Supporting Information Appendix

Ketoreductase Catalyzed Stereoselective Bioreduction of α-Nitro Ketones

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Chemicals

Unless otherwise specified, all reagents and solvent were purchased from commercial sources and used as received. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR were recorded on a Bruker Avance 400 spectrometer in $CDCl_3$ using tetramethylsilane (TMS) as internal standards. Coupling constant (*J*) values are given in Hz. Products were purified by flash column chromatography on silica gel purchased from Qingdao Haiyang Chemical Co., Ltd. Optical rotations were measured by a Rudolph AUTOPOL I Automatic Polarimeter. HRMS were recorded on a Bruker micrOTOF spectrometer. HPLC analysis were performed with Daicel Chiralpak OD-H column (25 cm × 4.6 mm × 5 µm), Chiralpak IA column (25 cm × 4.6 mm × 5 µm), Chiralpak IB column (25 cm × 4.6 mm × 5 µm), Chiralpak IC column (25 cm × 4.6 mm × 5 µm), Chiralpak AD-H column (25 cm × 4.6 mm × 5 µm), Chiralpak AS-H column (25 cm × 4.6 mm × 5 µm).

Molecular Biology

Reagents

Restriction enzymes (NdeI, NcoI, EcoRI and XhoI), PrimeSTAR® HS DNA Polymerase were purchased from TaKaRa (Japan). One Step Cloning Kit ClonExpress® II was purchased from Vazyme (Nanjing, China). PurePlasmid Mini Kit and Gel Extraction Kit were purchased from CWBIO (China). Chemically competent cells of *E. coli* DH5α and *E. coli* BL21 (DE3) were purchased from Transgen (China). Oligonucleotides were purchased from Genewiz (China) in standard, desalted form and used without further purification (Table S16). Synthetic genes (pET28a-LtCR, pET28a-RasADH, pET28a-CgCR, pET28a-KRED1-Pglu, pET28a-SsCR, pET28a-SeKRED, pET28a-LbADH, pET28a-LkADH, pET28a-SyADH, pET28a-TdADH, pET28a-KdoADH) were purchased from Genewiz (China) (Table S3). All other reagents were purchased from Sangon Biotech (China) unless otherwise specified. LB medium contained yeast extract (5 g/L), tryptone (10 g/L), NaCl (10 g/L). Antibiotics were used at the following concentration: kanamycin: 50 µg/mL, chloramphenicol: 25 µg/mL.

Cloning procedures

Cloning genes into pET28a vector

PCR products were amplified from genomic DNA of *Saccharomyces cerevisiae* s288c using the PrimeSTAR® HS DNA Polymerase with a T100 Thermal Cycler. The reaction began with an initial denaturing step for 180 s at 98 °C followed by 30 cycles of 10 s at 98 °C, 15 s at 55 °C and 90 s at 72 °C with a final extension step at 72 °C for 300 s. The resulting PCR products were ligated with linearized vectors, which were double digested at appropriate restriction sites (NdeI/XhoI or NcoI/XhoI), through homologous recombination using the One Step Cloning Kit ClonExpress® II. In general, a 10 µL reaction mixture containing 2 µL of 5×CE II Buffer, 1 µL of Exnase II, 50-200 ng linearized vector and 20-200 ng PCR amplicon was incubated at 37 °C for 30 min, and the resulting solution was used to transform chemically competent *E. coli* DH5α cells. Colony PCR and sequencing (Genewiz, China) were performed to confirm the sequence fidelity of the recombinant plasmids.

Cloning glucose dehydrogenase (GDH) into multiple cloning site 1 (MCS1) of pACYC-duet vector

PCR product was amplified with the previously constructed pET28b-GDH[1] as the template using the PrimeSTAR® HS DNA Polymerase with a T100 Thermal Cycler. The reaction began with an initial denaturing step for 180 s at 98 °C followed by 30 cycles of 10 s at 98 °C, 15 s at 55 °C and 90 s at 72 °C with a final extension step at 72 °C for 300 s. The resulting PCR products were ligated with pACYC-duet vector linearized at NcoI/EcoRI restriction sites through homologous recombination using the One Step Cloning Kit ClonExpress® II. In general, a 10 μL reaction mixture containing 2 μL of 5×CE II Buffer, 1 μL of Exnase II, 50-200 ng linearized vector and 20-200 ng PCR amplicon was incubated at 37 ºC for 30 min, and the resulting solution was used to transform chemically competent *E. coli* DH5α cells. Colony PCR and sequencing (Genewiz, China) were performed to confirm the sequence fidelity of the recombinant plasmids. Such constructed plasmid was designated as pACYC-duet-GDH (MCS1).

Cloning RasADH and GDH into pRSF-duet vector

PCR product of RasADH was amplified with the constructed pET28a-RasADH as the template using the PrimeSTAR® HS DNA Polymerase with a T100 Thermal Cycler. The reaction began with an initial denaturing step for 180 s at 98 °C followed by 30 cycles of 10 s at 98 °C, 15 s at 55 °C and 90 s at 72 °C with a final extension step at 72 °C for 300 s. The resulting PCR products were ligated with pRSF-duet vector linearized at NcoI/EcoRI restriction sites through homologous recombination using the One Step Cloning Kit ClonExpress® II. In general, a 10 μL reaction mixture containing 2 μL of 5×CE II Buffer, 1 μL of Exnase II, 50-200 ng linearized vector and 20-200 ng PCR amplicon was incubated at 37 ºC for 30 min, and the resulting solution was used to transform chemically competent *E. coli* DH5α cells. Colony PCR and sequencing (Genewiz, China) were performed to confirm the sequence fidelity of the recombinant plasmids. Such constructed plasmid was designated as pRSF-duet-RasADH (MCS1).

PCR product of GDH was amplified with the previously constructed pET28b-GDH as the template using the PrimeSTAR® HS DNA Polymerase with a T100 Thermal Cycler. The reaction began with an initial denaturing step for 180 s at 98 °C followed by 30 cycles of 10 s at 98 °C, 15 s at 55 °C and 90 s at 72 °C with a final extension step at 72 °C for 300 s. The resulting PCR products were ligated with plasmid pRSF-RasADH(1) linearized at NdeI/XhoI restriction sites through homologous recombination using the One Step Cloning Kit ClonExpress® II. In general, a 10 μL reaction mixture containing 2 μL of 5×CE II Buffer, 1 μL of Exnase II, 50-200 ng linearized vector and 20-200 ng PCR amplicon was incubated at 37 ºC for 30 min, and the resulting solution was used to transform chemically competent *E. coli* DH5α cells. Colony PCR and sequencing (Genewiz, China) were performed to confirm the sequence fidelity of the recombinant plasmids. Such constructed plasmid was designated as pRSF-duet-RasADH (MCS1)-GDH (MCS2).

Plasmid pRSF-duet-GDH (MCS1)-RasADH (MCS2) was constructed using the similar method.

Enzymology

Reagents

Nickel(II)-nitrilotriacetic acid (Ni-NTA) agarose was purchased from Sangon. Amicon ultracentrifugal filters were purchased from EMB Millipore. PD-10 desalting columns were purchased from GE Healthcare. Isopropylthio-β-D-galactoside (IPTG) was obtained from Sangon. Lysis buffer consisted of 50 mM NaPi, 300 mM NaCl, 10 mM imidazole, 10% glycerol, pH 7.5. Wash buffer consisted of 50 mM NaPi, 300 mM NaCl, 20 mM imidazole, 10% glycerol, pH 7.5. Elution buffer consisted of 50 mM NaPi, 300 mM NaCl, 250 mM imidazole, 10% glycerol, pH 7.5. Storage buffer consisted of 50 mM NaPi, 300 mM NaCl, 10% glycerol, pH 7.5.

Expression and purification of His_6-tagged recombinant proteins

An approximately 12 h culture of *E. coli* BL21 (DE3) cells freshly transformed with the appropriate plasmid and grown in LB medium supplemented with kanamycin (50 µg/mL) was diluted 1 : 100 into 0.5 L of the same medium in a 2 L flask. The culture was shaken at 37 °C until the optical density at 600 nm reached 0.6-0.8, then the flask was placed in an ice/water bath for ca. 30 min before the addition of isopropylthio-β-D-galactoside (IPTG) to a final concentration of 100 µM. The culture was shaken for an additional 12-14 h at 18 ºC. All the following purification steps were carried out at 4 °C. The cells (1.5-2 g wet mass from 0.5 L culture) were collected by centrifugation, and then resuspended in 20 mL of lysis buffer. The cells were lysed by sonication on ice and debris was removed by centrifugation at 37,000 x g for 30 min at 4 °C. The supernatant was loaded onto a column containing 2-3 mL of Ni-NTA resin previously equilibrated with lysis buffer. After equilibration of the resin with the lysate in an orbital shaker for ca. 30 min, the flow-through was discarded and the resin was washed with 2 × 20 mL of wash buffer. Resin-bound protein was eluted with elution buffer. Fractions of 1 mL were collected and the absorbance at 280 nm was measured by a NanoDrop One spectrophotometer. Fractions with strong absorbance at 280 nm were pooled and concentrated in an Amicon Ultra centrifugal filter unit with 10 kDa molecular weight cut off (MWCO) to a final volume of 2.5 mL. Imidazole and excess salt was removed by passing the protein solution through a PD-10 desalting column previously equilibrated with storage buffer. Protein was eluted with 3.5 mL of storage buffer and stored in aliquots at -80 ºC. The protein concentrations were measured by a NanoDrop One spectrophotometer with calculated extinction coefficient and molecular weight.

Co-expression of pET28a-RasADH and pACYC-duet-GDH (MCS1)

An approximately 12 h culture of *E. coli* BL21 (DE3) cells freshly co-transformed with plasmids pET28a-RasADH and pACYC-duet-GDH (MCS1), and grown in LB medium supplemented with kanamycin (50 µg/mL) and chloramphenicol (25 µg/mL) was diluted 1 : 100 into 0.5 L of the same medium in a 2 L flask. The culture was shaken at 37 °C until the optical density at 600 nm reached 0.6-0.8, then the flask was placed in an ice/water bath for ca. 30 min before the addition of isopropylthio-β-D-galactoside (IPTG) to a final concentration of 100 µM. The culture was shaken for an additional 12-14 h at 18 ºC. The cells (1.5-2 g wet mass from 0.5 L culture) were collected by centrifugation.

Expression of pRSF-duet-RasADH (MCS1)-GDH (MCS2) and pRSF-duet-GDH (MCS1)-RasADH (MCS2)

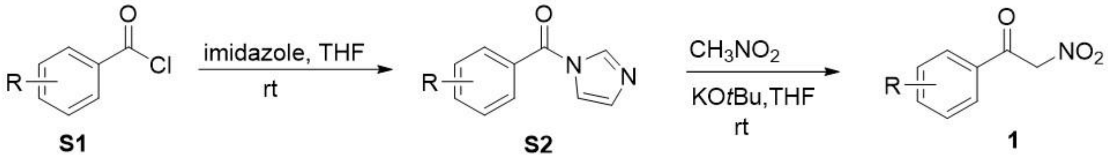
An approximately 12 h culture of *E. coli* BL21 (DE3) cells freshly transformed with plasmids pRSF-duet-RasADH (MCS1)-GDH (MCS2) or pRSF-duet-GDH (MCS1)-RasADH (MCS2), and grown in LB medium supplemented with kanamycin (50 μg/mL) was diluted 1 : 100 into 0.5 L of the same medium in a 2 L flask. The culture was shaken at 37 °C until the optical density at 600 nm reached 0.6-0.8, then the flask was placed in an ice/water bath for ca. 30 min before the addition of isopropylthio-β-D-galactoside (IPTG) to a final concentration of 100 μM. The culture was shaken for an additional 12-14 h at 18 ºC. The cells (1.5-2 g wet mass from 0.5 L culture) were collected by centrifugation.

References

[1] Z. Li, Z. Wang, G. Meng, H. Lu, Z. Huang and F. Chen, *Asian. J. Org. Chem.* 2018, **7**, 763–769.

General procedures for the synthesis of substrates

Method A

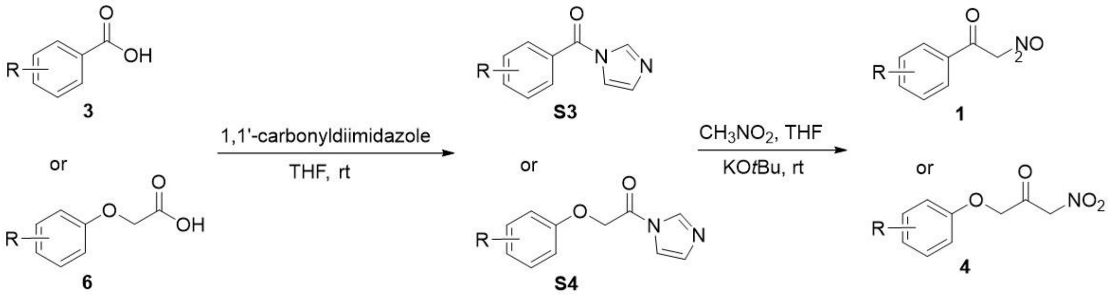


Scheme S1. General procedures for the synthesis of substrates using method A.[1]

To a stirred solution of imidazole (2 equiv.) in anhydrous THF (100 mL) was dropwise added benzoyl chloride **S1** (1 equiv.). The resulting mixture was stirred vigorously at room temperature overnight. Thus formed white precipitate was filtered and washed with THF. The combined filtrate was concentrated to give crude **S2** as a light yellow oil which was used in the next step without further purification.

To a stirred solution of KO*t*Bu (1.5 equiv.) in anhydrous THF (75 mL) was dropwise added CH_3NO_2 (6 equiv.) and the resulting mixture was stirred at room temperature for 2 h, at which time crude **S2** in THF was added dropwise. The resulting mixture was then stirred vigorously at room temperature for 24 h. The nitronate salt was filtered, washed with CH_2Cl_2 (50 mL) and dissolved in cold water (100 mL). The aqueous solution was then acidified slowly with 6 M HCl to pH 4-5 and then extracted with CH_2Cl_2 (3 ×50 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated to give pale yellow solids **1**.

