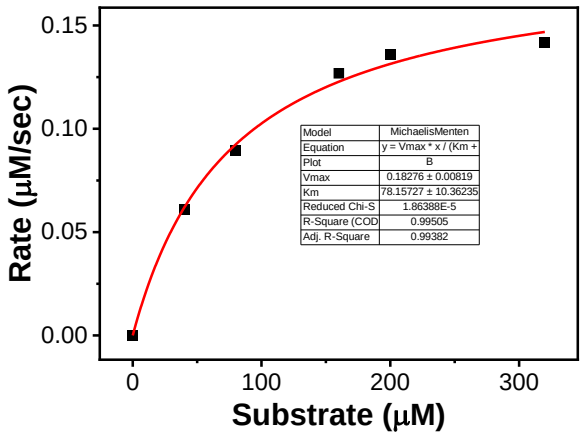


Figure S20. Michaelis–Menten plot of the hydrolysis of *p*-nitrophenyl acetate by **NP(1b)$_{5a}$** in a 25 mM HEPES buffer at 40 °C and pH 7.0. [NP] = 8.0 μM.

NMR Spectra of Key Compounds

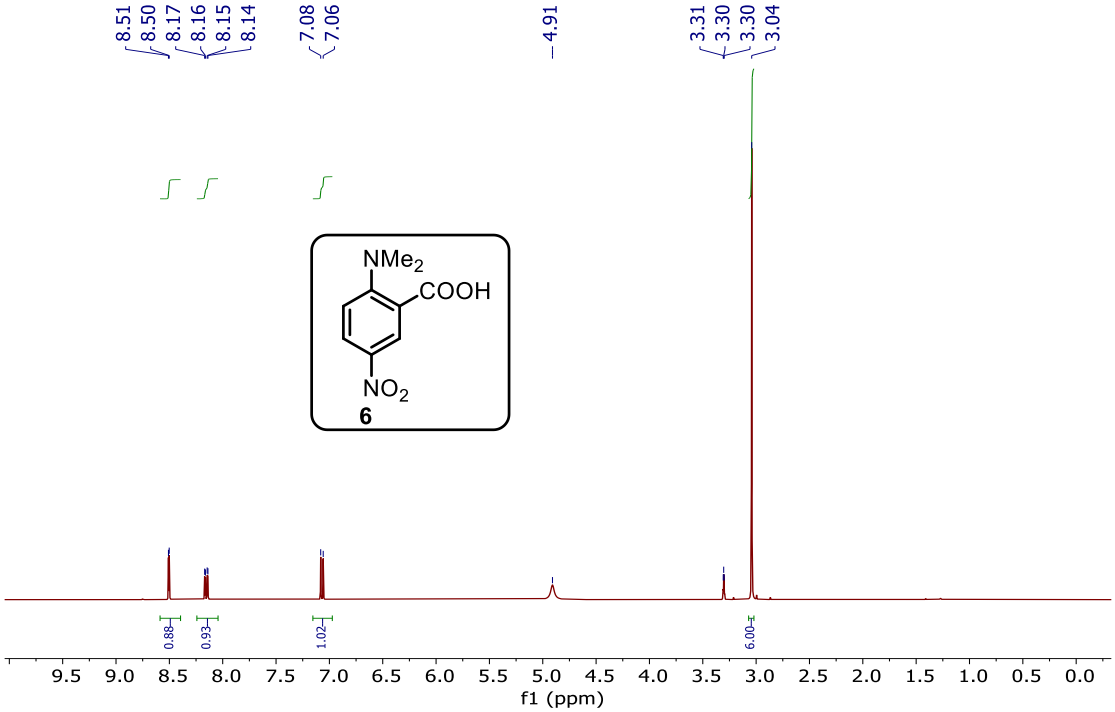


Figure S21. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **6** in CD_3OD.

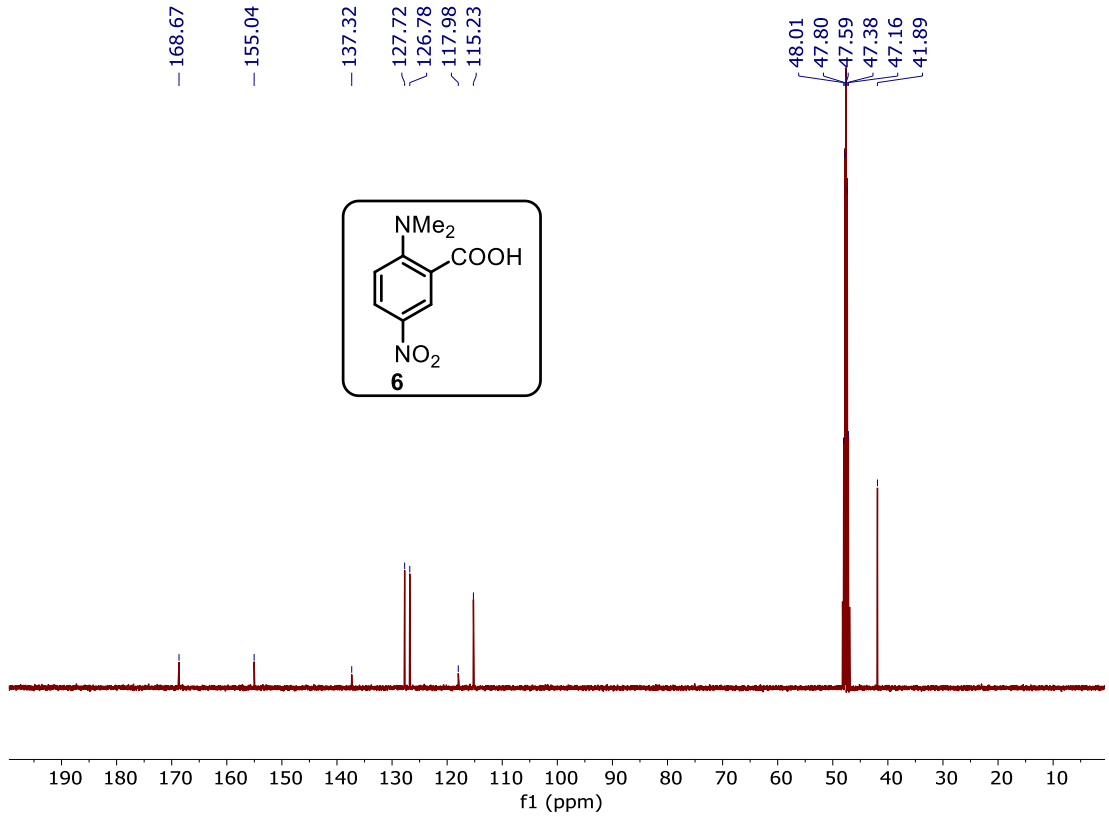


Figure S22. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **6** in CD_3OD.

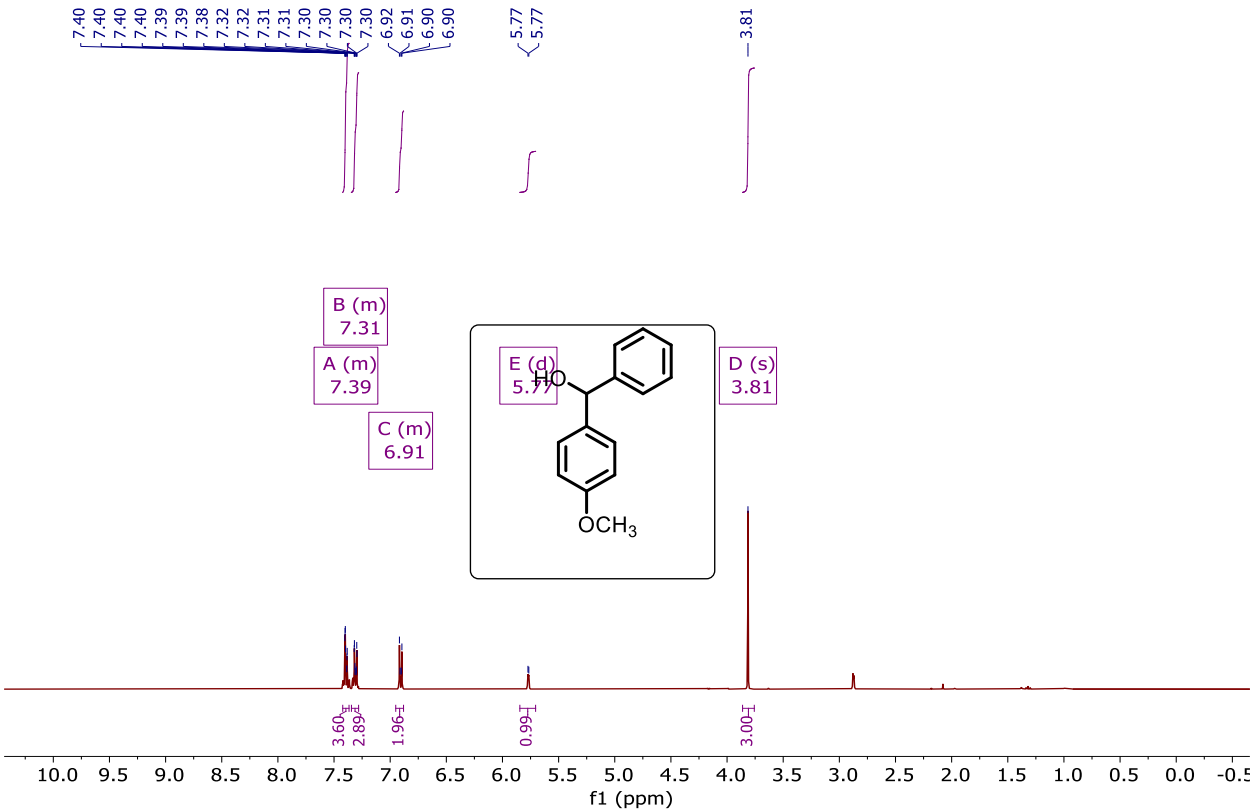


Figure S23. ^{1}H NMR(400 MHz, $CDCl_3$) spectrum of compound **8** in $CDCl_3$.

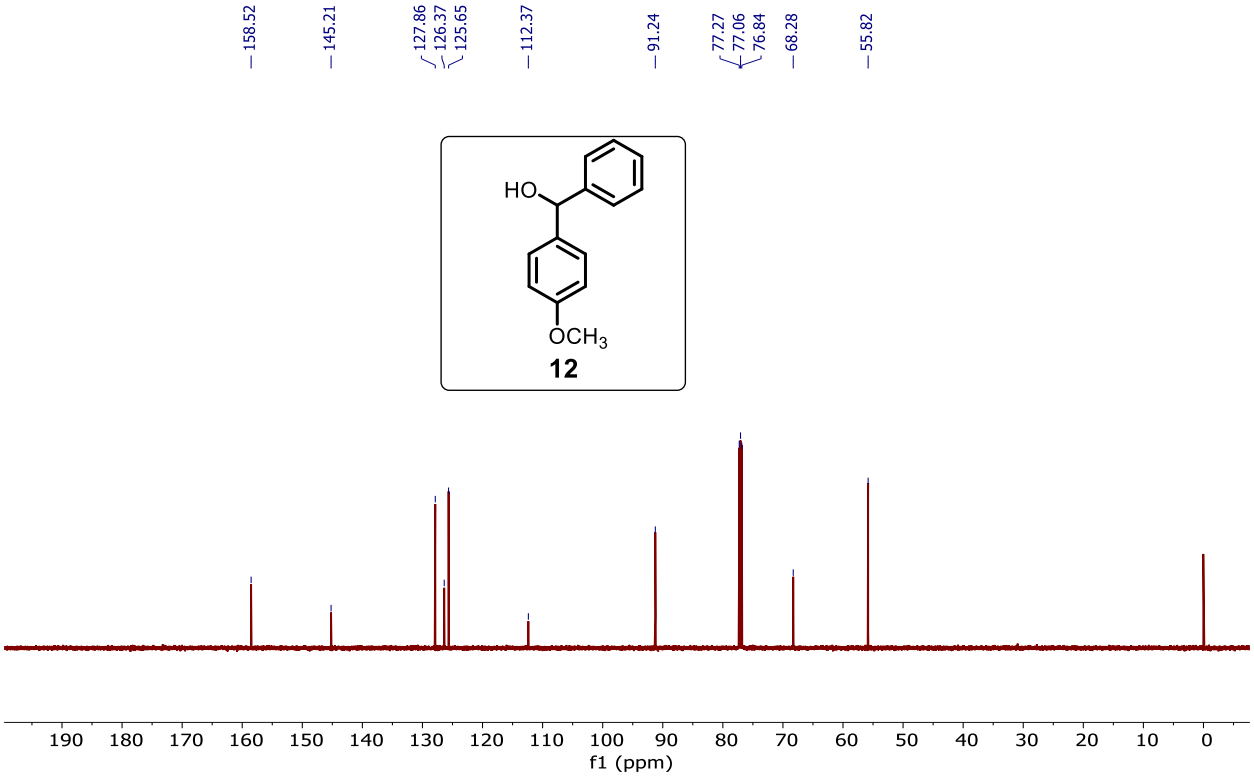


Figure S24. ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectrum of compound **8** in $CDCl_3$.

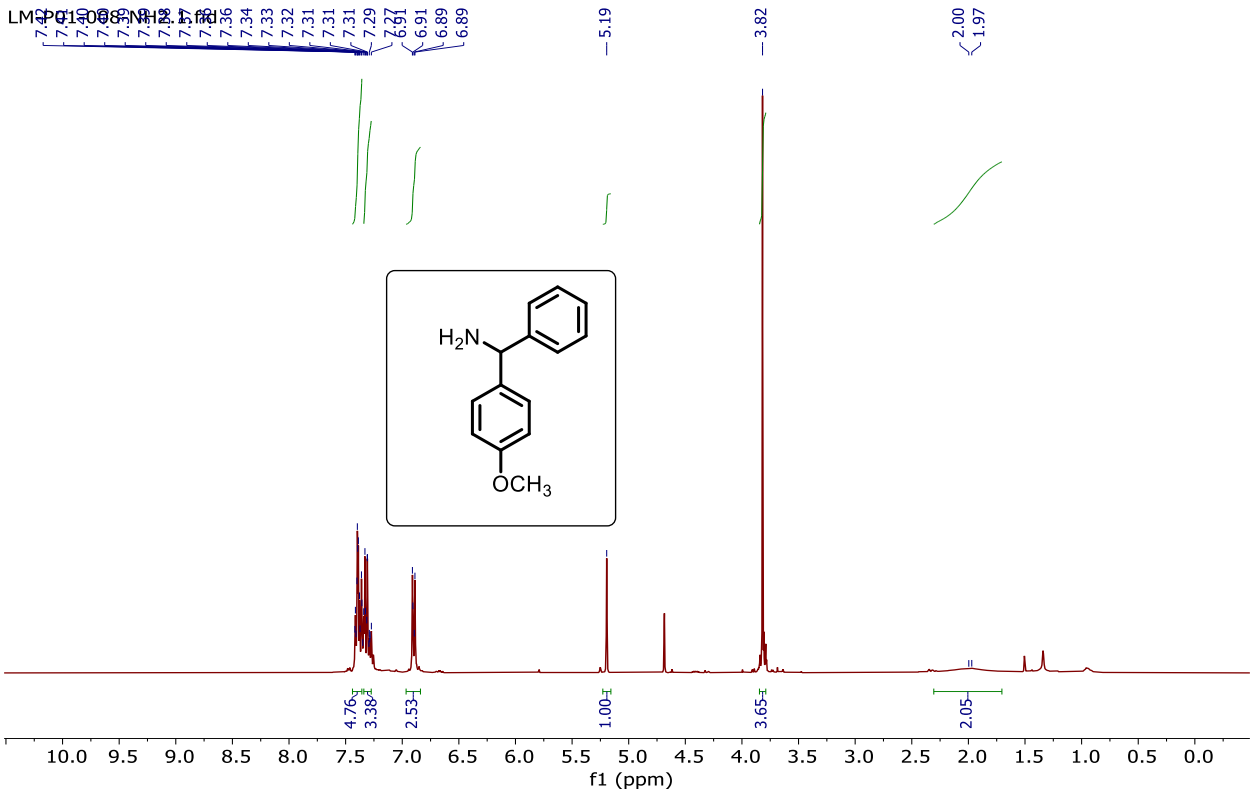


Figure S25. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **10** in $CDCl_3$.