Method B

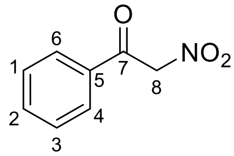
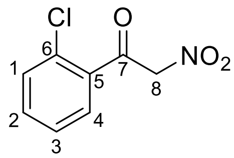
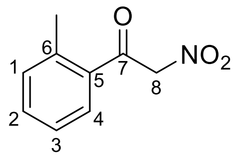


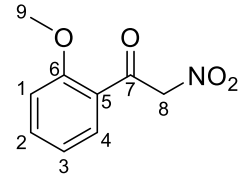
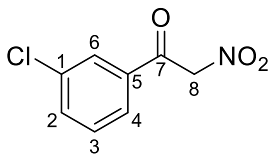
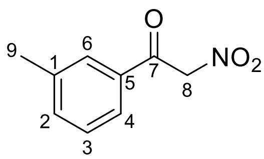
Scheme S2. General procedures for the synthesis of substrates using method B.[1]

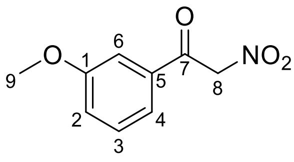
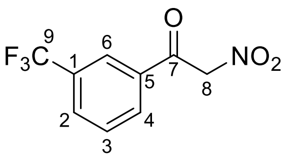
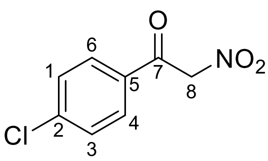
A solution of acid **3** or **6** (1 equiv.) and 1,1'-carbonyldiimidazole (1.2 equiv.) in anhydrous THF (150 mL) was refluxed for 1 h. The resulting mixture was concentrated to give crude **S3** or **S4** as a light yellow oil which was used in the next step without further purification.

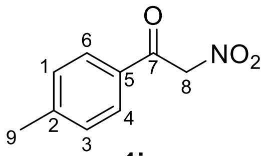
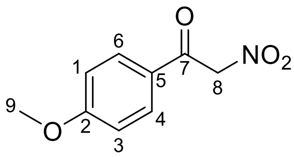
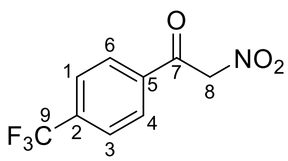
To a solution of KO*t*Bu (1.5 equiv.) in anhydrous THF (11 mL) was dropwise added CH_3NO_2 (6 equiv.) and the resulting mixture was stirred at room temperature for 2 h, at which time crude **S3** or **S4** in THF was added dropwise. The resulting mixture was stirred vigorously at room temperature for 24 h. The nitronate salt was filtered, washed with CH_2Cl_2 (50 mL) and dissolved in cold water (100 mL). The aqueous solution was acidified slowly with 6 M HCl to pH 4-5 and extracted with CH_2Cl_2 (3 × 50 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated to give an orange solid which was purified by flash chromatography to yield pale yellow solids **1** or **4**.

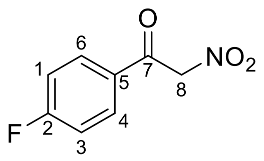
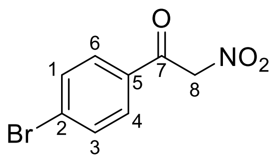
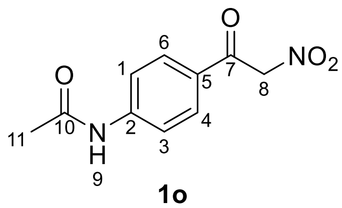
Table S1. Characterization of ketones 1a-1w and 4a-4j.

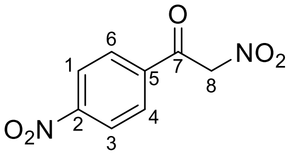
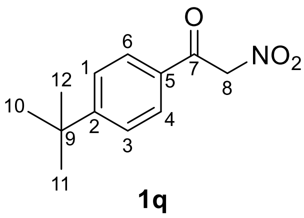
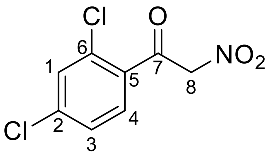
 **1a**	**2-nitro-1-phenylethan-1-one** (Method B, prepared from benzoic acid, pale yellow solid, yield 77%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.98-7.96 (m, 2H, Ar-H), 7.78-7.74 (m, 1H, Ar-H), 7.63-7.60 (m, 1H, Ar-H), 6.57 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.87 135.31 133.93 129.55, 128.92, 83.29.
 **1b**	**1-(2-chlorophenyl)-2-nitroethan-1-one** (Method B, prepared from 2-chlorobenzoic acid, pale yellow solids, yield 79%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.93-7.91 (m, 1H, Ar-H), 7.68-7.63 (m, 2H, Ar-H), 7.56-7.52 (m, 1H, Ar-H), 6.44 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 189.36, 134.71, 133.79, 131.75, 131.03, 128.02, 84.54.
 **1c**	**2-nitro-1-(o-tolyl)ethan-1-one** (Method A, prepared from 2-methylbenzoyl chloride, pale yellow solids, yield 86%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.87-7.84 (m, 1H, Ar-H), 7.59-7.55 (m, 1H, Ar-H), 7.43-7.39 (m, 2H, Ar-H), 6.45 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 190.92, 139.65, 133.79, 133.42, 132.73, 130.34, 126.70, 84.51, 21.55.

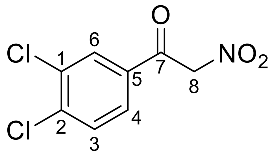
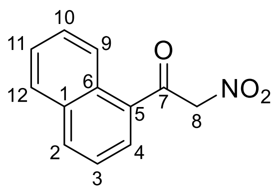
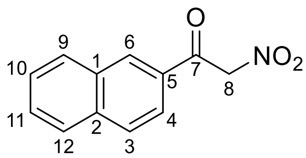
 **1d**	**1-(2-methoxyphenyl)-2-nitroethan-1-one** (Method B, prepared from 2-methoxybenzoic acid, pale yellow solids, yield 75%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.85-7.83 (m, 1H, Ar-H), 7.71-7.67 (m, 1H, Ar-H), 7.26-7.23 (m, 1H, Ar-H), 7.14-7.10 (m, 1H, Ar-H), 6.12 (s, 2H, C_8-H), 3.93 (s, 3H, C_9-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 187.90, 160.16, 136.79, 130.67, 123.56, 121.33, 113.38, 86.24, 56.51.
 **1e**	**1-(3-chlorophenyl)-2-nitroethan-1-one** (Method B, prepared from 3-chlorobenzoic acid, pale yellow solids, yield 68%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.00-7.99 (m, 1H, Ar-H), 7.93-7.91 (m, 1H, Ar-H), 7.84-7.82 (m, 1H, Ar-H), 7.67-7.63 (m, 1H, Ar-H), 6.57 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.02, 135.71, 134.92, 134.43, 131.48, 128.67, 127.50, 83.25.
 **1f**	**2-nitro-1-(m-tolyl)ethan-1-one** (Method B, prepared from 3-methylbenzoic acid, pale yellow solids, yield 65%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.79-7.75 (m, 2H, Ar-H), 7.58-7.56 (m, 1H, Ar-H), 7.51-7.47 (m, 1H, Ar-H), 6.52 (s, 2H, C_8-H), 2.40 (s, 3H, C_9-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.88, 139.11, 135.93, 133.95, 129.44, 129.21, 126.17, 83.27, 21.23.

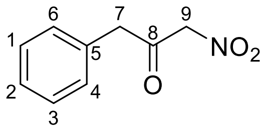
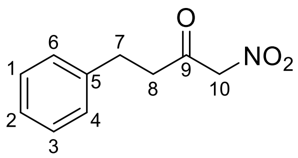
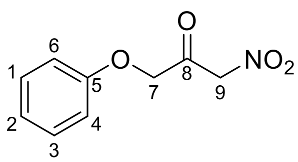
 **1g**	**1-(3-methoxyphenyl)-2-nitroethan-1-one** (Method B, prepared from 3-methoxybenzoic acid, pale yellow solids, yield 72%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.56-7.53 (m, 2H, Ar-H), 7.46 (m, 1H, Ar-H), 7.35-7.29 (m, 1H, Ar-H), 6.54 (s, 2H, C_8-H), 3.85 (s, 3H, C_9-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.72, 160.02, 135.20, 130.77, 121.35, 121.30, 113.41, 83.35, 55.98.
 **1h**	**2-nitro-1-(3-(trifluoromethyl)phenyl)ethan-1-one** (Method B, prepared from 3-(trifluoromethyl)benzoic acid, pale yellow solids, yield 77%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.28-8.27 (m, 2H, Ar-H), 8.16-8.14 (m, 1H, Ar-H), 7.91-7.87 (m, 1H, Ar-H), 6.67 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.17, 134.73, 132.80, 131.44 (q, J = 3.76 Hz), 130.86, 130.29 (q, J = 37.6 Hz), 125.49 (q, J = 3.84 Hz), 124.09 (q, J = 270.86 Hz).
 **1i**	**1-(4-chlorophenyl)-2-nitroethan-1-one** (Method B, prepared from 4-chlorobenzoic acid, pale yellow solids, yield 66%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.98-7.95 (m, 2H, Ar-H), 7.71-7.68 (m, 2H, Ar-H), 6.55 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.80, 140.30, 132.65, 130.80, 129.69, 83.20.

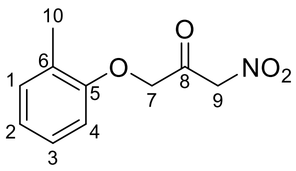
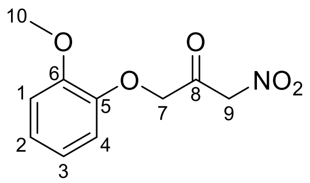
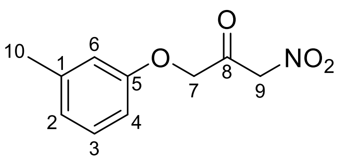
 **1j**	**2-nitro-1-(p-tolyl)ethan-1-one** (Method B, prepared from 4-methylbenzoic acid, pale yellow solids, yield 72%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.86-7.85 (m, 2H, Ar-H), 7.43-7.41 (m, 2H, Ar-H), 6.51 (s, 2H, C_8-H), 2.42 (s, 3H, C_9-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.31, 146.14, 131.46, 130.10, 129.02, 83.20, 21.78.
 **1k**	**1-(4-methoxyphenyl)-2-nitroethan-1-one** (Method B, prepared from 4-methoxybenzoic acid, pale yellow solids, yield 75%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ/ppm 7.89-7.87 (m, 2H, Ar-H), 7.03-7.01 (m, 2H, Ar-H), 5.86 (s, 2H, C_8-H), 3.93 (s, 3H, C_9-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 184.00, 165.04, 130.76, 126.44, 114.57, 81.06, 55.72.
 **1l**	**2-nitro-1-(4-(trifluoromethyl)phenyl)ethan-1-one** (Method B, prepared from 4-(trifluoromethyl)benzoic acid, pale yellow solids, yield 61%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.17-8.15 (m, 2H, Ar-H), 7.99-7.97 (m, 2H, Ar-H), 6.61 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.47, 137.13, 134.28, (q, *J* = 32.03 Hz), 129.77, 126.46 (q, *J* = 3.6 Hz), 124.02 (q, *J* = 271.21Hz), 83.33.

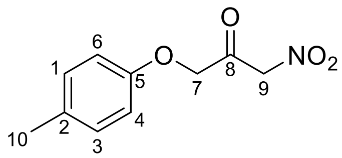
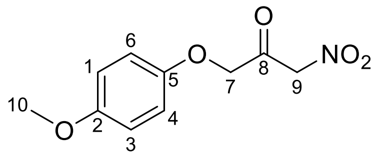
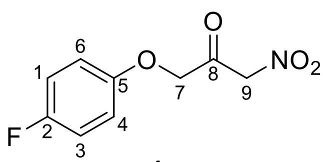
 **1m**	**1-(4-fluorophenyl)-2-nitroethan-1-one** (Method B, prepared from 4-fluorobenzoic acid, pale yellow solids, yield 76%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.06-8.03 (m, 2H, Ar-H), 7.47-7.43 (m, 2H, Ar-H), 6.54 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 187.52, 166.38 (d, *J* = 252.74 Hz), 132.12 (d, *J* = 9.86 Hz), 130.70 (d, *J* = 2.85 Hz), 116.72 (d, *J* = 22.26 Hz), 83.16.
 **1n**	**1-(4-bromophenyl)-2-nitroethan-1-one** (Method B, prepared from 4-bromobenzoic acid, pale yellow solids, yield 61%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.89-7.81 (m, 4H, Ar-H), 6.54 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.22, 132.98, 132.65, 130.83, 129.59, 83.16.
 **1o**	**N-(4-(2-nitroacetyl)phenyl)acetamide** (Method B, prepared from 4-acetamidobenzoic acid, pale yellow solids, yield 61%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 10.41(s, 1H, N-H), 7.92-7.89 (m, 2H, Ar-H), 7.79-7.75 (m, 2H, Ar-H), 6.45 (s, 2H, C_8-H), 2.12 (s, 3H, C_{11}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 187.10, 169.68, 145.54, 130.42, 128.30, 118.78, 82.99, 24.71.