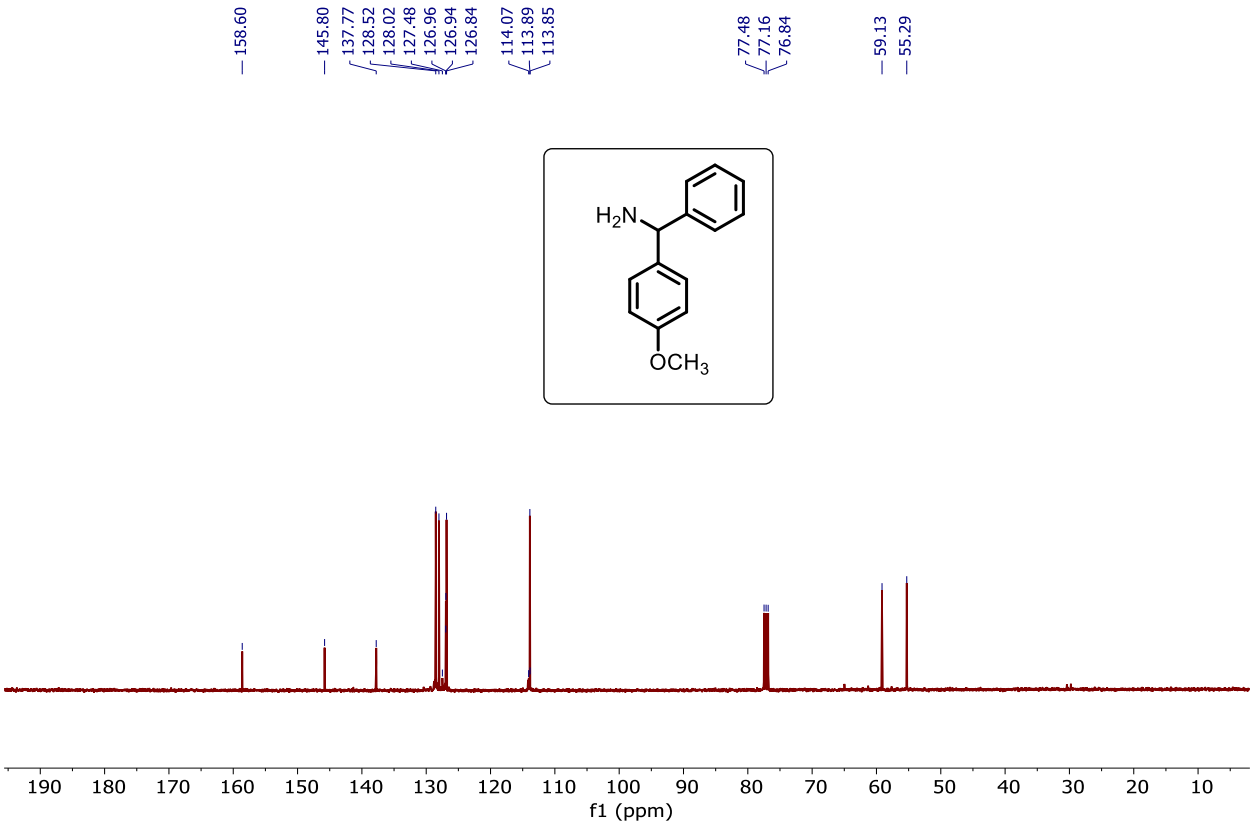


Figure S26. ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectrum of compound **10** in $CDCl_3$.

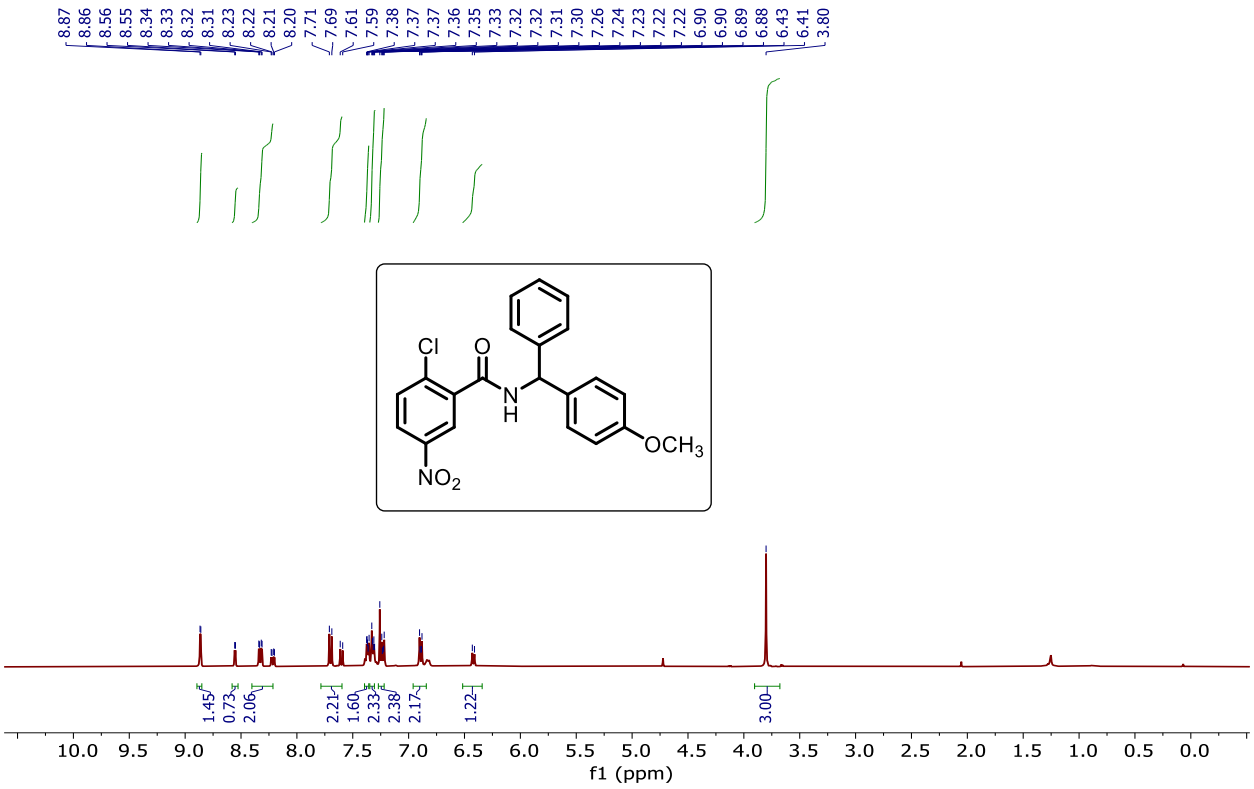


Figure S27. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11** in $CDCl_3$.

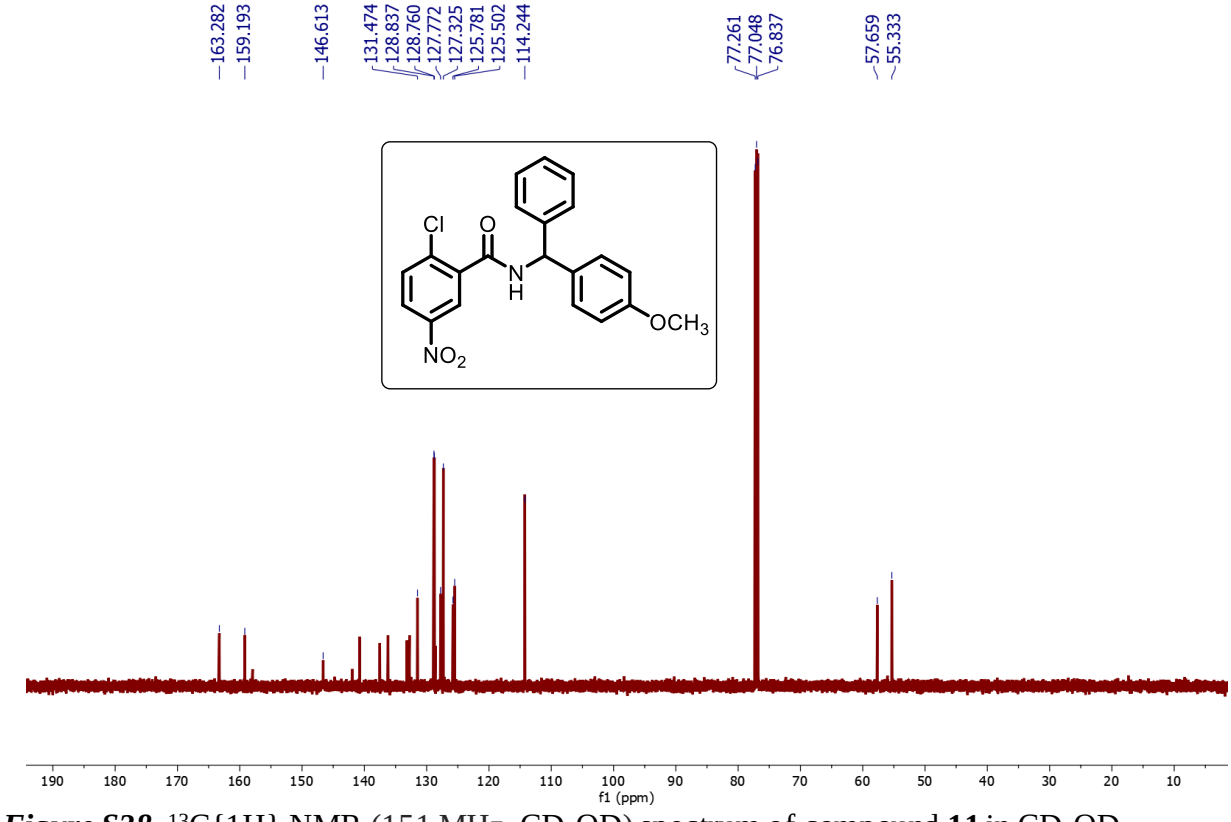


Figure S28. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **11** in CD_3OD.

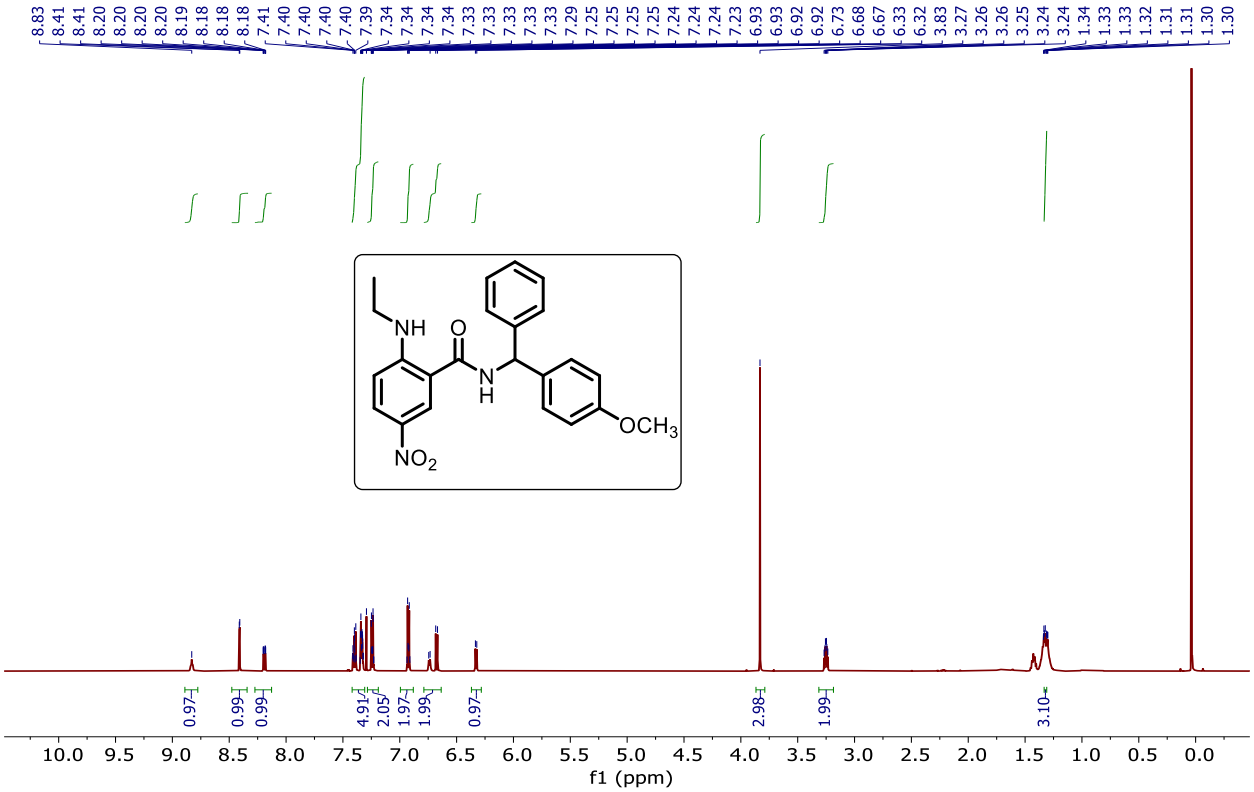


Figure S29. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **12** in $CDCl_3$.

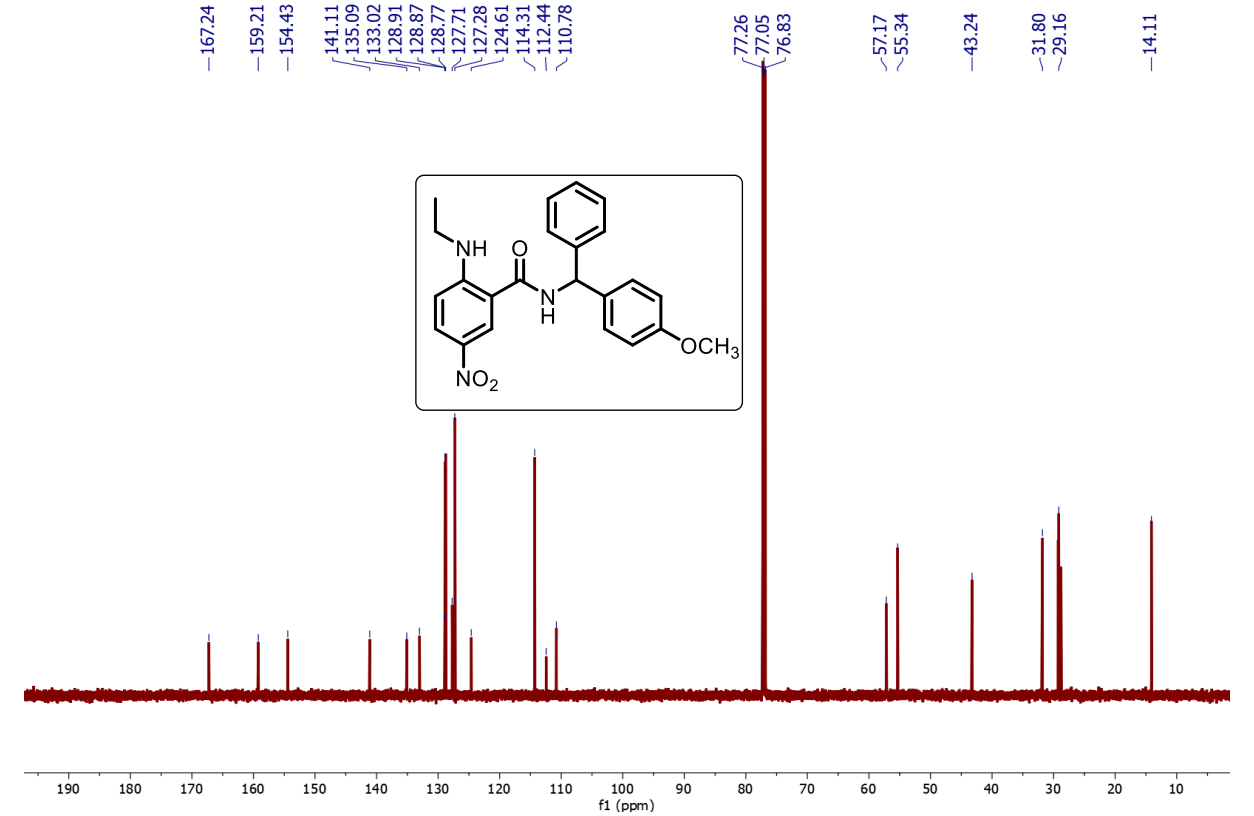


Figure S30. ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectrum of compound **12** in $CDCl_3$.