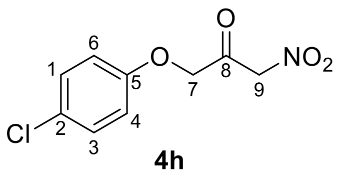
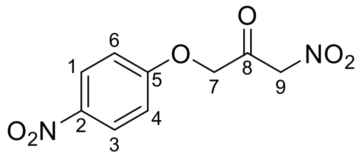
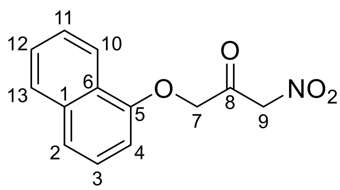
 **1p**	**2-nitro-1-(4-nitrophenyl)ethan-1-one** (Method B, prepared from 4-nitrobenzoic acid, pale yellow solids, yield 65%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.42-8.40 (m, 2H, Ar-H), 8.20-8.18 (m, 2H, Ar-H), 6.63 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.18, 151.18, 138.47, 130.39, 124.49, 83.37.
 **1q**	**1-(4-(tert-butyl)phenyl)-2-nitroethan-1-one** (Method B, prepared from 4-(*tert*-butyl)benzoic acid, pale yellow solids, yield 64%). ^{1}H NMR (DMSO$_3$, 400 MHz) δ/ppm 7.92-7.89 (m, 2H, Ar-H), 7.64-7.62 (m, 2H, Ar-H), 6.52 (s, 2H, C_8-H), 1.32 (s, 9H, C_{10}, C_{11}, C_{12}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.23, 158.62, 131.46, 128.91, 126.38, 83.19, 35,52, 31.14.
 **1r**	**1-(2,4-dichlorophenyl)-2-nitroethan-1-one** (Method B, prepared from 2,4-dichlorobenzoic acid, pale yellow solids, yield 56%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.96-7.94 (m, 1H, Ar-H), 7.83-7.82 (m, 1H, Ar-H), 7.66-7.64 (m, 1H, Ar-H), 6.42 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.42, 138.84, 133.23, 132.48, 131.36, 128.24, 84.45.

 **1s**	**1-(3,4-dichlorophenyl)-2-nitroethan-1-one** (Method B, prepared from 3,4-dichlorobenzoic acid, pale yellow solids, yield 80%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.18-8.17 (m, 1H, Ar-H), 7.92-7.87 (m, 2H, Ar-H), 6.56 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 187.26, 138.12, 134.06, 132.59, 131.83, 130.88, 128.77, 83.14.
 **1t**	**1-(naphthalen-2-yl)-2-nitroethan-1-one** (Method A, prepared from 1-naphthoyl chloride, reddish solid, yield 84%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.74-8.72 (m, 1H, Ar-H), 8.30-8.28 (m, 1H, Ar-H), 8.23-8.21 (m, 1H, Ar-H), 8.08-8.06 (m, 1H, Ar-H), 7.75-7.64 (m, 3H, Ar-H), 6.64 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 191.09, 135.46, 134.02, 131.10, 130.56, 130.06, 129.39, 129.33, 127.37, 125.37, 125.20, 84.55.
 **1u**	**1-(naphthalen-2-yl)-2-nitroethan-1-one** (Method A, prepared from 2-naphthoyl chloride, reddish solid, yield 83%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.68-8.67 (m, 1H, Ar-H), 8.14-8.04 (m, 3H, Ar-H), 7.98-7.96 (m, 1H, Ar-H), 7.77-7.66 (m, 2H, Ar-H), 6.68 (s, 2H, C_8-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 188.70, 136.13, 132.38, 131.64, 131.27, 130.20, 129.98, 129.26, 128.32, 127.87, 123.60, 83.28.

 **1v**	**1-nitro-3-phenylpropan-2-one** (Method B, prepared from 2-phenylacetic acid, pale yellow solids, yield 64%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.38-7.23 (m, 5H, Ar-H), 5.92 (s, 2H, C_9-H), 3.95 (s, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 196.94, 133.31, 130.35, 128.91, 127.55, 84.54, 46.47.
 **1w**	**1-nitro-4-phenylbutan-2-one** (Method B, prepared from 3-phenylpropanoic acid, pale yellow solids, yield 83%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.32-7.19 (m, 5H, Ar-H), 5.85 (s, 2H, C_{10}-H), 2.95-2.91 (m, 2H, C_8 -H), 2.88-2.82 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 198.42, 140.83, 128.83, 128.70, 126.54, 84.63, 41.51, 28.72.
 **4a**	**1-nitro-3-phenoxypropan-2-one** (Method B, prepared from 2-phenoxyacetic acid, pale yellow solids, yield 73%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.35-7.31 (m, 2H, Ar-H), 7.02-6.97 (m, 3H, Ar-H), 5.98 (s, 2H, C_9-H), 5.03 (s, 2H, C_7 -H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.54, 157.78, 130.03, 121.93, 115.02, 82.61, 71.10. HRMS Calcd. For $C_9H_8NO_4[M-H]^-$: 194.0459, Found: 194.0456.

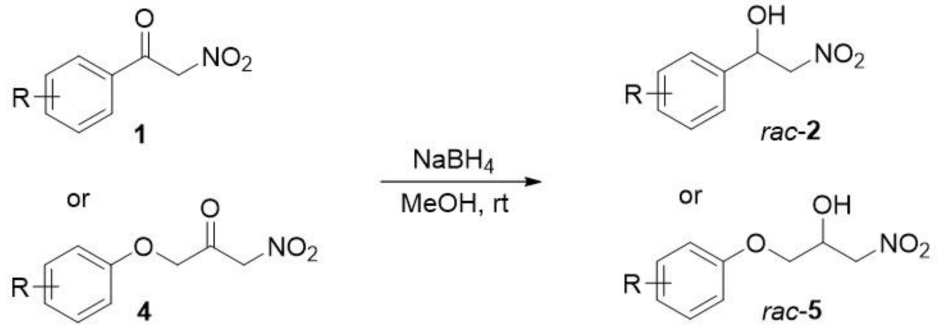
 **4b**	**1-nitro-3-(o-tolyloxy)propan-2-one** (Method B, prepared from 2-(o-tolyloxy)acetic acid, pale yellow solids, yield 77%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.20-7.14 (m, 2H, Ar-H), 6.93-6.88 (m, 2H, Ar-H), 6.00 (s, 2H, C_9-H), 5.01 (s, 2H, C_7 -H), 2.24 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.87, 155.84, 131.13, 127.36, 126.41, 121.65, 111.92, 82.78, 71.44, 16.43. HRMS Calcd. For $C_{10}H_{10}NO_4[M-H]^-$: 208.0615, Found: 208.0610.
 **4c**	**1-(2-methoxyphenoxy)-3-nitropropan-2-one** (Method B, prepared from 2-(2-methoxyphenoxy)acetic acid, pale yellow solids, yield 69%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.04-6.95 (m, 3H, Ar-H), 6.91-6.86 (m, 1H, Ar-H), 5.96 (s, 2H, C_9-H), 4.97 (s, 2H, C_7 -H), 3.79 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.82, 149.64, 147.34, 122.87, 121.08, 115.21, 113.11, 82.64, 72.46, 56.05. HRMS Calcd. For $C_{10}H_{10}NO_5[M-H]^-$: 224.0564, Found: 224.0563.
 **4d**	**1-nitro-3-(m-tolyloxy)propan-2-one** (Method B, prepared from 2-(m-tolyloxy)acetic acid, pale yellow solids, yield 65%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.21-7.17 (m, 1H, Ar-H), 6.83-6.75 (m, 3H, Ar-H), 5.96 (s, 2H, C_9-H), 4.99 (s, 2H, C_7 -H), 2.29 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.57, 157.79, 139.64, 129.75, 122.68, 115.69, 111.95, 82,60, 71.08, 21.51. HRMS Calcd. For $C_{10}H_{10}NO_4[M-H]^-$: 208.0615, Found: 208.0614.

 **4e**	**1-nitro-3-(p-tolyloxy)propan-2-one** (Method B, prepared from 2-(p-tolyloxy)acetic acid, pale yellow solids, yield 74%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.13-7.11 (m, 2H, Ar-H), 6.88-6.85 (m, 2H, Ar-H), 5.96 (s, 2H, C_9-H), 4.98 (s, 2H, C_7 -H), 2.25 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.67, 155.71, 130.72, 130.34, 114.86, 82.61, 71.25, 20.50. HRMS Calcd. For $C_{10}H_{10}NO_4[M-H]^-$: 208.0615, Found: 208.0606.
 **4f**	**1-(4-methoxyphenoxy)-3-nitropropan-2-one** (Method B, prepared from 2-(4-methoxyphenoxy)acetic acid, pale yellow solids, yield 81%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 6.93-6.87 (m, 4H, Ar-H), 5.95 (s, 2H, C_9-H), 4.95 (s, 2H, C_7 -H), 3.72 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.85, 154.49, 151.80, 116.06, 115.10, 82.64, 71.87, 55.83. HRMS Calcd. For $C_{10}H_{10}NO_5[M-H]^-$: 224.0564, Found: 224.0565.
 **4g**	**1-(4-fluorophenoxy)-3-nitropropan-2-one** (Method B, prepared from 2-(4-fluorophenoxy)acetic acid, pale yellow solids, yield 63%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.17-7.12 (m, 2H, Ar-H), 7.01-6.98 (m, 2H, Ar-H), 5.96 (s, 2H, C_9-H), 5.01 (s, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.45, 157.45 (d, J = 235.32 Hz), 154.14 (d, J = 2.06 Hz), 116.49, 116.33 (d, J = 16.19 Hz), 82.55, 71.71. HRMS Calcd. For $C_9H_7FNO_4[M-H]^-$: 212.0365, Found: 212.0368.

 **4h**	**1-(4-chlorophenoxy)-3-nitropropan-2-one** (Method B, prepared from 2-(4-chlorophenoxy)acetic acid, pale yellow solids, yield 51%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.38-7.35 (m, 2H, Ar-H), 7.02-6.99 (m, 2H, Ar-H), 5.96 (s, 2H, C_9-H), 5.04 (s, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.20, 156.70, 129.76, 125.68, 116.85, 82.52, 71.35. HRMS Calcd. For $C_9H_7ClNO_4[M-H]^-$: 228.0069, Found: 228.0078.
 **4i**	**1-nitro-3-(4-nitrophenoxy)propan-2-one** (Method B, prepared from 2-(4-nitrophenoxy)acetic acid, pale yellow solids, yield 81%). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.25-8.21 (m, 2H, Ar-H), 7.21-7.18 (m, 2H, Ar-H), 5.98 (s, 2H, C_9-H), 5.24 (s, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 194.46, 163.03, 141.97, 126.29, 115.67, 82.41, 71.50. HRMS Calcd. For $C_9H_7N_2O_6[M-H]^-$: 239.0310, Found: 239.0315.
 **4j**	**1-(naphthalen-1-yloxy)-3-nitropropan-2-one** (Method B, prepared from 2-(naphthalen-1-yloxy)acetic acid, pale yellow solids, yield 66%). ^{1}H NMR ($DMSO_3$, 400 MHz) δ/ppm 8.31-8.28 (m, 1H, Ar-H), 7.92-7.90 (m, 1H, Ar-H), 7.58-7.54 (m, 3H, Ar-H), 7.46-7.42 (m, 1H, Ar-H), 6.99-6.97 (m, 1H, Ar-H), 6.14 (s, 2H, C_9-H), 5.21 (s, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 195.57, 153.20, 134.58, 127.97, 127.13, 126.40, 126.08, 125.13, 122.13, 121.47, 106.18, 82.97, 71.71. HRMS Calcd. For

	$C_{13}H_{10}NO_4$[M-H]$^-$: 244.0615, Found: 244.0614.

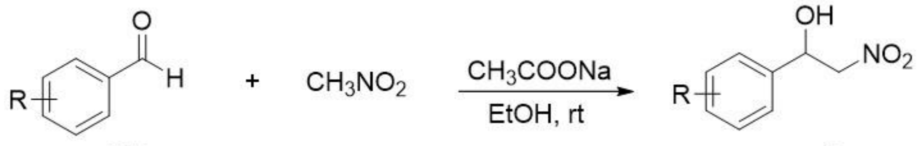
General procedures for the synthesis of *racemic* alcohols
Method C



Scheme S3. General procedures for the synthesis of *racemic* alcohols using method C.[2]

To a stirred solution of ketones **1** or **4** (1.0 eqiuv.) in methanol (5 mL) was added sodium borohydride (1.0 equiv.) in portion. When the reduction was completed (monitored by the TLC), a few drops of 1 M HCl were added. The solvent was evaporated *in vacuo*. Then water (10 mL) was added to the residue and the solution was extracted with DCM (3 x 10 mL). The organic layers were combined and dried over Na_2SO_4. The solvent was evaporated and the residue was purified by flash column chromatography (silica gel) using mixtures of petroleum ether /ethyl acetate or DCM/methanol as eluents to afford products *rac*-**2** or *rac*-**5**. Isolated yields: 45 -80%.

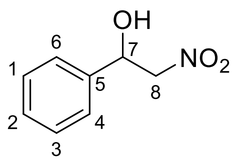
Method D

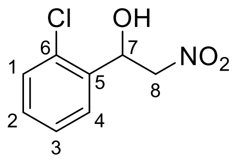
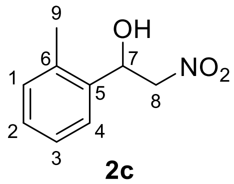
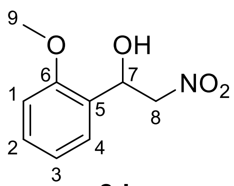
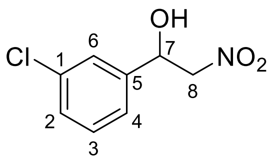
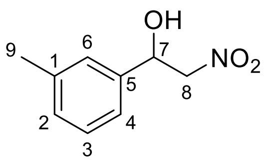


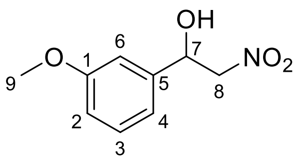
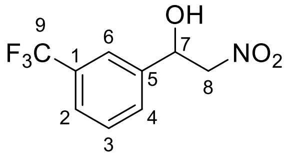
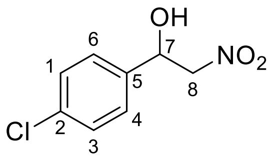
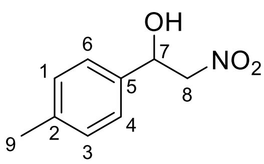
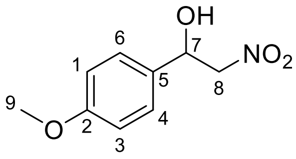
Scheme S4. General procedures for the synthesis of *racemic* alcohols using method D.[3]

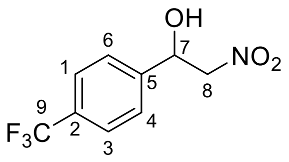
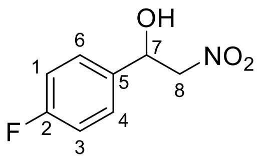
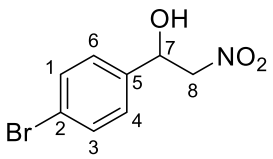
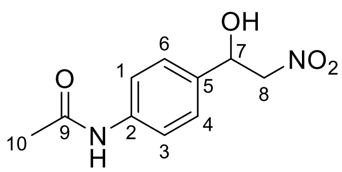
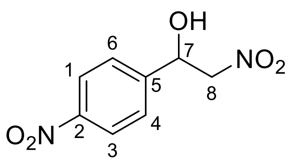
To a solution of aldehyde **S5** (1.0 equiv.) and nitromethane (1.4 equiv.) in ethanol (15 mL) was added sodium acetate (0.3 equiv.) at room temperature. The resulting suspension was stirred for 24 h, and was then filtered. The filtrate was concentrated *in vacuo* and the residue was purified by flash column chromatography to afford products *rac*-**2**. Isolated yields: 56-88%.