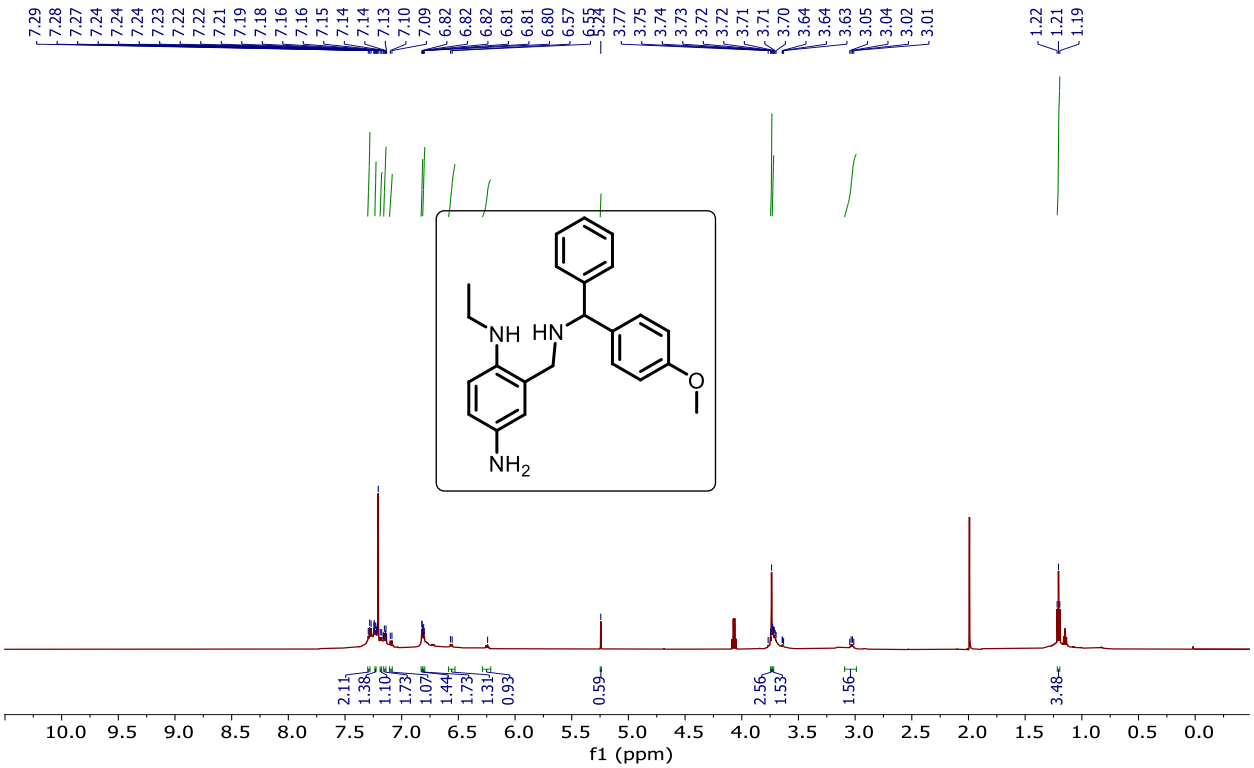


Figure S31. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **13** in $CDCl_3$.

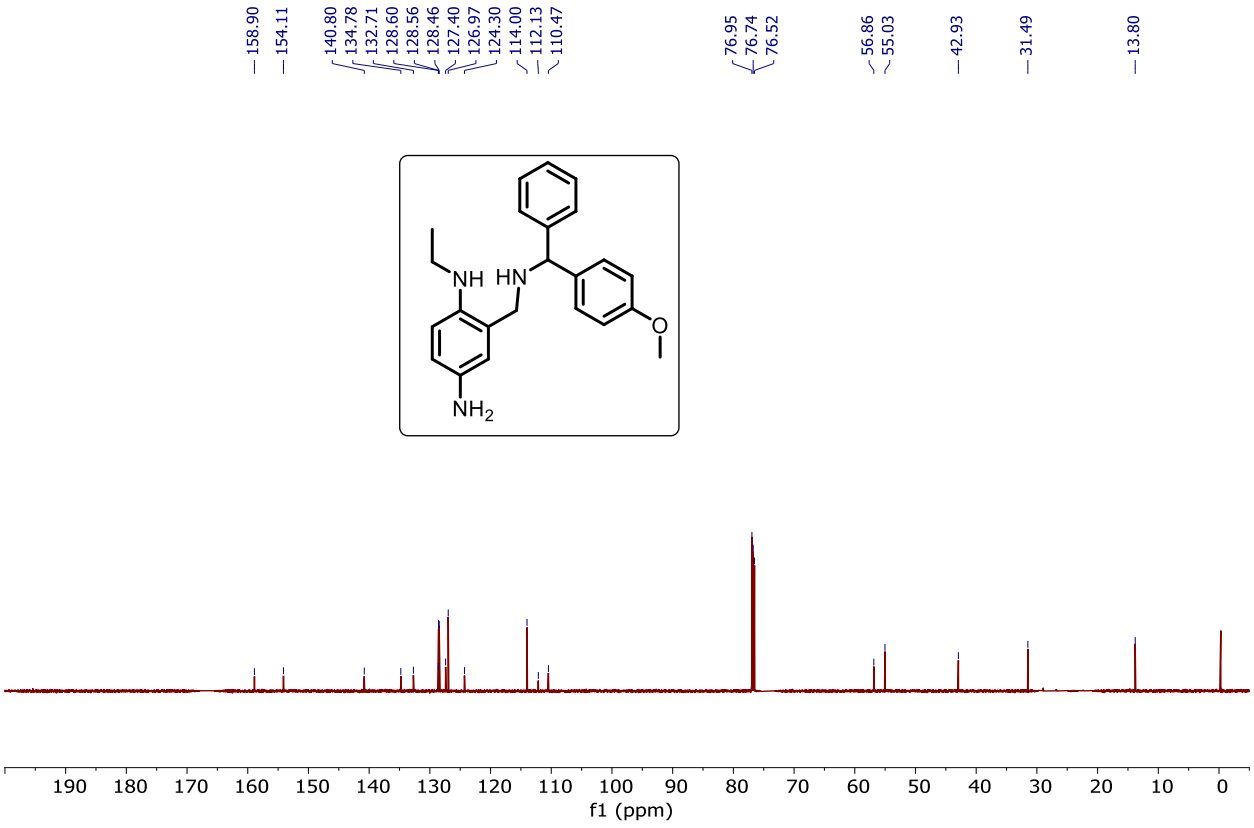


Figure S32. ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectrum of compound **13** in $CDCl_3$.

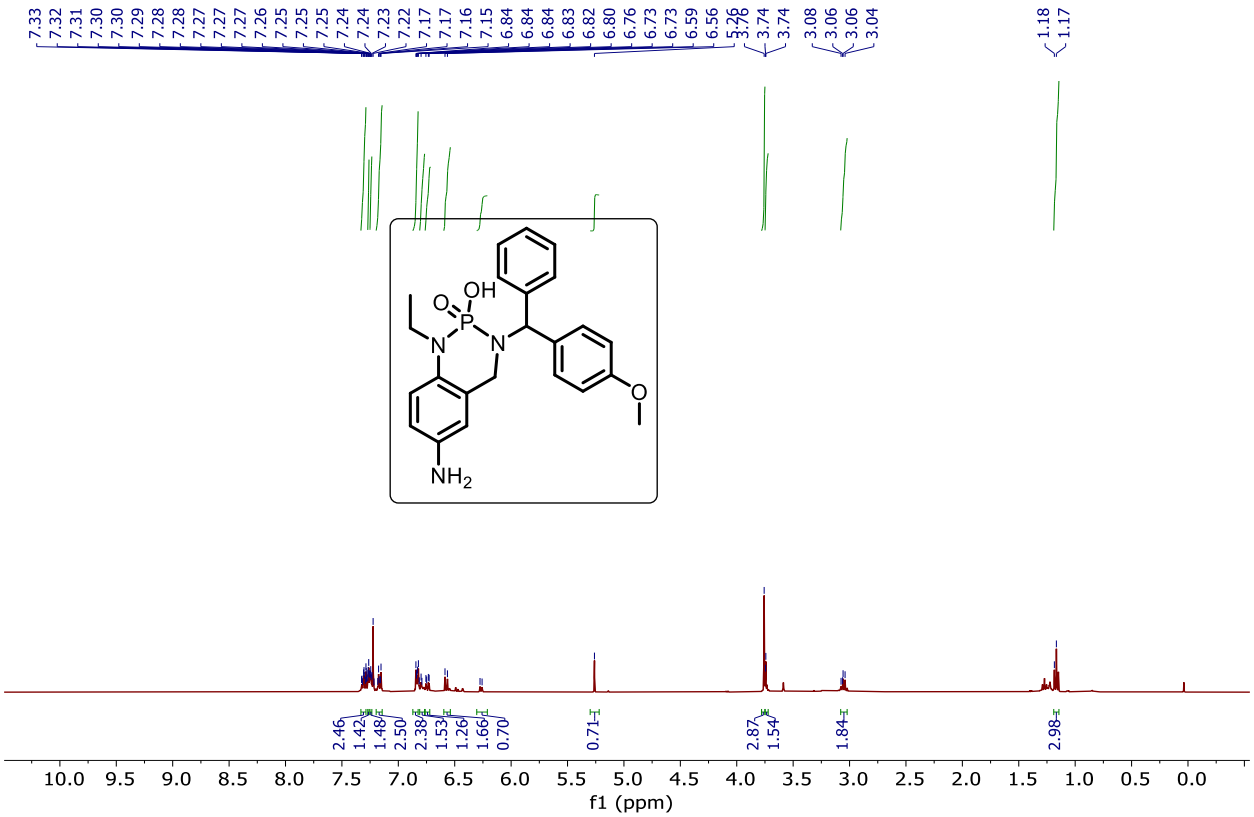


Figure S33. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **14** in $CDCl_3$.

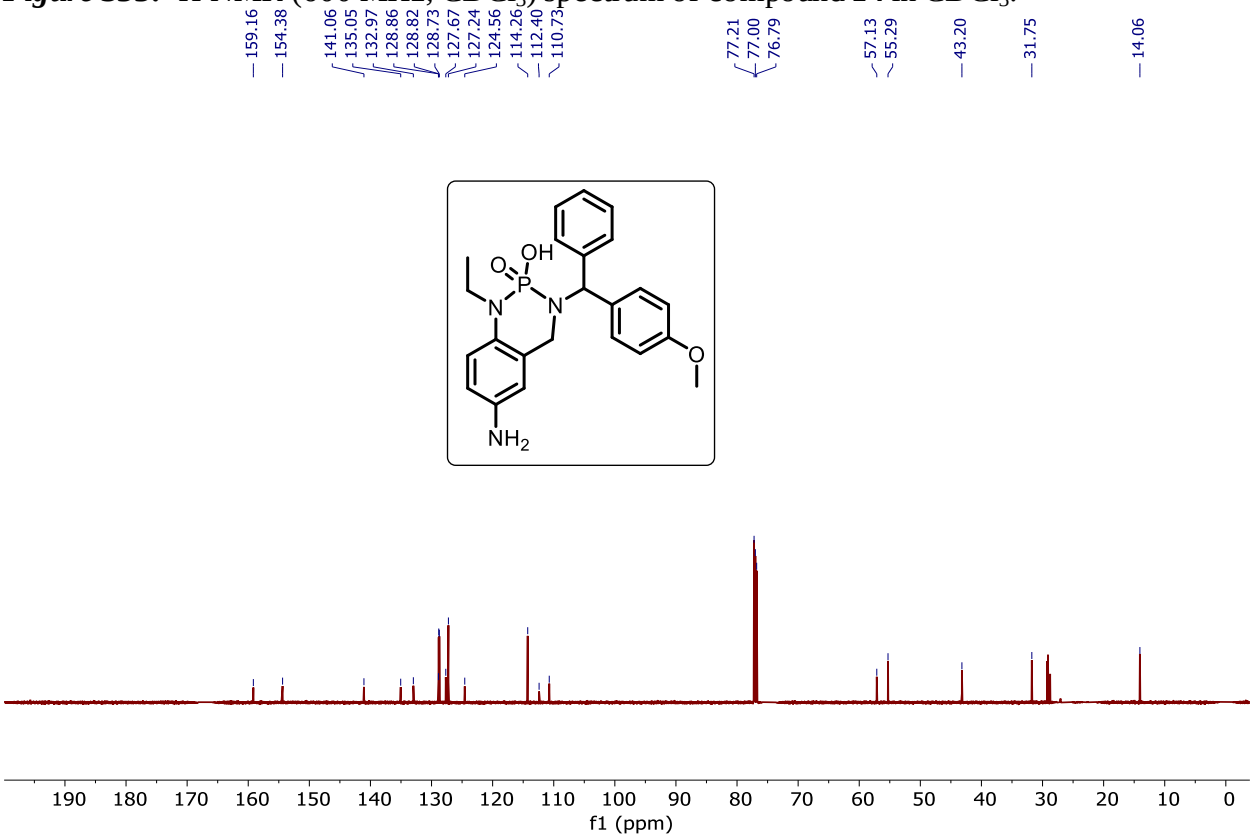


Figure S34. ^{13}C{1H} NMR (151 MHz, $CDCl_3$) spectrum of compound **14** in $CDCl_3$.