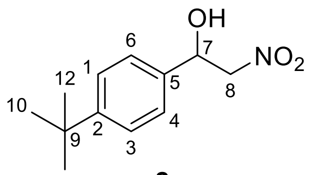
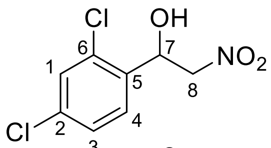
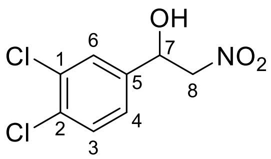
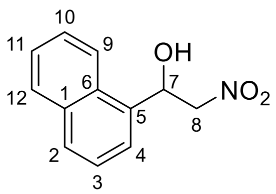
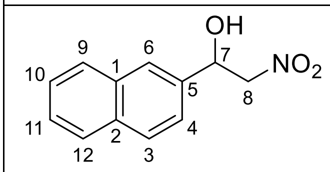
Table S2. Characterization of *racemic* alcohols 2a-2w and 5a-5j.

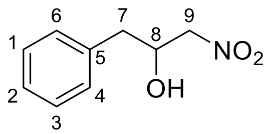
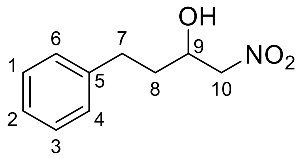
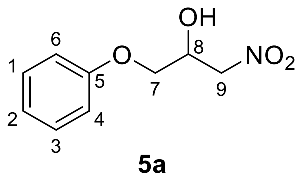
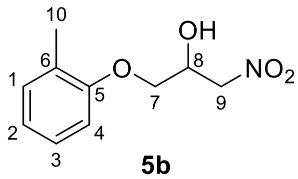
 **2a**	**2-nitro-1-phenylethan-1-ol** (Method B, prepared from benzaldehyde, colorless liquid). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.46-7.40 (m, 2H, Ar-H), 7.38-7.37 (m, 2H, Ar-H), 7.34-7.30 (m, 1H, Ar-H), 6.09 (d, 1H, *J* = 4.96 Hz, O-H), 5.30-5.25 (m, 1H, C_7-H), 4.87-4.83 (m, 1H, C_8-H), 4.60-4.54 (m, 1H, C_8-H).

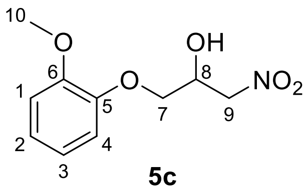
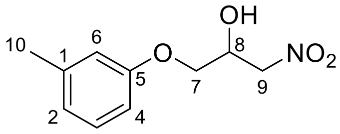
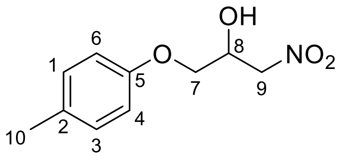
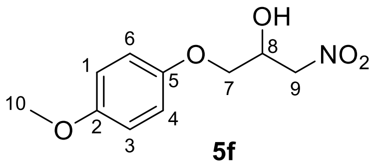
 **2b**	**1-(2-chlorophenyl)-2-nitroethan-1-ol** (Method D, prepared from 2-chlorobenzaldehyde, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.68-7.66 (m, 1H, Ar-H), 7.49 – 7.35 (m, 3H, Ar-H), 6.32 (d, 1H, *J* = 4.96 Hz, O-H), 5.64-5.59 (m, 1H, C_7-H), 4.85-4.81 (m, 1H, C_8-H), 4.53-4.51 (m, 1H, C_8-H).
 **2c**	**2-nitro-1-(o-tolyl)ethan-1-ol** (Method D, prepared from 2-methylbenzaldehyde, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.52-7.50 (m, 1H, Ar-H), 7.27 – 7.18 (m, 3H, Ar-H), 5.99 (d, 1H, *J* = 4.84 Hz, O-H), 5.50-5.45 (m, 1H, C_7-H), 4.83-4.80 (m, 1H, C_8-H), 4.51-4.46 (m, 1H, C_8-H), 2.37, (s, 3H, C_9-H).
 **2d**	**1-(2-methoxyphenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(2-methoxyphenyl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.50-7.48 (m, 1H, Ar-H), 7.34–7.29 (m, 1H, Ar-H), 7.03-6.98 (m, 2H, Ar-H), 5.96 (d, 1H, *J* = 5.24 Hz, O-H), 5.58-5.53 (m, 1H, C_7-H), 4.77-4.73 (m, 1H, C_8-H), 4.42-4.36 (m, 1H, C_8-H), 3.84 (s, 3H, C_9-H).
 **2e**	**1-(3-chlorophenyl)-2-nitroethan-1-ol** (Method D, prepared from 3-chlorobenzaldehyde, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.53 (s, 1H, Ar-H), 7.43-7.37 (m, 3H, Ar-H), 6.23 (d, 1H, *J* = 5.08 Hz, O-H), 5.33-5.29 (m, 1H, C_7-H), 4.93-4.88 (m, 1H, C_8-H), 4.64-4.58 (m, 1H, C_8-H).
 **2f**	**2-nitro-1-(m-tolyl)ethan-1-ol** (Method C, prepared from 2-nitro-1-(m-tolyl)ethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.29-7.22 (m, 3H, Ar-H), 7.14-7.12 (m, 1H, Ar-H), 6.05 (d, 1H, *J* = 4.96 Hz, O-H), 5.26-5.21 (m, 1H, C_7-H), 4.85-4.81 (m, 1H, C_8-H), 4.58-4.52 (m, 1H, C_8-H), 2.32 (s, 3H, C_9-H).

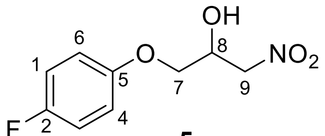
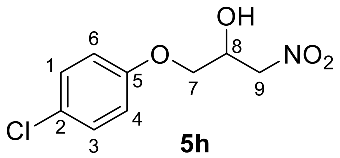
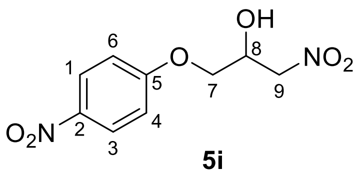
 **2g**	**1-(3-methoxyphenyl)-2-nitroethan-1-ol** (Method D, prepared from 3-methoxybenzaldehyde, colorless liquid). [1]H NMR (400 MHz, DMSO) δ/ppm 7.31-7.27 (m, 1H, Ar-H), 7.03-7.00 (m, 2H, Ar-H), 6.90-6.87 (m, 1H, Ar-H), 6.09 (d, 1H, *J* = 5.24 Hz, O-H), 5.28-5.23 (m, 1H, C_7-H), 4.88-4.84 (m, 1H, C_8-H), 4.59-4.53 (m, 1H, C_8-H), 3.77 (m, 3H, C_9-H).
 **2h**	**2-nitro-1-(3-(trifluoromethyl)phenyl)ethan-1-ol** (Method D, prepared from 3-(trifluoromethyl)benzaldehyde, colorless liquid). [1]H NMR (400 MHz, DMSO) δ/ppm 7.83 (s, 1H, Ar-H), 7.78-7.73 (m, 1H, Ar-H), 7.70 – 7.68 (m, 1H, Ar-H), 7.65-7.61 (m, 1H, Ar-H), 6.31 (d, 1H, *J* = 5.06 Hz, O-H), 5.43-5.39 (m, 1H, C_7-H), 4.97-4.93 (m, 1H, C_8-H), 4.68-4.62 (m, 1H, C_8-H).
 **2i**	**1-(4-chlorophenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(4-chlorophenyl)-2-nitroethan-1-one, colorless liquid). [1]H NMR (400 MHz, DMSO) δ/ppm 7.49-7.43 (m, 4H, Ar-H), 6.19 (d, 1H, *J* = 4.96 Hz, O-H), 5.31-5.26 (m, 1H, C_7-H), 4.88-4.84 (m, 1H, C_8-H), 4.60-4.54 (m, 1H, C_8-H).
 **2j**	**2-nitro-1-(p-tolyl)ethan-1-ol** (Method D, prepared from 4-methylbenzaldehyde, colorless liquid). [1]H NMR (400 MHz, DMSO) δ/ppm 7.34-7.32 (m, 2H, Ar-H), 7.20-7.18 (m, 2H, Ar-H), 6.02 (d, 1H, *J* = 5.04 Hz, O-H), 5.26-5.22 (m, 1H, C_7-H), 4.83-4.79 (m, 1H, C_8-H), 4.58-4.52 (m, 1H, C_8-H), 2.31 (s, 3H, C_9-H).
 **2k**	**1-(4-methoxyphenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(4-methoxyphenyl)-2-nitroethan-1-one, colorless liquid). [1]H NMR (400 MHz, $CDCl_3$) δ/ppm 7.36-7.33 (m, 2H, Ar-H), 6.96-6.93 (m, 2H, Ar-H), 5.45-5.42 (m, 1H, C_7-H), 4.66-4.59 (m, 1H, C_8-H), 4.52-4.48 (m, 1H, C_8-H), 3.84, (s, 3H, C_9-H).

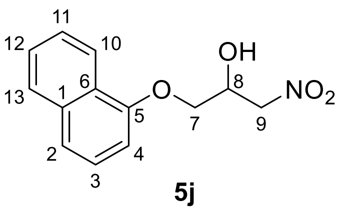
 **2l**	**2-nitro-1-(4-(trifluoromethyl)phenyl)ethan-1-ol** (Method C, prepared from 1-(4-bromophenyl)-2-nitroethan-1-one, coreless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.76-7.74 (m, 2H, Ar-H), 7.70-7.68 (m, 2H, Ar-H), 6.33 (d, 1H, *J* = 4.96 Hz, O-H), 5.41-5.37 (m, 1H, C_7-H), 4.95-4.91 (m, 1H, C_8-H), 4.65-4.59 (m, 1H, C_8-H).
 **2m**	**1-(4-fluorophenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(4-fluorophenyl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.51-7.47 (m, 2H, Ar-H), 7.23-7.18 (m, 2H, Ar-H), 6.14 (d, 1H, *J* = 4.96 Hz, O-H), 5.31-5.26 (m, 1H, C_7-H), 4.86-4.82 (m, 1H, C_8-H), 4.61-4.55 (m, 1H, C_8-H).
 **2n**	**1-(4-bromophenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(4-bromophenyl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.59-7.56 (m, 2H, Ar-H), 7.42-7.40 (m, 2H, Ar-H), 6.19 (d, 1H, *J* = 4.96 Hz, O-H), 5.29-5.25 (m, 1H, C_7-H), 4.88-4.84 (m, 1H, C_8-H), 4.60-4.54 (m, 1H, C_8-H).
 **2o**	**N-(4-(1-hydroxy-2-nitroethyl)phenyl)acetamide** (Method C, prepared from N-(4-(2-nitroacetyl)phenyl)acetamide, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 9.95 (s, 1H, N-H), 7.57-7.55 (m, 2H, Ar-H), 7.36-7.34 (m, 2H, Ar-H), 6.01 (d, 1H, *J* = 4.92 Hz, O-H), 5.22-5.20 (m, 1H, C_7-H), 4.82-4.78 (m, 1H, C_8-H), 4.57-4.52 (m, 1H, C_8-H), 2.04 (s, 3H, C_{10}-H).
 **2p**	**2-nitro-1-(4-nitrophenyl)ethan-1-ol** (Method C, prepared from 2-nitro-1-(4-nitrophenyl)ethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 8.26-8.23 (m, 2H, Ar-H), 7.76-7.73 (m, 2H, Ar-H), 6.43 (d, 1H, *J* = 5 Hz, O-H), 5.46-5.42