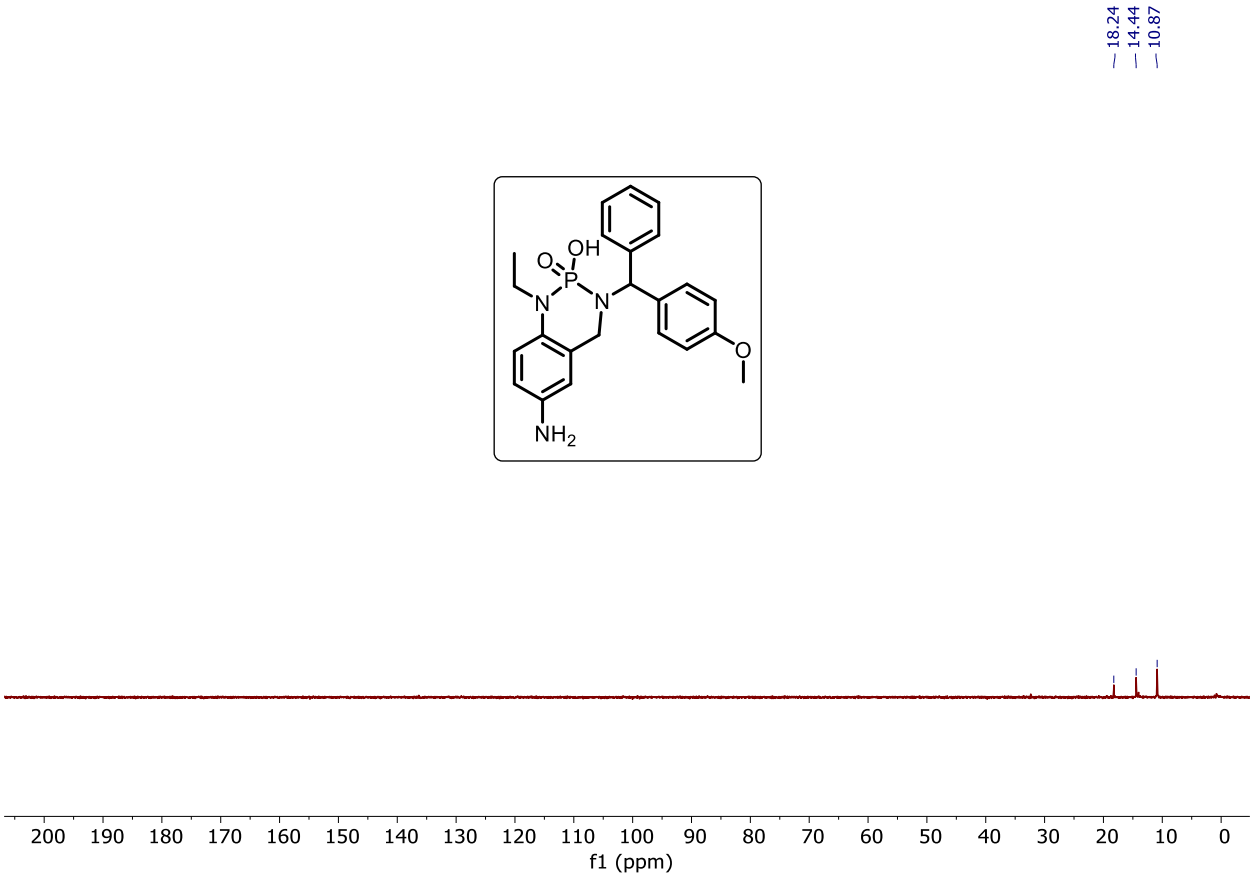


Figure S35. ^{31}P NMR spectrum of compound **14** in $CDCl_3$.

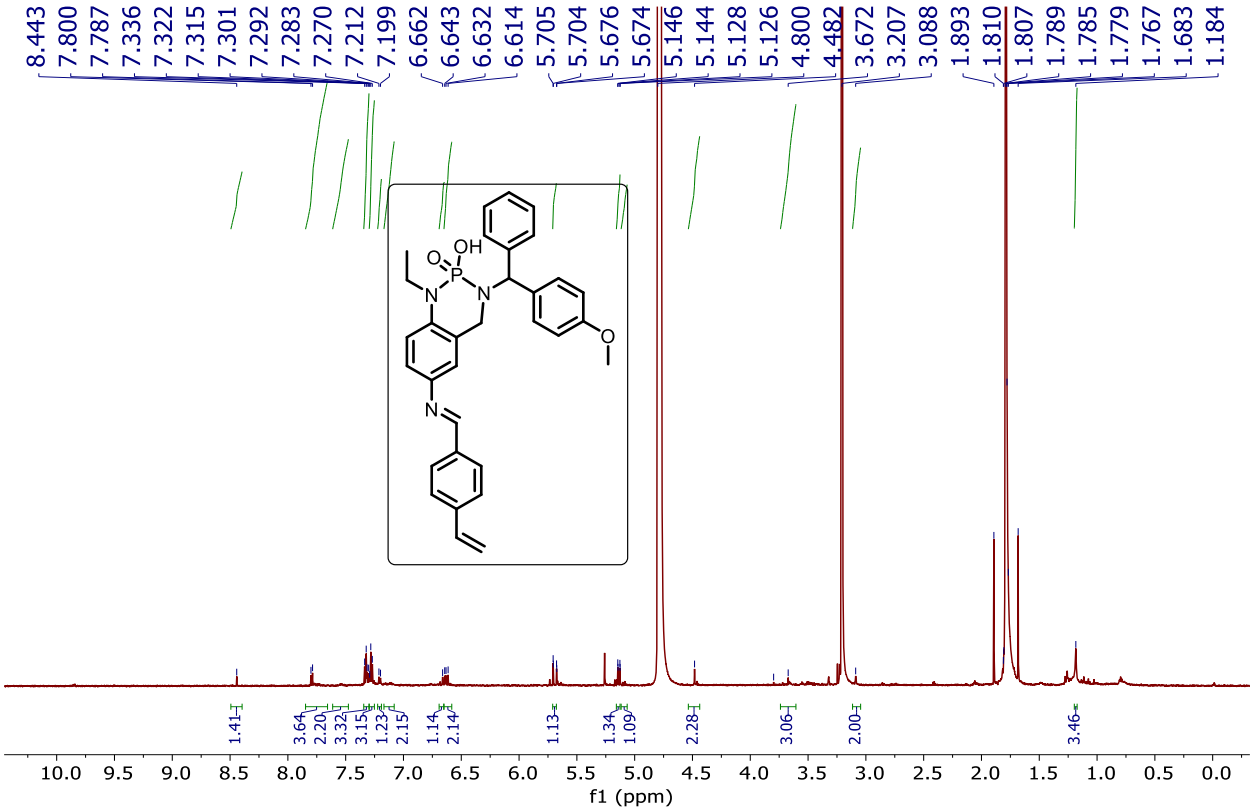


Figure S36. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **1** in CD_3OD.

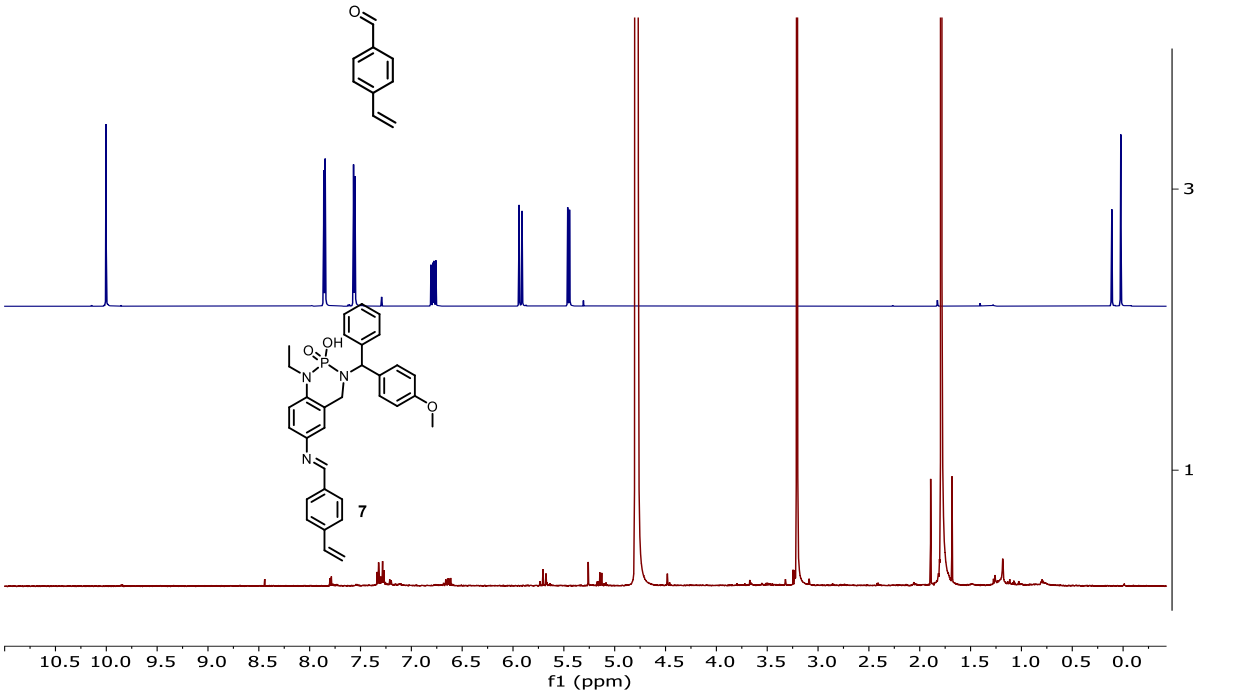


Figure S37. Stacked ^{1}H NMR(400 MHz) spectra of (a) vinyl benzaldehyde in $CDCl_3$, (b) the compound **1** in CD_3OD.

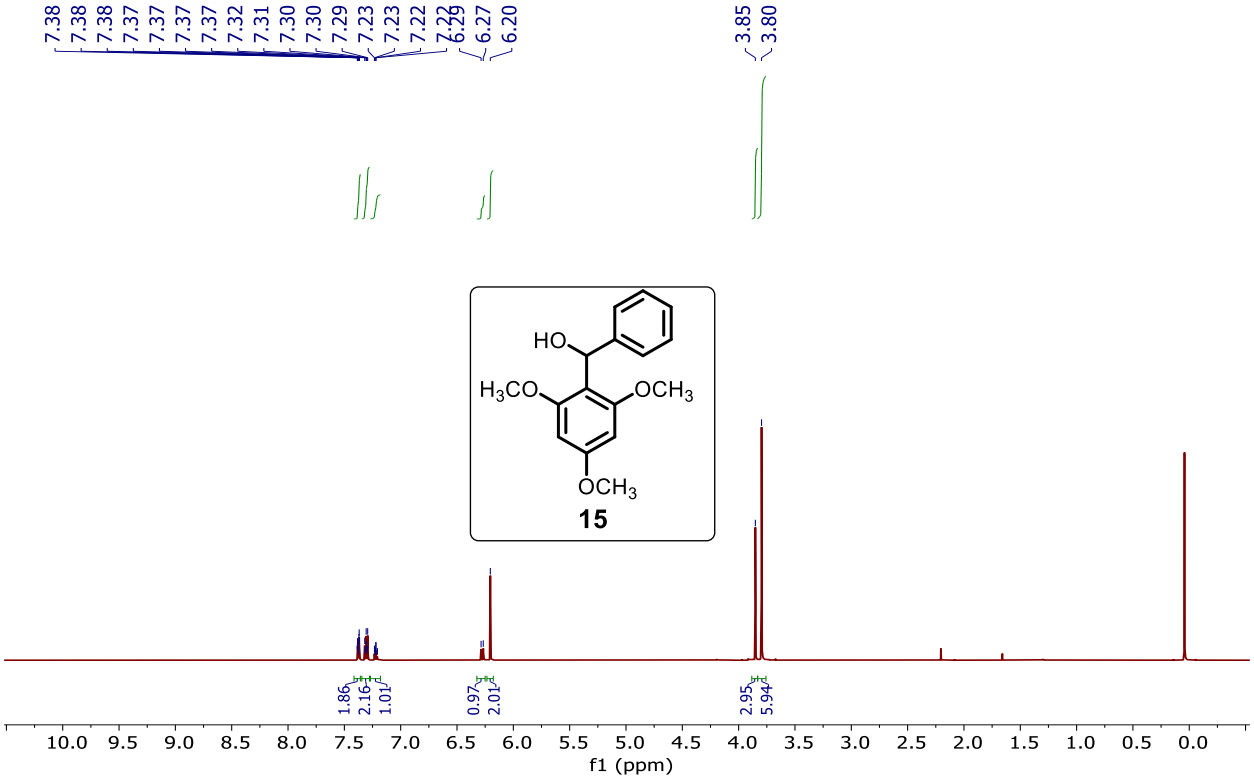


Figure S38. ^{1}H NMR(600 MHz, CD_3OD) spectrum of compound **15** in CD_3OD.

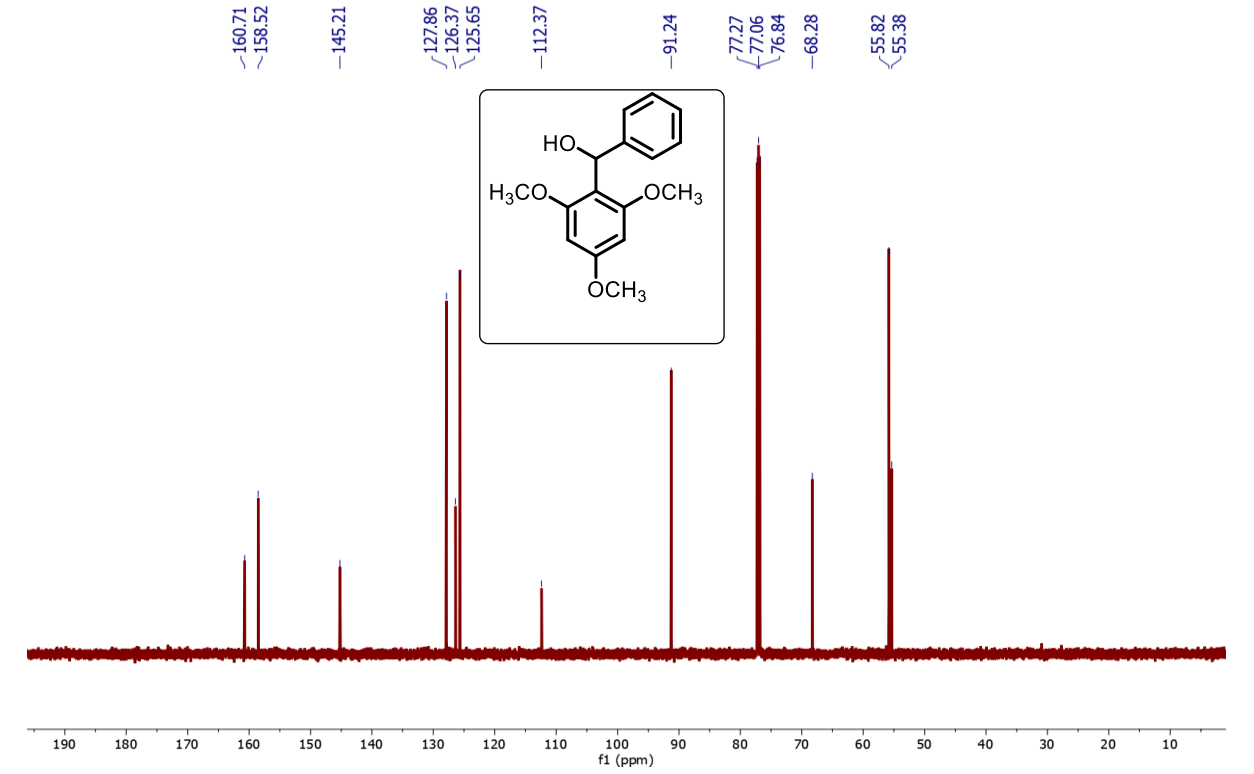


Figure S39. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **15** in CD_3OD.