	(m, 1H, C_7-H), 4.97-4.93 (m, 1H, C_8-H), 4.68-4.61 (m, 1H, C_8-H).
 **2q**	**1-(4-(*tert*-butyl)phenyl)-2-nitroethan-1-ol** (Method C, prepared from 1-(4-*(tert*-butyl)phenyl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.42-7.36 (m, 4H, Ar-H), 6.01 (s, 1H, O-H), 5.27-5.23 (m, 1H, C_7-H), 4.85-4.81 (m, 1H, C_8-H), 4.59-4.53 (m, 1H, C_8-H), 1.29, (s, 9H, C_{10}, C_{11}, C_{12}-H).
 **2r**	**1-(2,4-dichlorophenyl)-2-nitroethan-1-ol** (Method D, prepared from 2,4-dichlorobenzaldehyde, colorless liquid). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.68-7.65 (m, 2H, Ar-H), 7.53-7.50 (m, 1H, Ar-H), 6.40 (d, 1H, J = 5 Hz, O-H), 5.59-5.55 (m, 1H, C_7-H), 4.85-4.81 (m, 1H, C_8-H), 4.55-4.49 (m, 1H, C_8-H).
 **2s**	**1-(3,4-dichlorophenyl)-2-nitroethan-1-ol** (Method D, prepared from 3,4-dichlorobenzaldehyde, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.73-7.72 (m, 1H, Ar-H), 7.66–7.64 (m, 1H, Ar-H), 7.47-7.44 (m, 1H, Ar-H), 6.31 (d, 1H, J = 5.04 Hz, O-H), 5.34-5.30 (m, 1H, C_7-H), 4.93-4.89 (m, 1H, C_8-H), 4.65-4.60 (m, 1H, C_8-H).
 **2t**	**1-(naphthalen-1-yl)-2-nitroethan-1-ol** (Method C, prepared from 1-(naphthalen-1-yl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (DMSO, 400 MHz) δ/ppm 8.17-8.15 (m, 1H, Ar-H), 8.01-7.99 (m, 1H, Ar-H), 7.94-7.92 (m, 1H, Ar-H), 7.76-7.74 (m, 1H, Ar-H), 7.67-7.62 (m, 1H, Ar-H), 7.60-7.54 (m, 2H, Ar-H), 6.30 (d, 1H, J = 5.02 Hz O-H), 6.07-6.02 (m, 1H, C_7-H), 5.01-4.97 (m, 1H, C_8-H), 4.70-4.64 (m, 1H, C_8-H).
 **2u**	**1-(naphthalen-2-yl)-2-nitroethan-1-ol** (Method C, prepared from 1-(naphthalen-2-yl)-2-nitroethan-1-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.98-7.91 (m, 4H, Ar-H), 7.60 – 7.52 (m, 3H, Ar-H), 6.25 (d, 1H, J = 4.72 Hz, O-H),

	5.47-5.43 (m, 1H, C_7-H), 4.98-4. 94 (m, 1H, C_8-H), 4.70-4.65 (m, 1H, C_8-H).
 **2v**	**1-nitro-3-phenylpropan-2-ol** (Method D, prepared from 2-phenylacetaldehyde, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.37-7.16 (m, 5H, Ar-H), 5.51 (d, 1H, *J* = 5.84 Hz, O-H), 4.65-4.60 (m, 1H, C_9-H), 4.40-4.29 (m, 2H, C_8-H, C_9-H), 2.81-2.71 (m, 2H, C_7-H).
 **2w**	**1-nitro-4-phenylbutan-2-ol** (Method D, prepared from 3-phenylpropanal, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.32-7.17 (m, 5H, Ar-H), 5.45 (d, 1H, *J* = 6.32 Hz, O-H), 4.73-4.69 (m, 1H, C_{10}-H), 4.42-4.36 (m, 1H, C_{10}-H), 4.14-4.07 (m, 1H, C_9-H), 2.77-2.60 (m, 2H, C_7-H), 1.78-1.64 (m, 2H, C_8-H).
 **5a**	**1-nitro-3-phenoxypropan-2-ol** (Method C, prepared from 1-nitro-3-phenoxypropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.33-7.28 (m, 2H, Ar-H), 6.99-6.95 (m, 3H, Ar-H), 5.86 (d, 1H, *J* = 5.64 Hz, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.61-4.55 (m, 1H, C_9-H), 4.53-4.46 (m, 1H, C_8-H), 4.07-3.97 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.62, 130.00, 121.40, 115.02, 79.53, 69.46, 67.28. HRMS Calcd. For $C_9H_{10}NO_4[M-H]^-$: 196.0615. Found: 196.0619.
 **5b**	**1-nitro-3-(o-tolyloxy)propan-2-ol** (Method C, prepared from 1-nitro-3-(o-tolyloxy)propan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.18-7.14 (m, 2H, Ar-H), 6.93-6.84 (m, 2H, Ar-H), 5.85 (d, 1H, *J* = 5.68 Hz, O-H), 4.91-4.87 (m, 1H, C_9-H), 4.64-4.58 (m, 1H, C_9-H), 4.55-4.49 (m, 1H, C_8-H), 4.06-3.96 (m, 2H, C_7-H), 2.18 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 156.64, 130.94, 127.44, 126.45, 121.10, 111.82, 79.71, 69.62, 67.39, 16.37. HRMS Calcd. For $C_{10}H_{12}NO_4[M-H]^-$: 210.0772. Found: 210.0771.

 **5c**	**1-(2-methoxyphenoxy)-3-nitropropan-2-ol** (Method C, prepared from 1-(2-methoxyphenoxy)-3-nitropropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.01-6.87 (m, 4H, Ar-H), 5.84-5.83 (s, 1H, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.60-4.55 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.03-3.94 (m, 2H, C_7-H), 3.35 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 149.80, 148.14, 122.21, 121.22, 114.85, 112.92, 79.63, 70.72, 67.38, 56.04.
 **5d**	**1-nitro-3-(m-tolyloxy)propan-2-ol** (Method C, prepared from 1-nitro-3-(m-tolyloxy)propan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.20-7.16 (m, 1H, Ar-H), 6.79-6.74 (m, 3H, Ar-H), 5.85 (d, 1H, *J* = 5.64 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.05-3.94 (m, 2H, C_7-H), 2.29 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.63, 139.51, 129.72, 122.14, 115.67, 112.03, 79.54, 69.41, 67.29, 21.56.
 **5e**	**1-nitro-3-(p-tolyloxy)propan-2-ol** (Method C, prepared from 1-nitro-3-(p-tolyloxy)propan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.11-7.09 (m, 2H, Ar-H), 6.86-6.81 (m, 2H, Ar-H), 5.84 (d, 1H, *J* = 5.68 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.59-4.54 (m, 1H, C_9-H), 4.51-4.44 (m, 1H, C_8-H), 4.01-3.92 (m, 2H, C_7-H), 2.24 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 156.53, 130.32, 130.09, 114.90, 79.55, 69.61, 67.31, 20.55. HRMS Calcd. For $C_{10}H_{12}NO_4$[M-H]$^-$: 210.0772. Found: 210.0772.
 **5f**	**1-(4-methoxyphenoxy)-3-nitropropan-2-ol** (Method C, prepared from 1-(4-methoxyphenoxy)-3-nitropropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 6.92-6.86 (m, 4H, Ar-H), 5.83 (d, 1H, *J* = 5.68 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.59-4.53 (m, 1H, C_9-H),

	4.50-4.43 (m, 1H, C_8-H), 3.99-3.90 (m, 2H, C_7-H), 3.71 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 154.11, 152.65, 116.05, 115.09, 79.57, 70.19, 67.34, 55.83. HRMS Calcd. For $C_{10}H_{12}NO_5[M-H]^-$: 226.0721. Found: 226.0728.
 **5g**	**1-(4-fluorophenoxy)-3-nitropropan-2-ol** (Method C, prepared from 1-(4-fluorophenoxy)-3-nitropropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.16-7.09 (m, 2H, Ar-H), 7.01-6.95 (m, 2H, Ar-H), 5.86 (d, 1H, *J* = 5.6 Hz, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.51-4.45 (m, 1H, C_8-H), 4.03-3.95 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 157.16 (d, *J* = 234.79 Hz), 155.00 (d, *J* = 1.96 Hz), 116.44, 116.29 (d, *J* = 13.85 Hz), 79.47, 70.21, 67.24. HRMS Calcd. For $C_9H_9FNO_4[M-H]^-$: 214.0521. Found: 214.0529.
 **5h**	**1-(4-chlorophenoxy)-3-nitropropan-2-ol** (Method C, prepared from 1-(4-chlorophenoxy)-3-nitropropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 7.37-7.31 (m, 2H, Ar-H), 7.01-6.96 (m, 2H, Ar-H), 5.88 (d, 1H, *J* = 5.64 Hz, O-H), 4.87-4.84 (m, 1H, C_9-H), 4.60-4.55 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.07-3.97 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 157.53, 129.75, 125.10, 116.85, 79.42, 69.93, 67.17. HRMS Calcd. For $C_9H_9ClNO_4[M-H]^-$: 230.0226. Found: 230.0230.
 **5i**	**1-nitro-3-(4-nitrophenoxy)propan-2-ol** (Method C, prepared from 1-nitro-3-(4-nitrophenoxy)propan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 8.25-8.21 (m, 2H, Ar-H), 7.20-7.16 (m, 2H, Ar-H), 5.97 (d, 1H, *J* = 5.56 Hz, O-H), 4.90-4.87 (m, 1H, C_9-H), 4.64-4.58 (m, 1H, C_9-H), 4.56-4.51 (m, 1H, C_8-H), 4.19-4.18 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 163.95, 141.56,

	126.36, 115.63, 79.23, 70.43, 67.00. HRMS Calcd. For $C_9H_9N_2O_6$[M-H]$^-$: 241.0466. Found: 241.0471.
 **5j**	**1-(naphthalen-1-yloxy)-3-nitropropan-2-ol** (Method C, prepared from 1-(naphthalen-1-yloxy)-3-nitropropan-2-one, colorless liquid). ^{1}H NMR (400 MHz, DMSO) δ/ppm 8.27-8.25 (m, 1H, Ar-H), 7.89-7.87 (m, 1H, Ar-H), 7.57-7.50 (m, 3H, Ar-H), 7.45-7.41 (m, 1H, Ar-H), 6.98-6.97 (m, 1H, Ar-H), 5.99 (d, 1H, *J* = 5.48 Hz, O-H), 5.03-4.99 (m, 1H, C_9-H), 4.76-4.70 (m, 1H, C_9-H), 4.69-4.64 (m, 1H, C_8-H), 4.25-4.16 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 154.11, 134.49, 127.87, 127.01, 126.61, 125.80, 125.33, 122.26, 120.80, 105.73, 79.66, 69.91, 67.35.

References

[1] H. H. Nguyen and M. J. Kurth, *Org. Lett.* 2013, **15**, 362-365.

[2] C. Rodríguez, W. Borzęcka, J. H. Sattler, W. Kroutil, I. Lavandera and V. Gotor, *Org. Biomol. Chem.* 2014, **12**, 673-681.

[3] M. Zhou, D. Dong, B. Zhu, H. Geng, Y. Wang and X. Zhang, *Org. Lett.* 2013, **15**, 5524-5527.

Table S3. The details of genes used in this study.

Name	Accession No.	Source	aa
YDR541c	AAB64983.1	*Saccharomyces cerevisiae*	344
YGL157w	NP_011358.3	*Saccharomyces cerevisiae*	347
YPL113c	NP_015212.1	*Saccharomyces cerevisiae*	396
YHR104w	NP_011972	*Saccharomyces cerevisiae*	327
YNL274c	NP_014125	*Saccharomyces cerevisiae*	350
YDR368w	NP_010656	*Saccharomyces cerevisiae*	312
YGL039w	NP_011476	*Saccharomyces cerevisiae*	348
YNL331c	NP_014068.1	*Saccharomyces cerevisiae*	376
Ymr226c	NP_013953.1	*Saccharomyces cerevisiae*	267
YOL151w	NP_014490.1	*Saccharomyces cerevisiae*	342
YAL060w	NP_009341.2	*Saccharomyces cerevisiae*	382
YOR120w	NP_014763.1	*Saccharomyces cerevisiae*	312
YGL185c	NP_011330.1	*Saccharomyces cerevisiae*	379
LtCR	XP_002554048.1	*Lachancea thermotolerans*	281
RasADH	EU485985	*Ralstonia sp.* DSMZ 6428	250
CgCR	XP_447302.1	*Candida glabrata*	310
KRED1-Pglu	AKP95857.1	*Pichia glucozyma*	252
SsCR	AF160799.1	*Sporidiobolus salmonicolor*	343
SeKRED	XP_018221648.1	*Saccharomyces eubayanus*	342
LbADH	CAD66648.1	*Lactobacillus brevis*	252
LkADH	WP_054768785.1	*Lactobacillus kefiri*	252
SyADH	EU427523.1	*Sphingobium yanoikuyae*	263
TdADH	XP_003678559.1	*Torulaspora delbrueckii*	342
KdoADH	CDO95209.1	*Kluyveromyces dobzhanskii*	342

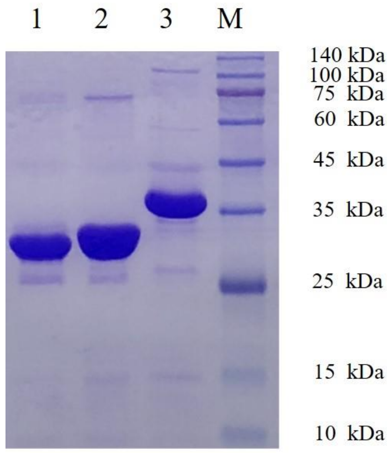


Figure S1. SDS-PAGE analysis of *N*-terminal-His$_6$-SyADH, *N*-terminal-His$_6$-RasADH and *N*-terminal-His$_6$-YGL039w after IMAC purification. Coomassie staining. M: RealBand 3-color Regular Range Protein Marker (Sangon Biotech, China). Lane 1: *N*-terminal-His$_6$-SyADH. Lane 2: *N*-terminal-His$_6$-RasADH. Lane 3: *N*-terminal-His$_6$-YGL039w.