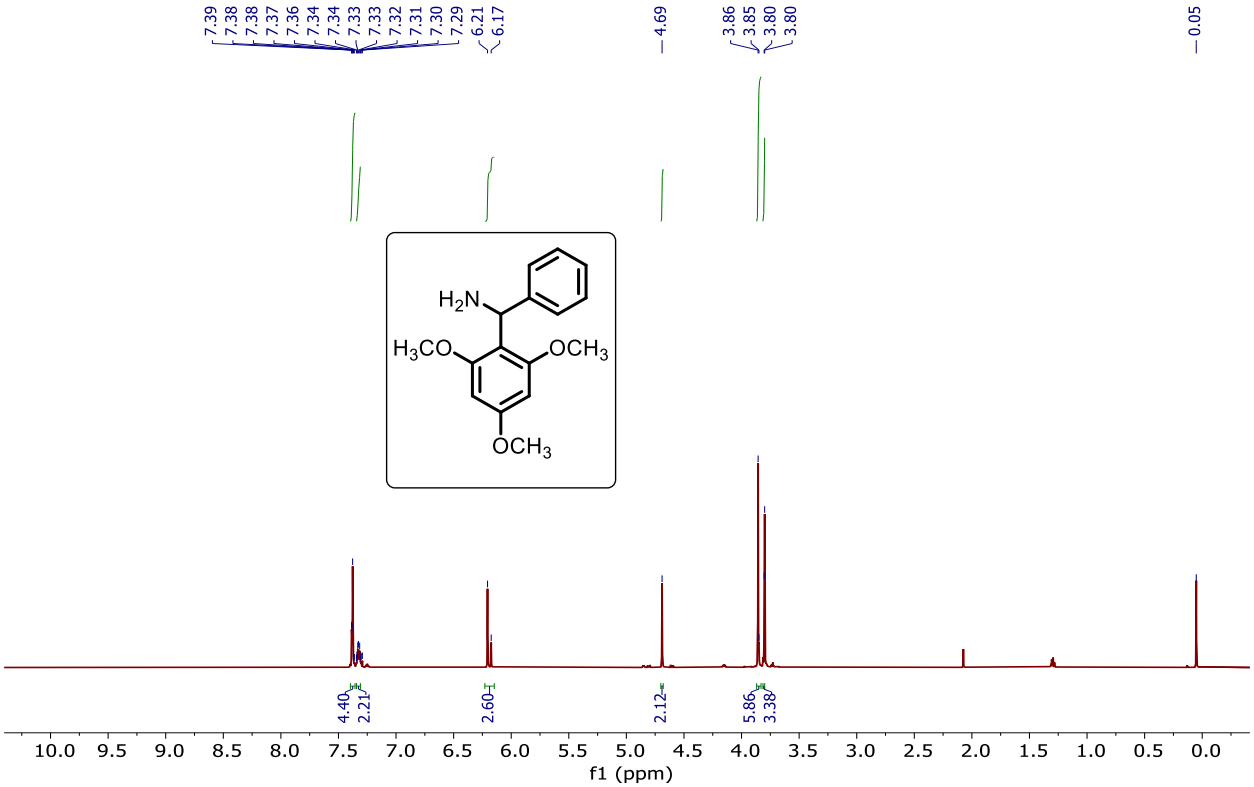


Figure S40. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **17** in CD_3OD.

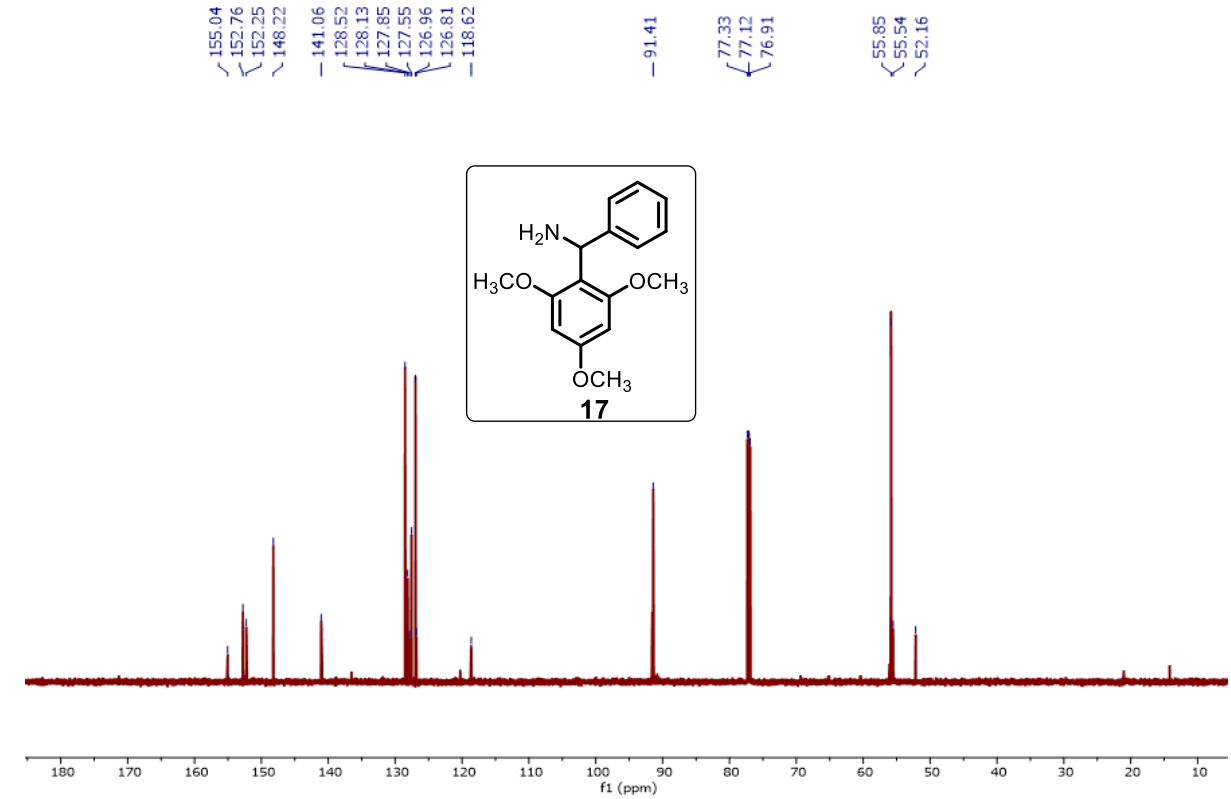


Figure S41. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **17** in CD_3OD.

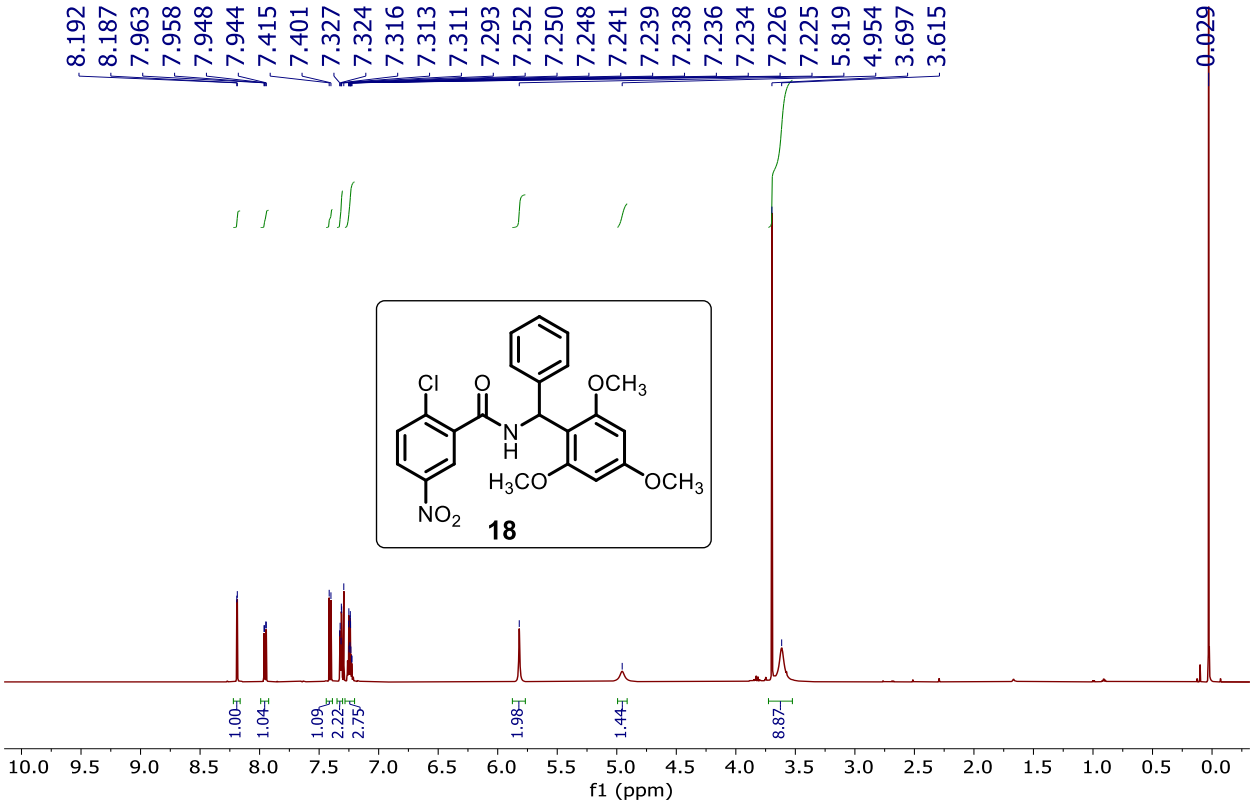


Figure S42. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **18** in CD_3OD.

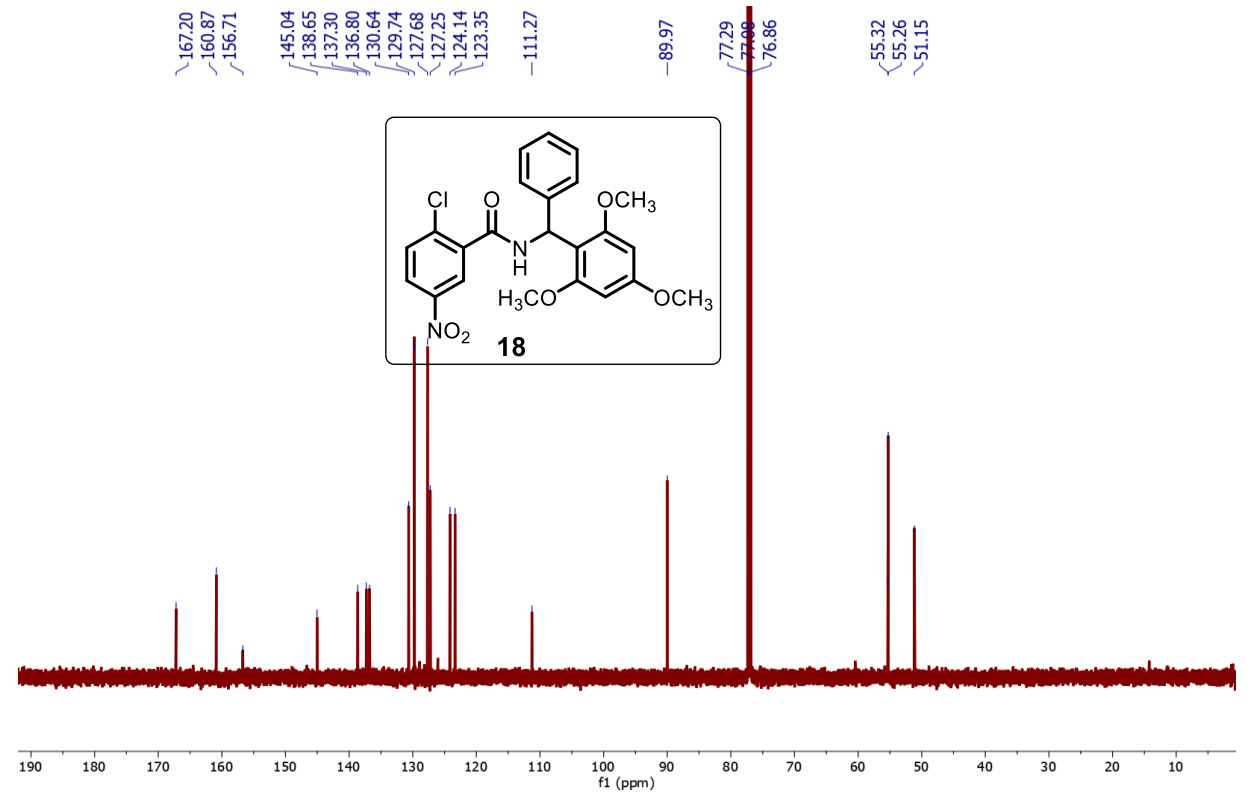


Figure S43. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **18** in CD_3OD.

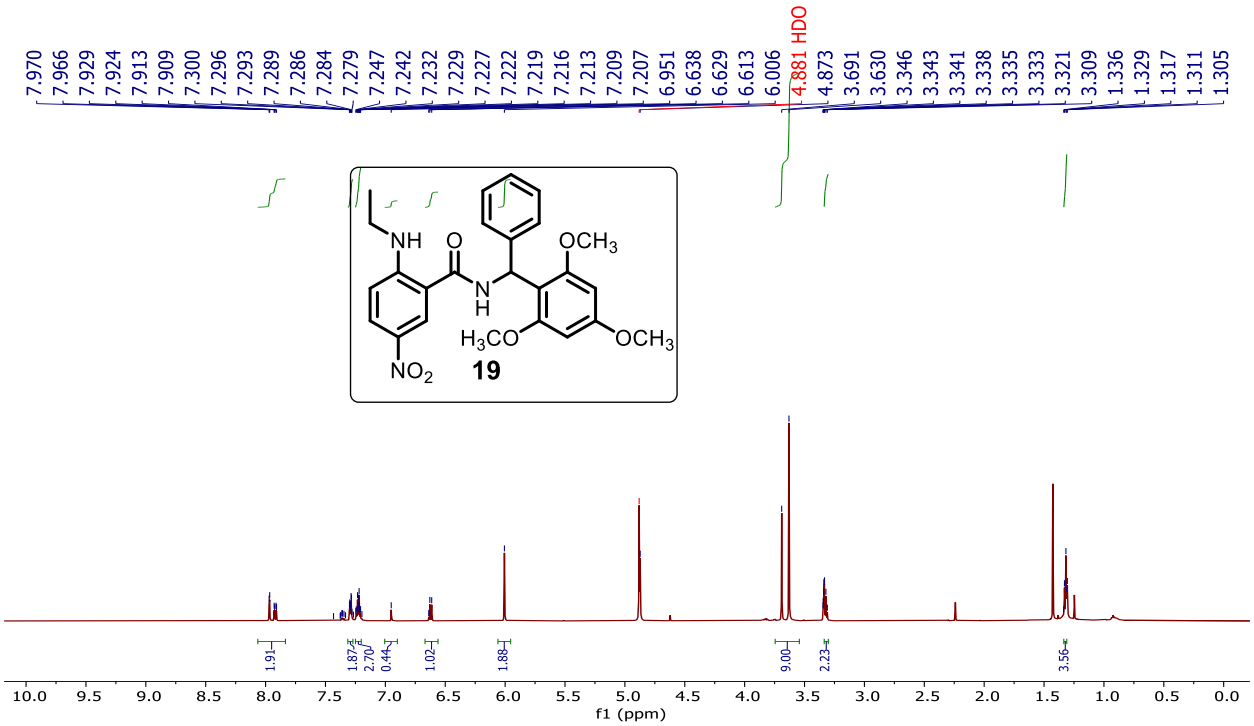


Figure S44. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **19** in CD_3OD.