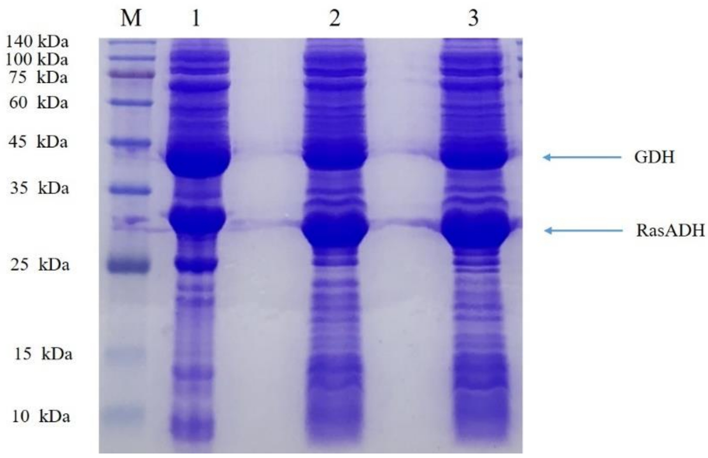


Figure S2. SDS-PAGE analysis of coexpression of RasADH and GDH. Coomassie staining. M: RealBand 3-color Regular Range Protein Marker (Sangon Biotech, China). Lane 1: coexpression of RasADH and GDH using two gene-two plasmid method (plasmids pET28a-RasADH and pACYC-duet-GDH (MCS1)). Lane 2: coexpression of RasADH and GDH using two gene-one plasmid method (plasmid pRSF-duet-RasaDH (MCS1)-GDH (MCS2)). Lane 3: coexpression of RasADH and GDH using two gene-one plasmid method (plasmid pRSF-duet-GDH (MCS1)-RasADH (MCS2)).

YGL039w catalyzed reduction of 1a under different pHs

To a solution of 10 mM ketone substrate, 20 mM glucose and 0.2 mM $NADP^+$ in 50 mM buffer of appropriate pHs, were added YGL039w and glucose dehydrogenase (GDH) (0.3 mg/mL each, 7.4 μM YGL039w and 7.3 μM GDH). The 1.5 mL Eppendorf tube containing 1 mL of the above mixture was shaken at 180 rpm and 30 °C. After 0.5 h, the reaction mixture was extracted with EtOAc (5 mL) and the organic layer was concentrated and subjected to ^{1}H NMR analysis.

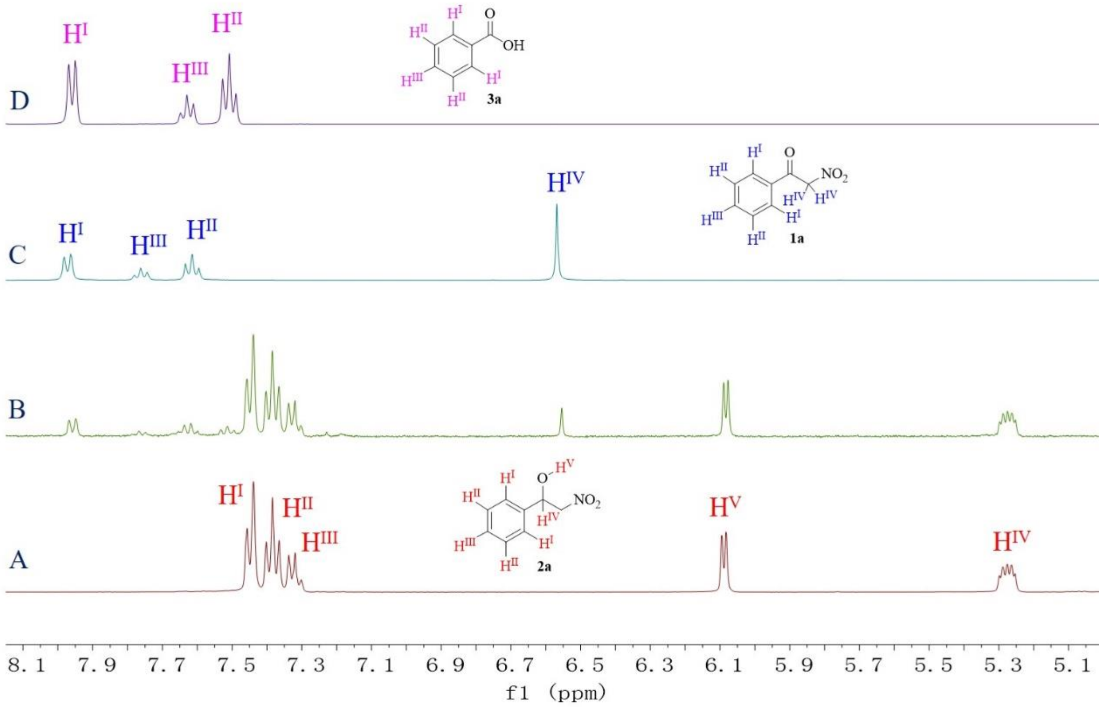


Figure S3. ^{1}H NMR spectra of the products obtained by incubation of YGL039w with ketone 1a. A. NMR spectrum of authentic racemic alcohol **2a**. B. NMR spectrum of YGL039w (0.3 mg/mL, 7.4 μM) catalyzed reduction of **1a** for 0.5 h at pH 5. C. NMR spectrum of authentic ketone **1a**. D. NMR spectrum of authentic benzoic acid **3a**.

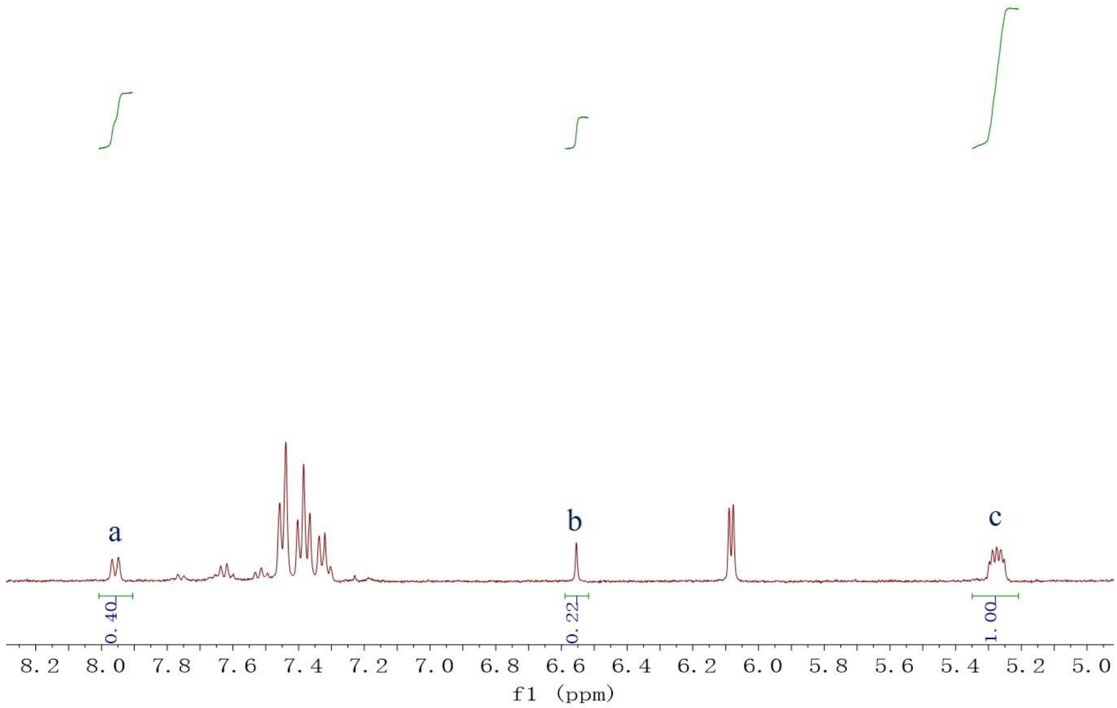


Figure S4. ^{1}H NMR spectrum of the products obtained by incubation of YGL039w (0.3 mg/mL, 7.4 μM) with ketone 1a for 0.5 h at pH 5 (spectrum B from Figure S3 with integration).

Calculation of reaction conversion using ^{1}H NMR:

As shown in Figure S3, we can assign signals in the ^{1}H NMR spectrum of the reaction mixture (spectrum B) by comparing this spectrum to the ^{1}H NMR spectra of **1a**, **2a** or **3a** (spectra C, A or D).

The spectrum in Figure S4 is the same spectrum B of Figure S3, but with integrations for certain signals. With the above knowledge, we assign signal c (with integration of 1) as H^{IV} (1 proton) of the desired product **2a**, signal b (with integration of 0.22) as H^{IV} (2 protons) of unreacted ketone **1a**, signal a (with integration of 0.40) as the sum of H^{I} (2 protons) of unreacted **1a** and H^{I} (2 protons) of the side product **3a**.

Hence, the conversion of **2a** is calculated as follows: 1 / (1 + 0.40/2) * 100% = 83%.

The percentage of remaining **1a** is calculated as follows: (0.22/2) / (1 + 0.40/2) * 100% = 9%.

The percentage of the side product **3a** is calculated as follows: (0.4/2 - 0.22/2) / (1 + 0.40/2) * 100% = 8%.

Table S4. YGL039w catalyzed reduction of 1a under different pHs

Entry	pH	Enzyme loading (mg/mL)	Reaction time (h)	**1a** [%]	**2a** [%]	**3a** [%]
1	4	0.3	0.5	35	64	1
2	**5**	**0.3**	**0.5**	**9**	**83**	**8**
3	6	0.3	0.5	25	71	4
4	7	0.3	0.5	24	73	3

5	8	0.3	0.5	40	60	0
6	**5**	**1**	**1**	**0**	**>99**	**0**

Screen KREDs against reduction of ketone 1a

To a solution of 10 mM ketone substrate, 20 mM glucose and 0.2 mM $NADP^+$ in 50 mM citric acid buffer (pH 5.0), were added KRED and glucose dehydrogenase (GDH) (1 mg/mL each enzyme). The 1.5 mL Eppendorf tube containing 1 mL of the above mixture was shaken at 180 rpm and 30 °C. After 1 h, the reaction mixture was extracted with EtOAc (5 mL) and the organic layer was concentrated and subjected to chiral HPLC analyses. The absolute configuration of the product was determined by comparing the elution order in chiral HPLC with known data.

Table S5. Screen KREDs against reduction of ketone 1a

Entry	Enzyme	Conversion [%]	ee of **2a** [%]
1	**YGL039w**	**>99**	**99 (*S*)**
2	YGL157w	54	93 (*S*)
3	YNL274c	39	84 (*S*)
4	SsCR	86	79 (*S*)
5	YDR368w	27	65 (*S*)
6	YHR104w	28	54 (*S*)
7	YNL331c	55	*racemic*
8	**RasADH**	**>99**	**98 (*R*)**
9	YOL151w	34	62 (*R*)
10	YDR541c	21	59 (*R*)
11	Ymr226c	23	33 (*R*)
12	YPL113c	33	28 (*R*)
13	YOR120w	23	24 (*R*)
14	YAL060w	61	20 (*R*)

YGL039w and RasADH catalyzed reduction of class I ketones (1) in analytical scale

To a solution of 10 mM ketone substrate, 20 mM glucose and 0.2 mM $NADP^+$ in 50 mM citric acid buffer (pH 5.0), were added KRED and glucose dehydrogenase (GDH) (appropriate concentrations as indicated in the following Table S6). The 1.5 mL Eppendorf tube containing 1 mL of the above mixture was shaken at 180 rpm and 30 °C. After certain amounts of time, the reaction mixture was extracted with EtOAc (5 mL) and the organic layer was concentrated and subjected to ^{1}H NMR and chiral HPLC analyses.

The ee of the products was determined using chiral HPLC and the absolute configuration of certain products was determined by comparing the elution order in chiral HPLC with known data (Table S7).

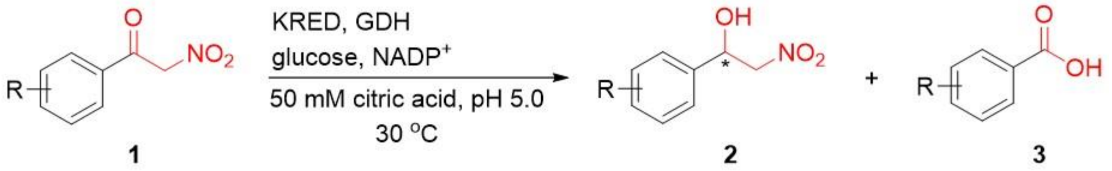
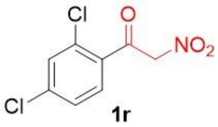
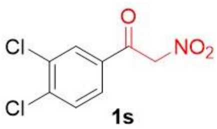
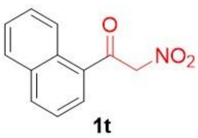
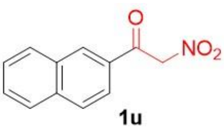
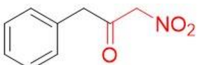
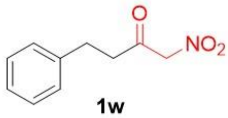


Table S6. YGL039w and RasADH catalyzed synthesis of β-nitro alcohols 2.