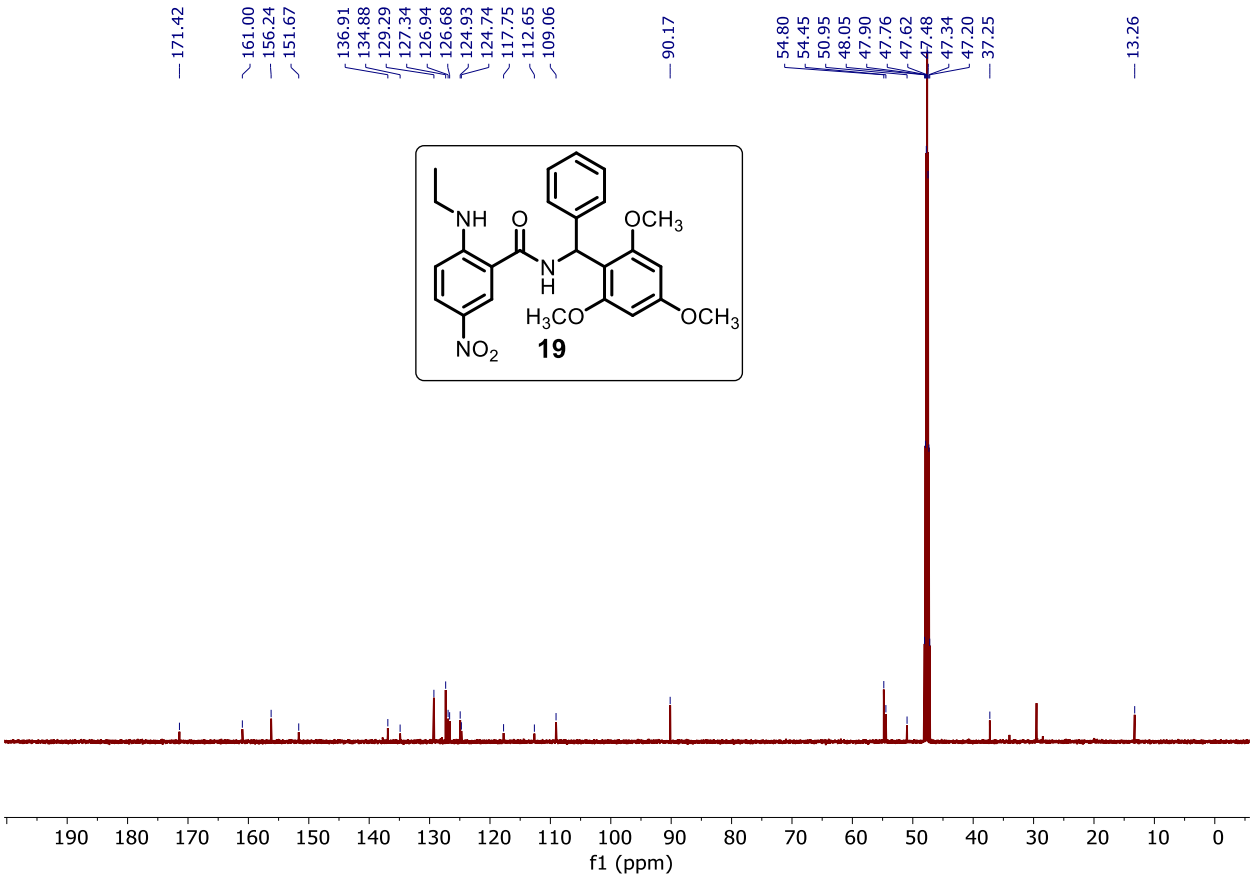


Figure S45. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **19** in CD_3OD.

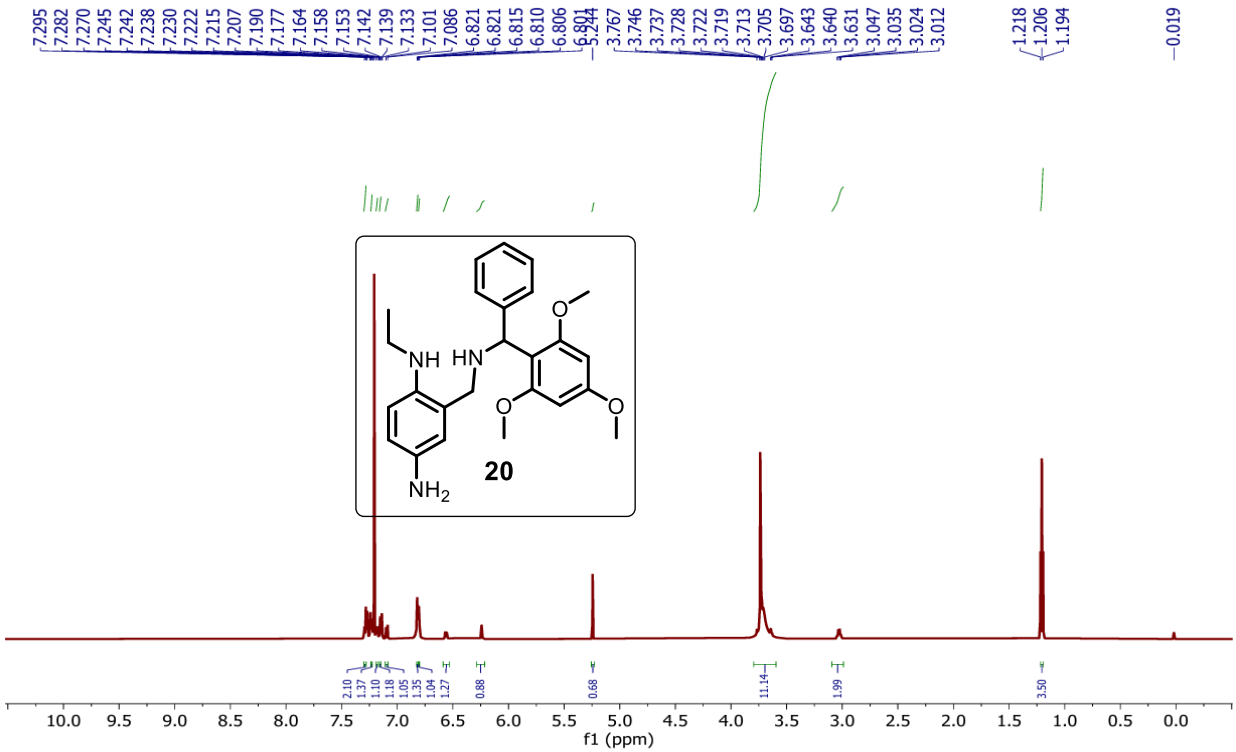


Figure S46. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **20** in $CDCl_3$.

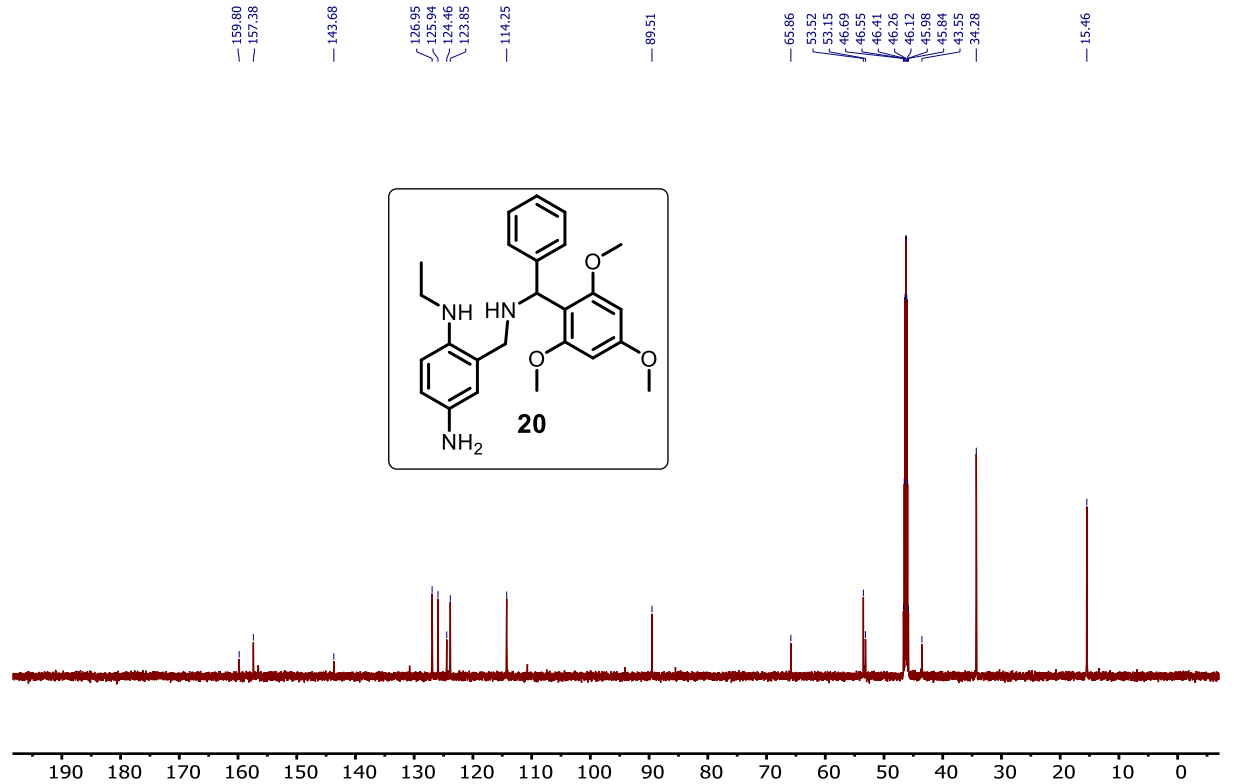


Figure S47. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **20** in CD_3OD.

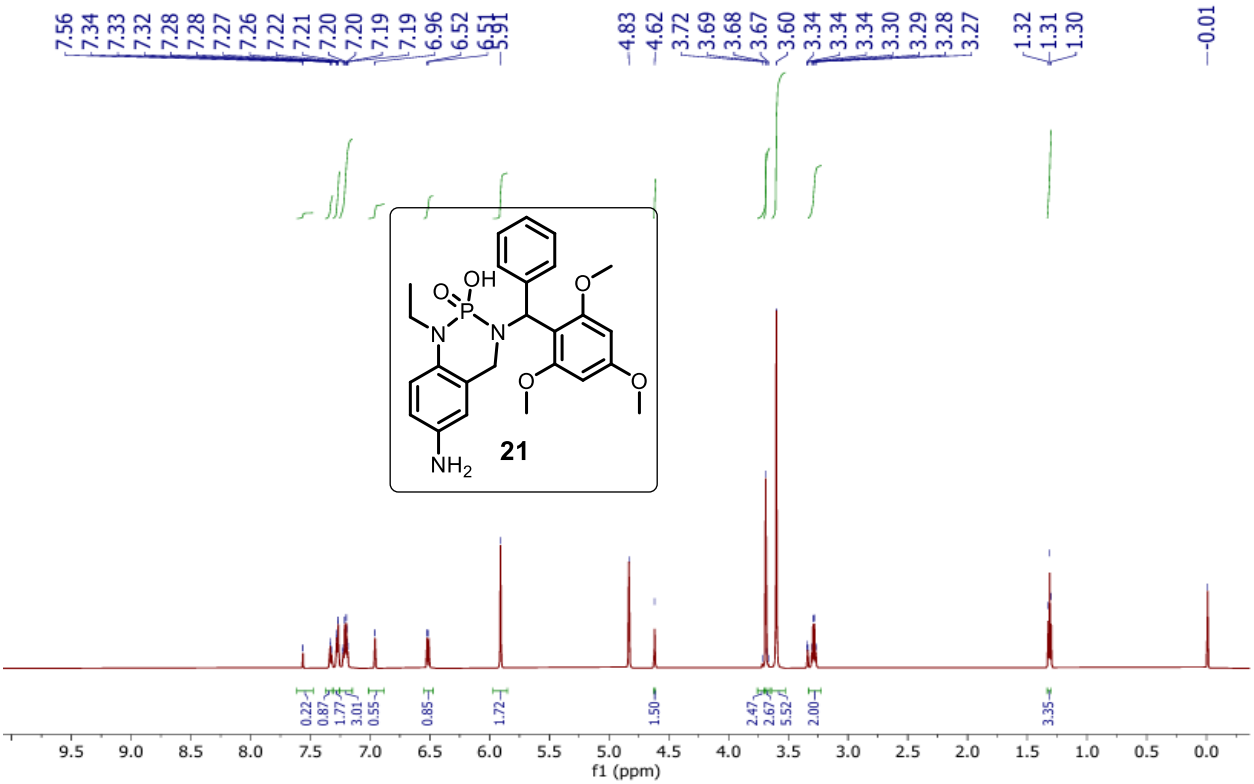


Figure S48. ^{1}H NMR (600 MHz, CD_3OD) spectrum of compound **21** in CD_3OD.

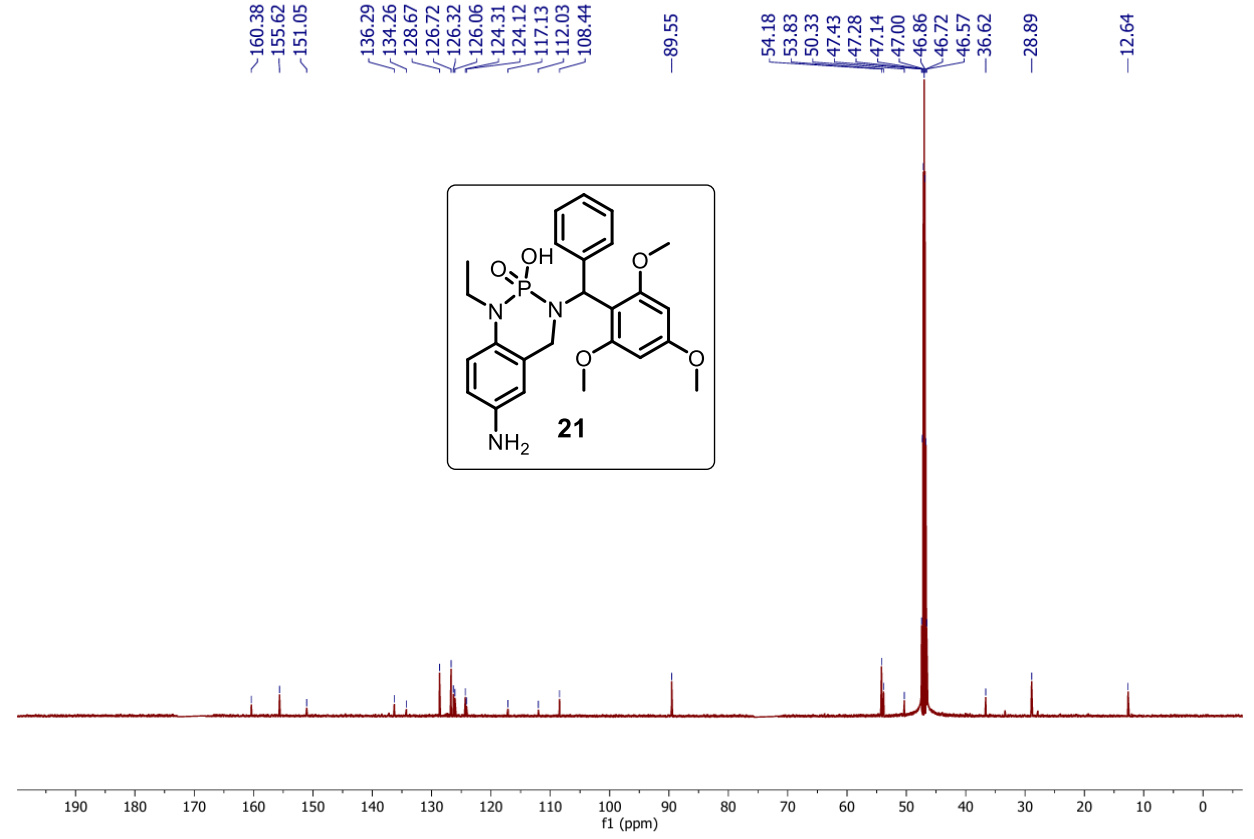


Figure S49. ^{13}C{1H} NMR (151 MHz, CD_3OD) spectrum of compound **21** in CD_3OD.