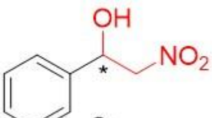
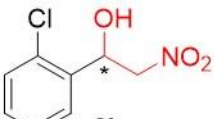
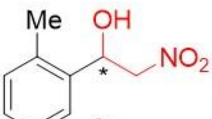
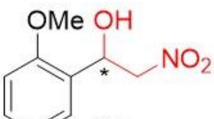
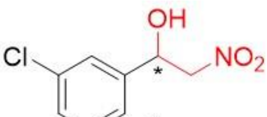
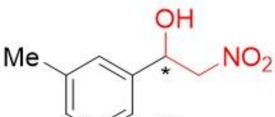
	YGL039w				RasADH			
Substrate	**1** [%][a]	**2** [%][a]	**3** [%][a]	ee of **2** [%][b]	**1** [%]	**2** [%]	**3** [%]	ee of **2** [%]
1a, R = H	0	>99	0	99, *S*[c]	0	>99	0	98, *R*
1b, R = *o*-Cl	37	63	0	90, *N.D.*[g]	0	>99	0	>99,
1c, R = *o*-Me	88 (69[d])	12 (31[d])	0 (0[d])	74, *S*	52 (16[e])	48 (81[e])	0 (3[e])	>99, *R*
1d, R = *o*-OMe	10	50	40	31, *S*	2	79	19	84, *R*
1e, R = *m*-Cl	27	73	0	29, *S*	53 (28[e])	47 (72[e])	0 (0[e])	96, *R*
1f, R = *m*-Me	5	95	0	93, *S*	62 (6[e])	38 (94[e])	0 (0[e])	91, *R*
1g, R = *m*-OMe	0	73	27	92, *S*	18	59	23	79, *R*
1h, R = *m*-CF_3	13	87	0	92, *S*	61 (0[e])	39 (>99[e])	0 (0[e])	85, *R*
1i, R = *p*-Cl	0	>99	0	98, *S*	2	98	0	98, *R*
1j, R = *p*-Me	4	96	0	96, *S*	0	>99	0	86, *R*

1k, R = *p*-OMe	0	96	4	>99, *S*	0	>99	0	99, *R*
1l, R = *p*-CF_3	45	43	12	72, *S*	9	85	6	98, *R*
1m, R = *p*-F	7	93	0	68, *S*	15	85	0	96, *R*
1n, R = *p*-Br	0	76	24	96, *S*	4	86	10	98, *R*
1o, R = *p*-NHC(O)CH_3	20	55	25	96, *S*	1	99	0	89, *R*
1p, R = *p*-NO_2	9	62	29	77, *S*	0	88	12	98, *R*
1q, R = *p*-*t*Bu	65	35	0	66, *S*	69	31	0	>99, *R*
 **1r**	20	80	0	32, *S*	29 (0[f])	71 (>99[f])	0 (0[f])	99, *R*
 **1s**	46	45	9	82, *S*	34	55	11	92, *R*
 **1t**	82	18	0	37, *R*	95 (63[d])	5 (37[d])	0 (0[d])	92, *R*
 **1u**	70 (26[d])	30 (74[d])	0 (0[d])	99, *S*	74 (14[e])	26 (86[e])	0 (0[e])	96, *R*
 **1v**	18	82	0	83, *R*	35	65	0	17, *S*

 **1w**	41	48	11	6, *R*	22	64	14	90, *R*

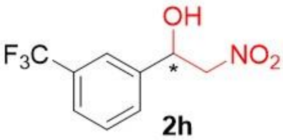
Unless otherwise stated, the reaction was carried out with 10 mM ketone substrate, 20 mM glucose, 0.2 mM $NADP^+$, 1 mg/mL KRED (24.7 μM YGL039w or 34.6 μM RasADH) and 1 mg/mL GDH (24.3 μM) in 1 mL of 50 mM citric acid, pH 5.0 at 30 °C and 180 rpm for 1 h. [a] The reaction conversion was determined using ^{1}H NMR. [b] The ee was determined using chiral HPLC. [c] The absolute configuration was determined by comparing the elution order in chiral HPLC with known data. [d] The reaction was performed with 5 mg/mL KRED (123.7 μM YGL039w or 173.1 μM RasADH) and 1 mg/mL GDH (24.3 μM) for 2 h. [e] The reaction was performed with 3 mg/mL KRED (74.2 μM YGL039w or 103.8 μM RasADH) and 1 mg/mL GDH (24.3 μM) for 2 h. [f] The reaction was performed with 1 mg/mL KRED (24.7 μM YGL039w or 34.6 μM RasADH) and 1 mg/mL (24.3 μM) GDH for 2 h. [g] The absolute configuration was not determined (*N.D.*).

Table S7. Chiral HPLC methods utilized for the determination of ee of alcohols 2

Product	Chiral HPLC method
 **2a**	Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 16.4 min, t_R' = 20.5 min [1].
 **2b**	Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 99:1, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 26.8 min, t_R' = 28.5 min.
 **2c**	Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 18.4 min, t_R' = 20.0 min [1].
 **2d**	Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 14.2 min, t_R' = 17.4 min [1].
 **2e**	Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R = 12.5 min, t_R' = 16.0 min.[2]
 **2f**	Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R = 22.6 min, t_R' = 26.8 min.[2]

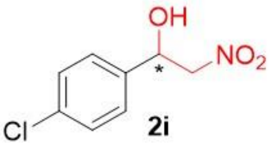
2g

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 24.5 min, t_R' = 32.9 min.[3]



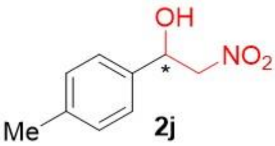
2h

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 11.3 min, t_R' = 13.2 min.[4]



2i

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 16.3 min, t_R' = 21.0 min.[3]

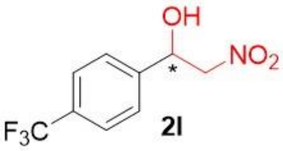


2j

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R = 18.6 min, t_R' = 23.5 min.[2]

2k

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R = 18.8 min, t_R' = 24.1 min.[5]

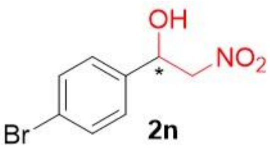


2l

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R=9.2 min, t_R'=11.5 min.[2]

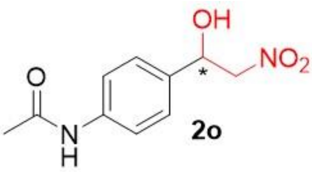
2m

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R = 16.1 min, t_R' = 18.7 min. [2]



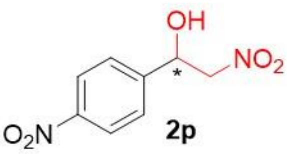
2n

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 15.2 min, t_R' = 20.3 min.[5]



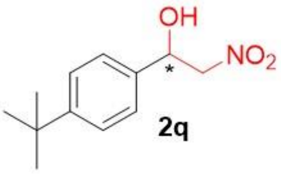
2o

Chiracel® IC, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 230 nm UV lamp, 24 °C, t_R = 33.9 min, t_R' = 40.6 min.[6]



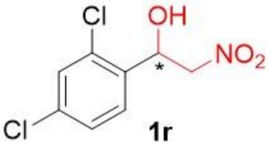
2p

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R = 24.7 min, t_R' = 32.3 min.[5]



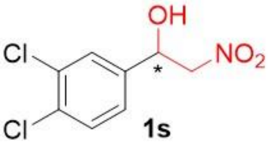
2q

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R = 12.0 min, t_R' = 17.9 min.[2]



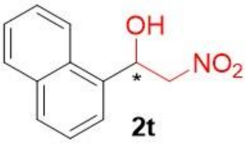
1r

Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R =16.6 min, t_R' = 20.0 min.[7]



1s

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 15.0 min, t_R' = 20.7 min.[8]

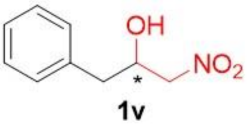


2t

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 254 nm UV lamp, 26 °C, t_R = 24.7 min, t_R' = 40.0 min.[8]

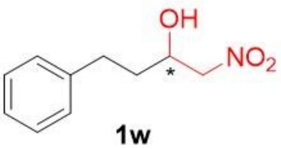
2u

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 254 nm UV lamp, 24 °C, t_R = 20.8 min, t_R' = 29.5 min.[9]



1v

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 21.0 min, t_R' = 27.2 min.[10]



1w

Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.9 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 12.3 min, t_R' = 15.5 min.[11]

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[1] Y. ji, G. Qi and Z. M. A. Judeh, *Eur. J. Org. Chem.* 2011, **25**, 4892–4898.

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Screen KREDs against reduction of ketone 4a

To a solution of 10 mM ketone substrate, 20 mM glucose and 0.2 mM $NADP^+$ in 50 mM citric acid buffer (pH 5.0), were added KRED and glucose dehydrogenase (GDH) (1 mg/mL each enzyme). The 1.5 mL Eppendorf tube containing 1 mL of the above mixture was shaken at 180 rpm and 30 °C. After 1 h, the reaction mixture was extracted with EtOAc (5 mL) and the organic layer was concentrated and subjected to chiral HPLC analyses. The absolute configuration of the product was determined by comparing the elution order in chiral HPLC with known data.

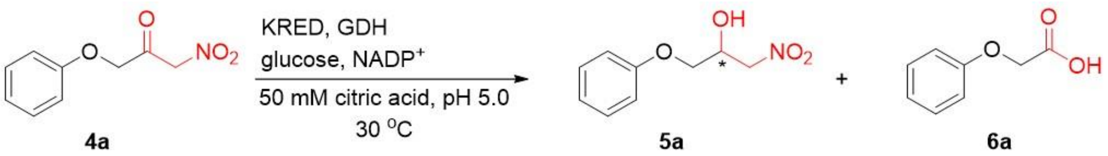


Table S8. Screen KREDs against reduction of ketone 4a

Entry	Enzyme	ee of **5a** [%][a]
1	**YGL039w**	**96**
2	LbADH	94
3	SeKRED	87
4	YAL060w	83
5	YGL185c	78
6	YNL331c	64
7	Ymr226c	34
8	LkADH	25
9	YOL151w	16
10	KRED1-Pglu	*racemic*
11	YOR120w	*racemic*
12	LtCR	*racemic*
13	YDR541c	*racemic*
14	**SyADH**	**96**
15	TdADH	90
16	KdoADH	71
17	RasADH	58
18	CgCR	39
19	YDR368w	30
20	YPL113c	19

[a] The major enantiomer formed in entries 1-9 (colored in red) eluted first (t_R = 9.6 min) in chiral HPLC, while the major enantiomer formed in entries 14-20 (colored in blue) eluted second (t_R = 11.9 min) in chiral HPLC.

YGL039w and SyADH catalyzed reduction of class II ketones (4) in analytical scale

To a solution of 10 mM ketone substrate, 20 mM glucose and 0.2 mM $NADP^+$ in 50 mM citric acid buffer (pH 5.0), were added KRED and glucose dehydrogenase (GDH) (appropriate concentrations as indicated in the following Table S9). The 1.5 mL Eppendorf tube containing 1 mL of the above mixture was shaken at 180 rpm and 30 °C. After certain amounts of time, the reaction mixture was extracted with EtOAc (5 mL) and the organic layer was concentrated and subjected to [1]H NMR and chiral HPLC analyses.

The ee of the products was determined using chiral HPLC and the absolute configuration of certain products was determined by comparing the elution order in chiral HPLC with known data (Table S10).

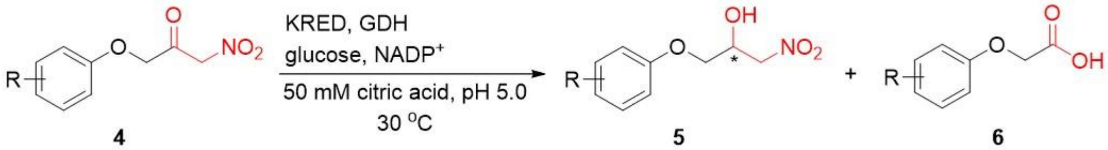
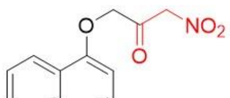
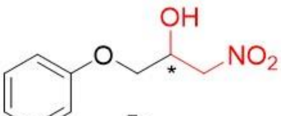
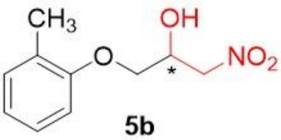
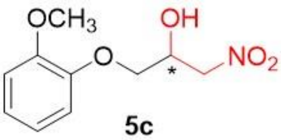
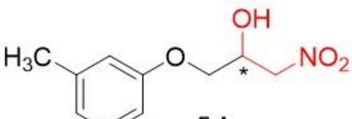
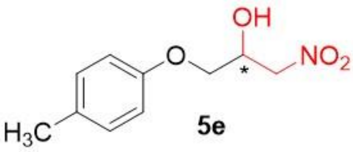
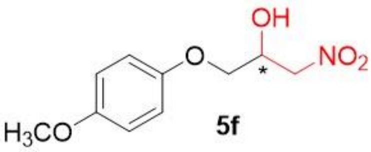
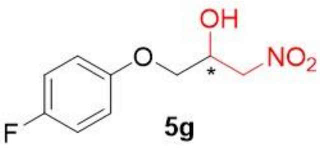
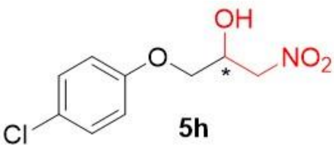
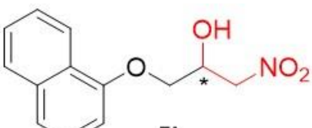


Table S9. YGL039w and SyADH catalyzed synthesis of β-nitro alcohols 5.

	YGL039w				SyADH			
Substrate	**4** [%][a]	**5** [%][a]	**6** [%][a]	ee of **5** [%][b]	**4** [%]	**5** [%]	**6** [%]	ee of **5** [%]
4a, R = H	0	>99	0	96, *R*[c]	0	75	25	96, *S*
4b, R = *o*-Me	10	90	0	94, *R*	4	80	16	57, *S*
4c, R = *o*-OMe	0	64	36	98, *R*	0	>99	0	97, *S*
4d, R = *m*-Me	0	83	17	85, *R*	0	>99	0	77, *S*
4e, R = *p*-Me	16	75	9	99, *R*	0	95	5	86, *S*
4f, R = *p*-OMe	0	>99	0	98, *R*	0	>99	0	97, *S*
4g, R = *p*-F	0	83	17	95, *R*	0	88	12	98, *S*
4h, R = *p*-Cl	0	83	17	92, *R*	0	77	23	94, *S*
4i, R = *p*-NO_2	0	93	7	55, *R*	0	74	26	>99, *S*
 **4j**	10	49	41	98, *R*	58	21	21	93, *S*

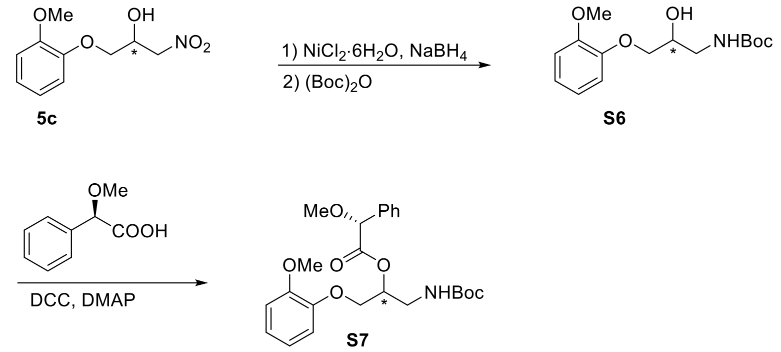
The reaction was carried out with 10 mM ketone substrate, 20 mM glucose, 0.2 mM $NADP^+$, 1 mg/mL KRED (24.7 μM YGL039w or 33.2 μM SyADH) and 1 mg/mL GDH (24.3 μM) in 1 mL of 50 mM citric acid, pH 5.0 at 30 °C and 180 rpm for 1 h. [a] The reaction conversion was determined using [1]H NMR. [b] The ee was determined using chiral HPLC. [c] The absolute configuration of **5c** was determined by [1]H NMR spectroscopy using Mosher's reagent (see Figure S5, S6, and the associated discussion for details); the absolute configuration of the rest of compounds (**5a**, **5b**, **5d** to **5j**) was assigned by analogy.