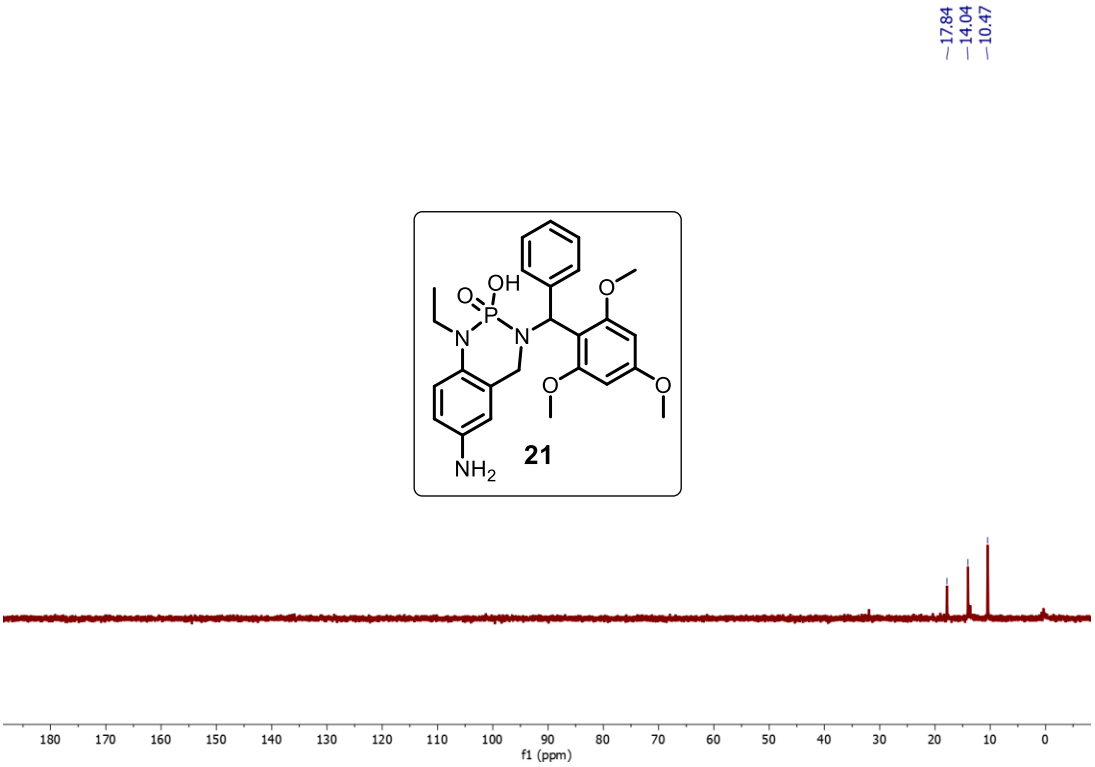


Figure S50. ^{31}P NMR spectrum of compound **21** in CD_3OD.

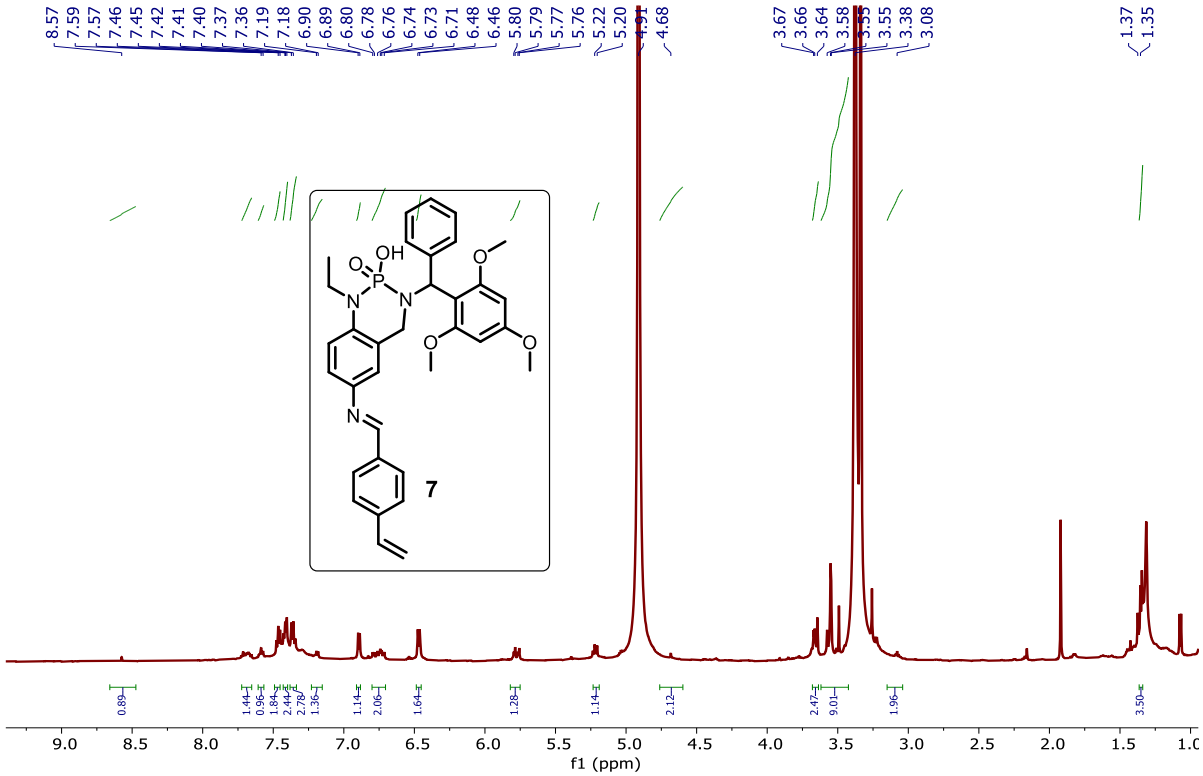


Figure S51. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **1b** in CD_3OD.

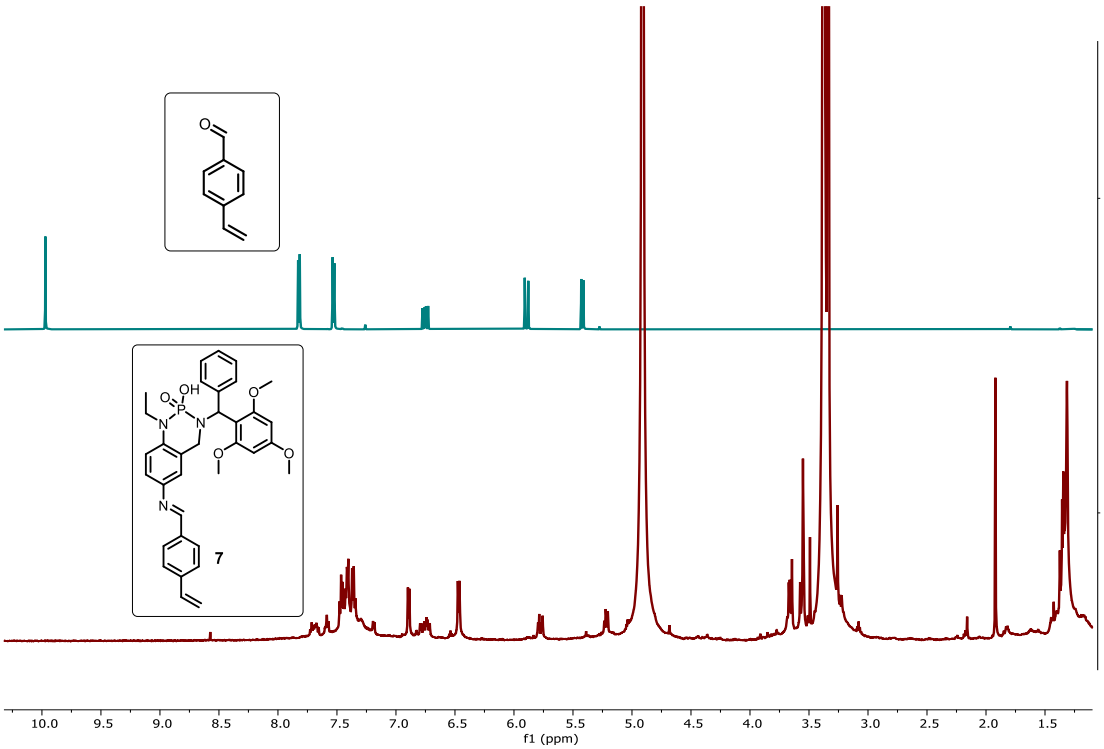
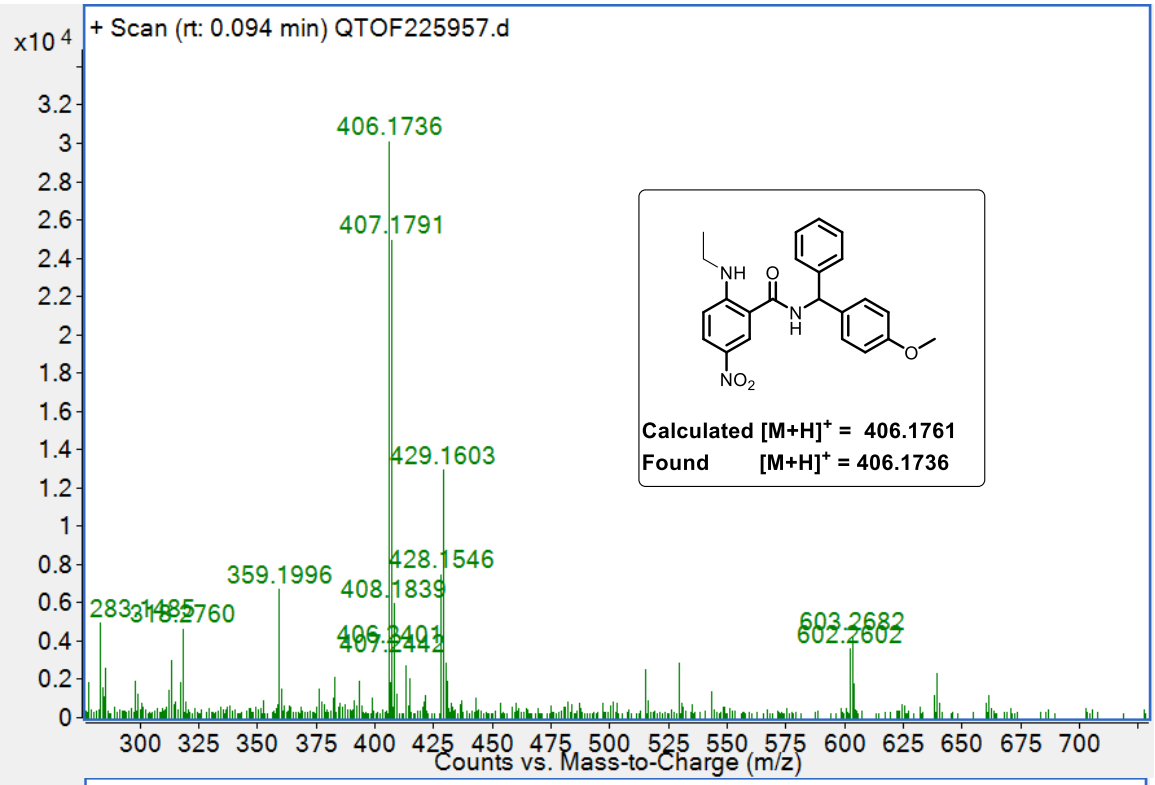
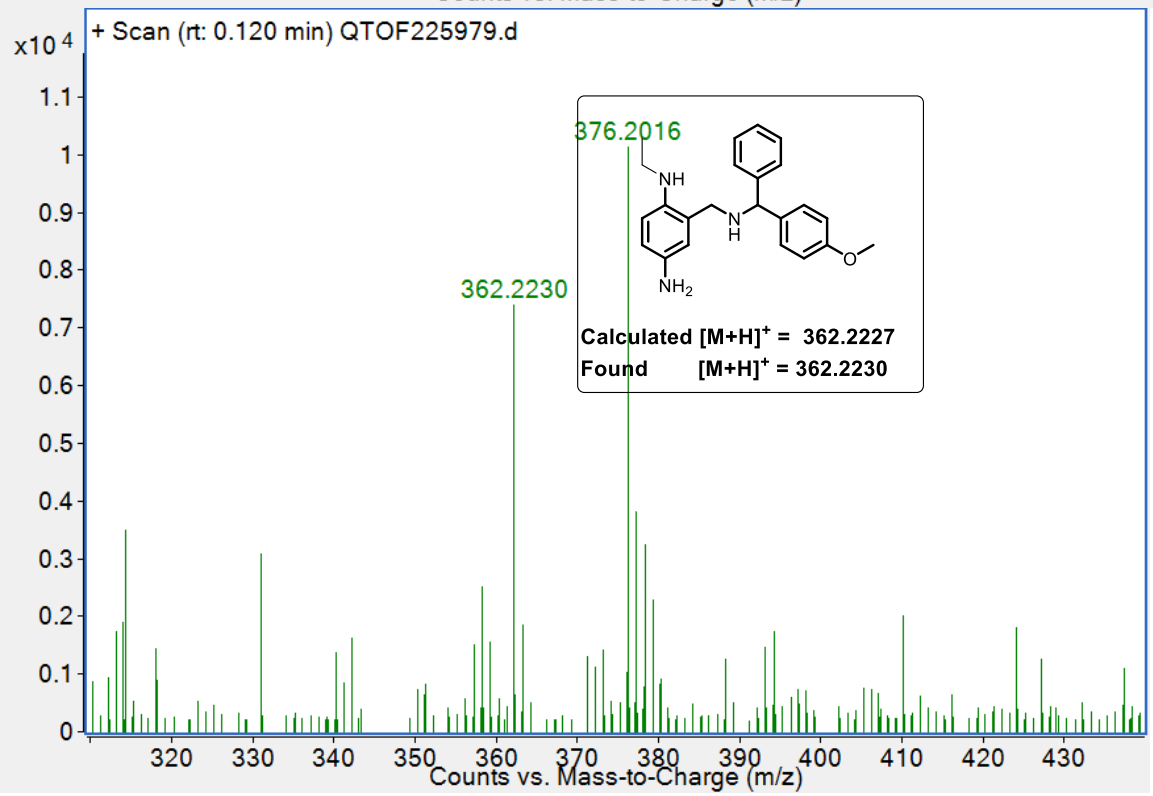
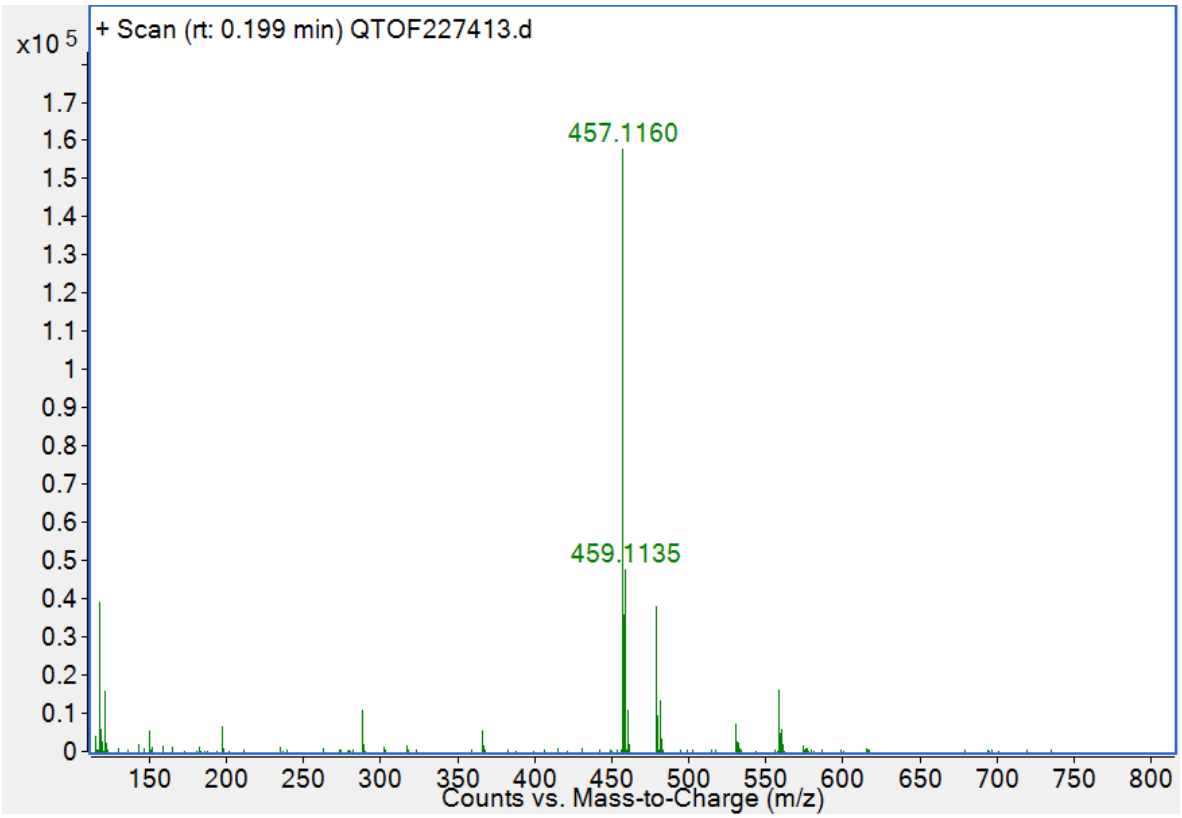


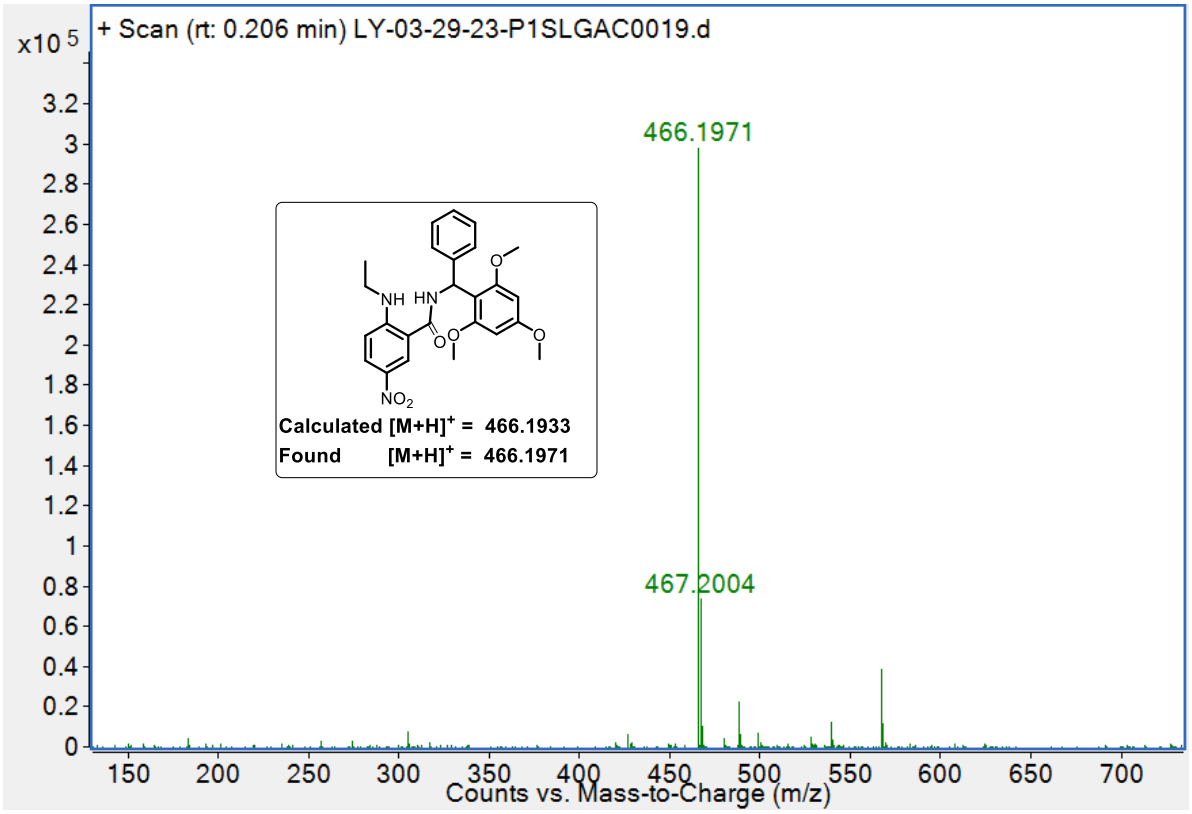
Figure S52. Stacked ^{1}H NMR(400 MHz) spectra of (a) vinyl benzaldehyde in $CDCl_3$, (b) the compound **1b** in CD_3OD.

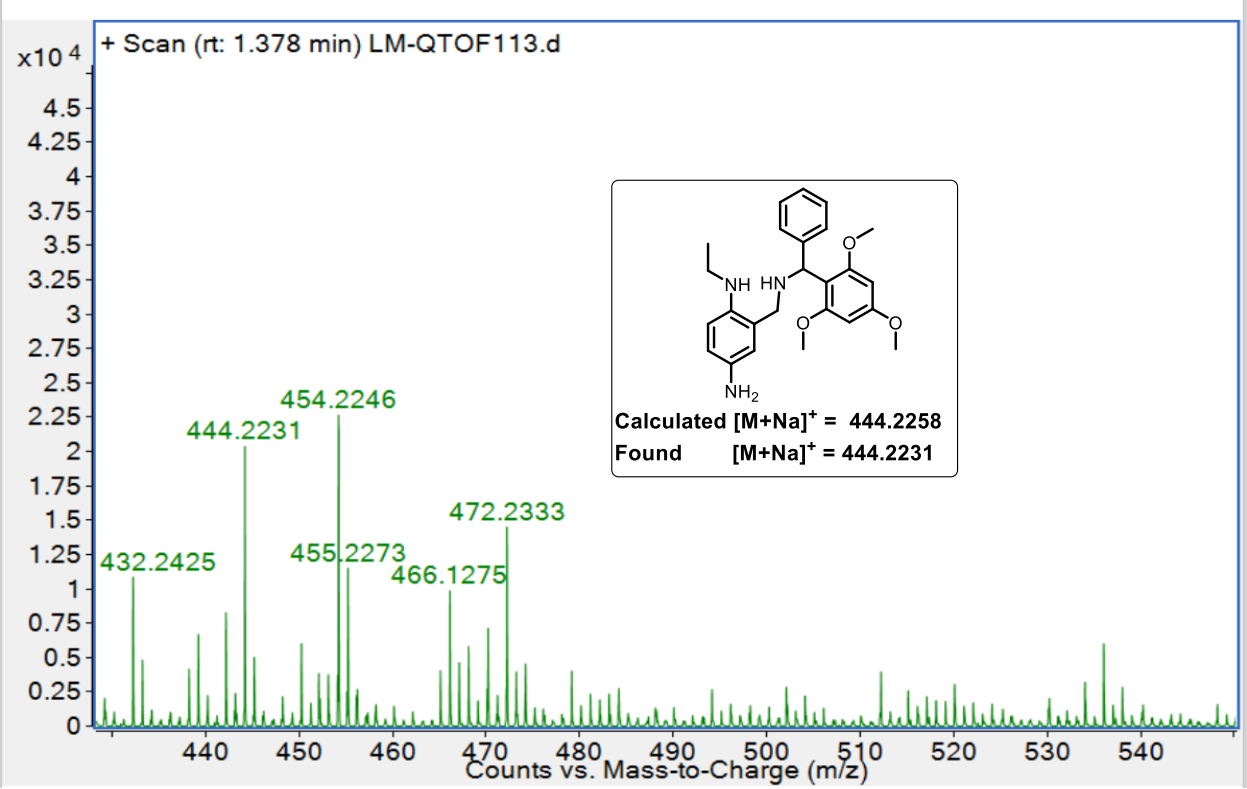
ESI-MS Spectra for New Compounds

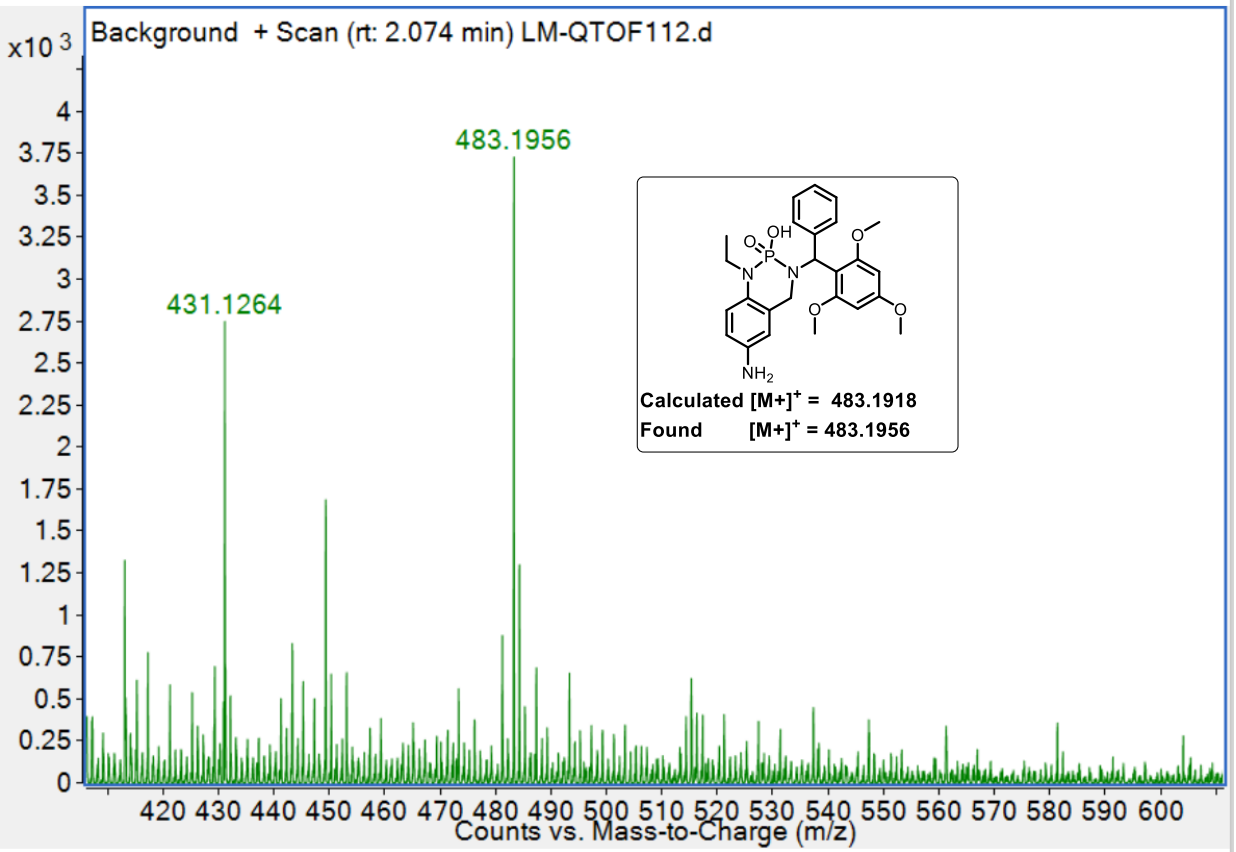


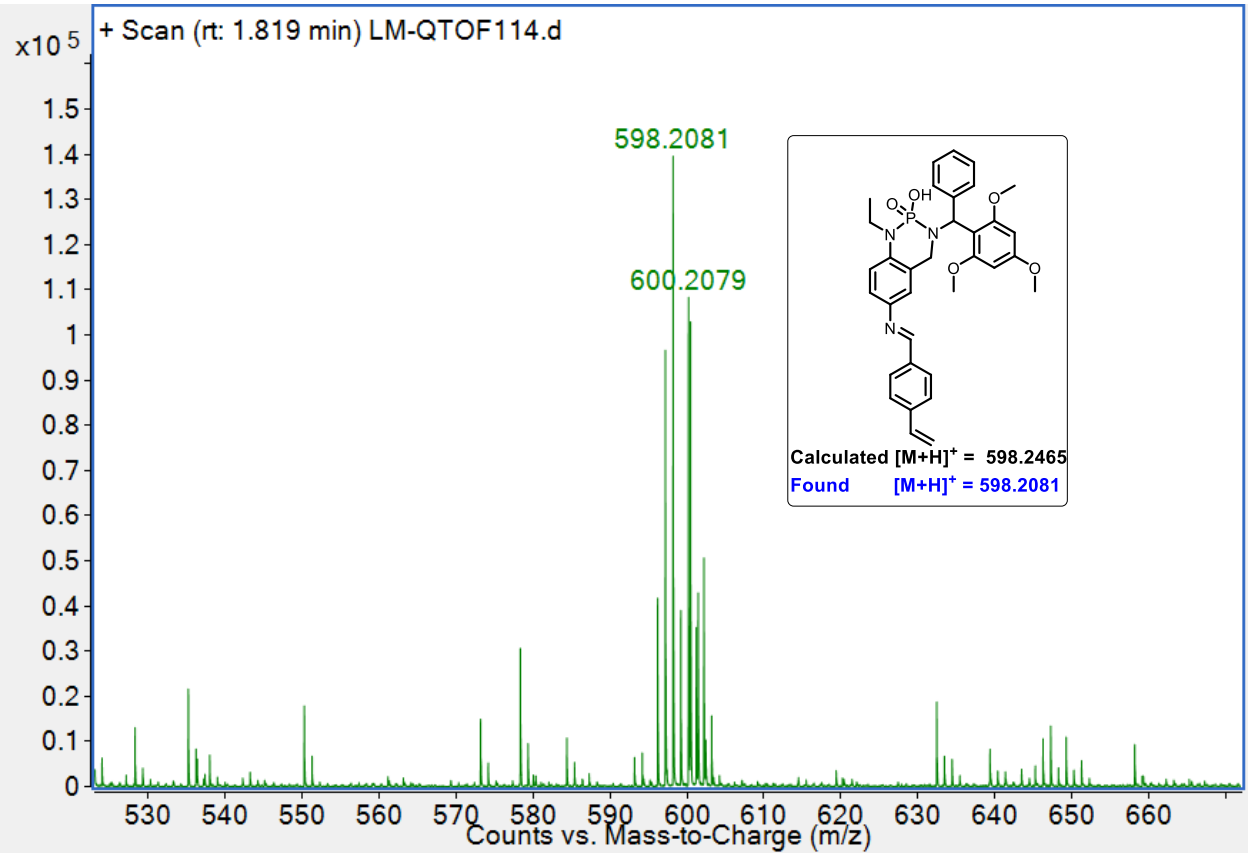



+ Scan (rt: 0.199 min) QTOF227413.d
x10 5
457.1160
459.1135
Counts vs. Mass-to-Charge (m/z)


+ Scan (rt: 0.206 min) LY-03-29-23-P1SLGAC0019.d
x10 5
466.1971
467.2004
Calculated [M+H]+ = 466.1933
Found [M+H]+ = 466.1971
Counts vs. Mass-to-Charge (m/z)


+ Scan (rt: 1.378 min) LM-QTOF113.d
x10 4
4.5
4.25
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
454.2246
444.2231
472.2333
432.2425
455.2273
466.1275
NH
HN
O
O
O
NH2
Calculated [M+Na]+ = 444.2258
Found [M+Na]+ = 444.2231
440 450 460 470 480 490 500 510 520 530 540
Counts vs. Mass-to-Charge (m/z)


Background + Scan (rt: 2.074 min) LM-QTOF112.d
x10 3
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
483.1956
431.1264
OH
O
P
N
N
O
O
NH2
Calculated [M+]+ = 483.1918
Found [M+]+ = 483.1956
420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570 580 590 600
Counts vs. Mass-to-Charge (m/z)


+ Scan (rt: 1.819 min) LM-QTOF114.d
x10 5
598.2081
600.2079
Calculated [M+H]+ = 598.2465
Found [M+H]+ = 598.2081
Counts vs. Mass-to-Charge (m/z)

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