Table S10. Chiral HPLC methods utilized for the determination of ee of alcohols 5

Product	Chiral HPLC method
 **5a**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 9.6 min, t_R' = 11.9 min.
 **5b**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 11.1 min, t_R' = 12.0 min.
 **5c**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 10.7 min, t_R' = 14.1 min.
 **5d**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 10.0 min, t_R' = 12.3 min.
 **5e**	Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 92:8, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 24.4 min, t_R' = 26.3 min.
 **5f**	Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=17.9 min, t_R'=20.2 min.
 **5g**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 12.0 min, t_R' = 16.4 min.
 **5h**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 14.2 min, t_R' = 20.9 min.
 **5i**	Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 21.8 min, t_R' = 24.8 min.
 **5j**	Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R = 20.7 min, t_R' = 23.2 min.

Determination of the absolute configuration of alcohols 5.

The absolute configuration of biosynthesized **5c** was determined by ^{1}H NMR spectroscopy using Mosher's reagent.

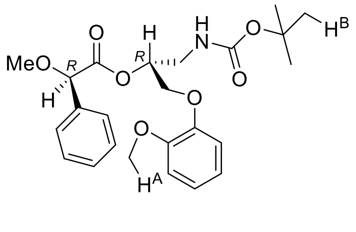


Scheme S5. Synthesis of the Mosher esters S7

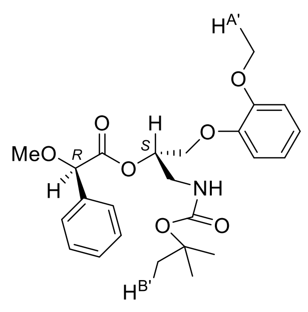
To an ice-cooled solution of enantioenriched **5c** (227 mg, 1 mmol, 1 equiv.) and $NiCl_2 \cdot 6H_2O$ (237 mg, 1 mmol, 1 equiv.) in MeOH (2 mL) was add $NaBH_4$ (114 mg, 3 mmol, 3 equiv.) slowly, and the resulting mixture was stirred at the same temperature until the nitro alcohol was completely consumed monitored by TLC. Then $(Boc)_2O$ (264 mg, 1.2 mmol, 1.2 equiv.) was added and the reaction was monitored by TLC. After completion of the reaction, the mixture was filtered and the filtrate was concentrated. The desired product **S6** was purified by flash chromatography on silica.

To an ice-cooled solution of **S6** (97 mg, 0.34 mmol, 1 equiv.), DCC (140 mg, 0.68 mmol, 2 equiv.), and DMAP (4.8 mg, 0.04 mmol, 0.12 equiv.) in DCM (1.5 mL) was added dropwise a solution of (*R*)-(-)-alpha-methoxyphenylacetic acid (61 mg, 0.37 mmol, 1.1 equiv.) in DCM (1 mL). The resulting mixture was stirred overnight and filtered. The filtrate was concentrated and the desired product **S7** was purified by flash chromatography on silica.

When (*R*)-**S6** and (*S*)-**S6** were coupled with *R*-Mosher's acid separately, diastereomeric esters (*R*,*R*)-**S7** and (*S*,*R*)-**S7** were generated, respectively. In ^{1}H NMR spectra, due to the shielding effect of the phenyl ring from the Mosher's acid part (**reference:** *Tetrahedron* **2005**, *64*, 8700-8708.), the methoxy protons H^{A} on the phenyl ring of ester (*R*,*R*)-**S7** would be shifted to upfield compared to the corresponding methoxy protons $H^{A'}$ of ester (*S*,*R*)-**S7** (see below two structures). On the other hand, the Boc protons $H^{B'}$ of ester (*S*,*R*)-**S7** would be shifted to upfield compared to the corresponding Boc protons H^{B} of ester (*R*,*R*)-**S7**.



(*R*,*R*)-**S7**



(*S*,*R*)-**S7**

Accordingly, the enantioenriched nitro alcohols **5c** from the YGL039w-catalyzed and SyADH-catalyzed reactions were reduced, Boc-protected, and coupled with *R*-Mosher's acid to give the corresponding esters, which we temporarily named as (*YGL039w*,*R*)-**S7** and (*SyADH*,*R*)-**S7**, respectively. We then acquired the ^{1}H NMR spectra of pure (*YGL039w*,*R*)-**S7**, pure (*SyADH*,*R*)-**S7**, and a mixture of (*YGL039w*,*R*)-**S7** and (*SyADH*,*R*)-**S7** (approximately 2:3 molar ratio).
With the knowledge regarding the above described ^{1}H NMR-based method, we analyzed and the acquired spectra and determined the configuration of the enzymatic products **5c** from the YGL039w-catalyzed and SyADH-catalyzed reduction reactions as *R* and *S*, respectively (Figure S5 and S6).
It is worth emphasizing that one key thing we have done for this experiment was acquiring the ^{1}H NMR spectrum of a mixture of (*YGL039w*,*R*)-S7 and (*SyADH*,*R*)-S7 with the known molar ratio, because it allows us unambiguously identify which peak is coming from (*YGL039w*,*R*)-S7 or (*SyADH*,*R*)-S7.
The absolute configuration of products **5a**, **5b**, **5d** to **5j** was then assigned by analogy.

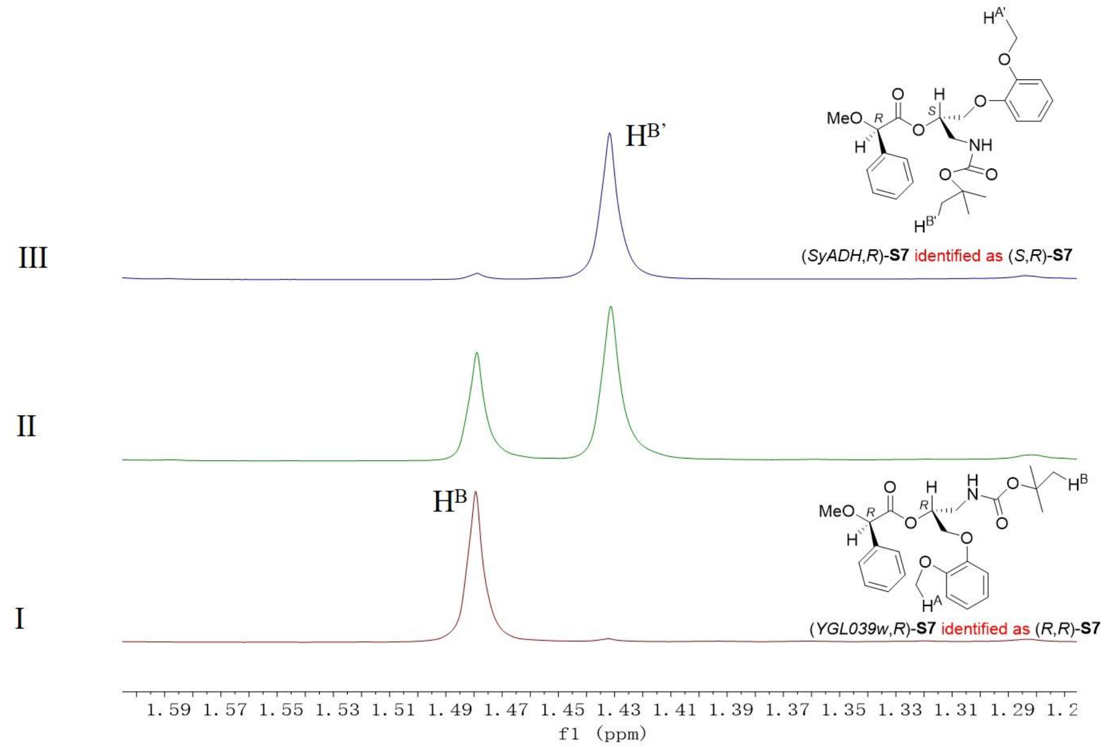


Figure S5. Determination of absolute configuration of **5c** by ^{1}H NMR spectroscopy using Mosher's reagent, zoom-in the Boc region. Trace I: ^{1}H NMR spectrum of pure (*YGL039w*,*R*)-**S7**. Trace II: ^{1}H NMR spectrum of a mixture of (*YGL039w*,*R*)-**S7** and (*SyADH*,*R*)-**S7** (approximately 2:3 molar ratio). Trace III: ^{1}H NMR spectrum of pure (*SyADH*,*R*)-**S7**.

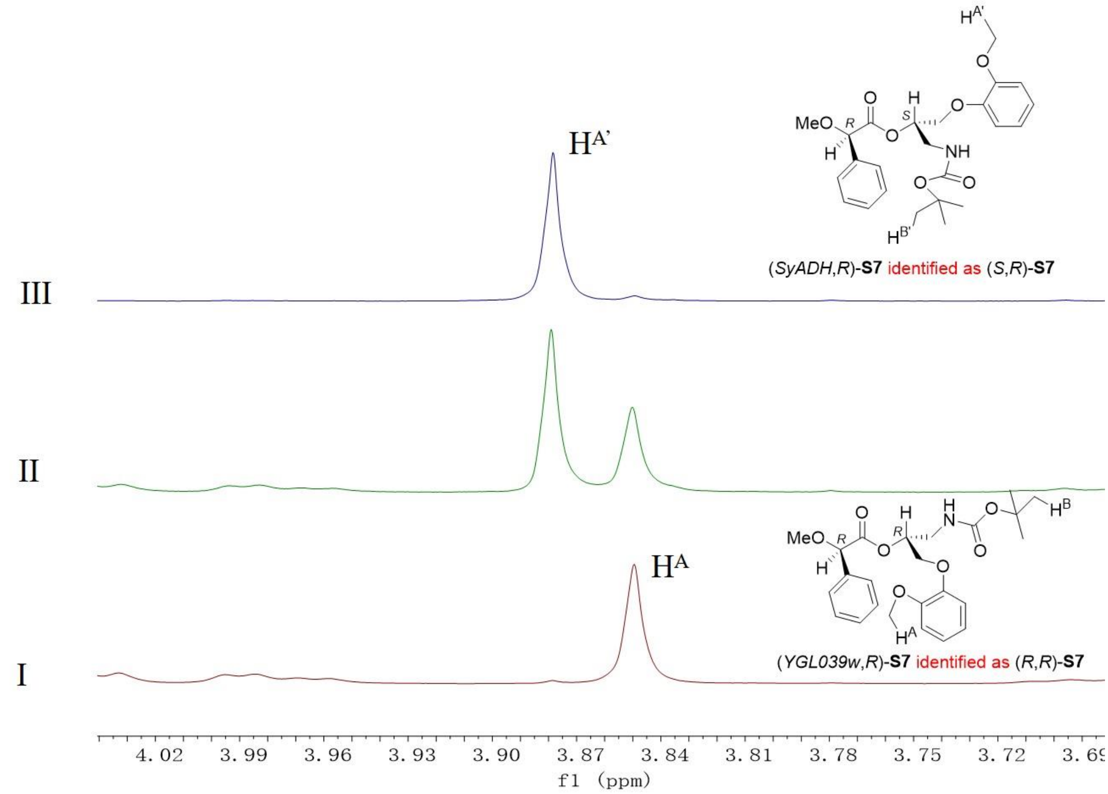
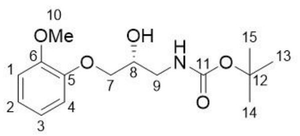
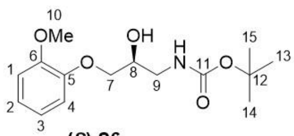
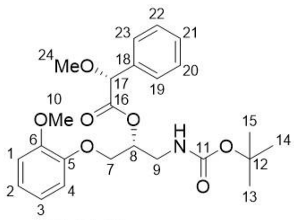
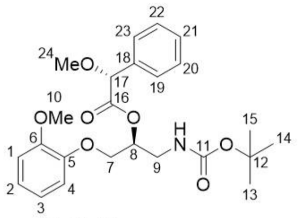


Figure S6. Determination of absolute configuration of **5c** by ^{1}H NMR spectroscopy using Mosher's reagent, zoom-in the region of methoxy on the phenyl ring. Trace I: ^{1}H NMR spectrum of pure (*YGL039w*,*R*)-**S7**. Trace II: ^{1}H NMR spectrum of a mixture of (*YGL039w*,*R*)-**S7** and (*SyADH*,*R*)-**S7** **(**approximately 2:3 molar ratio). Trace III: ^{1}H NMR spectrum of pure (*SyADH*,*R*)-**S7**.

Table S11. Characterization of S6 and S7

Product	Isolated yield (%)	NMR and HRMS	Optical rotation
 (*R*)-**S6** from YGL039w-catalyzed reaction	40	^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm 7.01-6.90 (m, 4H, Ar-H), 5.33-5.31 (m, 1H, N-H), 4.15-4.10 (m, 1H, C_8-H), 4.08-4.05 (m, 1H, C_7-H), 4.00-3.94 (m, 1H, C_7-H), 3.88 (s, 3H, C_{10}-H), 3.53-3.47 (m, 1H, C_9-H), 3.34-3.28 (m, 1H, C_9-H), 1.47 (s, 9H, $C_{13, 14, 15}$-H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ/ppm 156.93, 149.77, 147.97, 122.20, 121.10, 115.00, 111.87, 79.60, 72.18, 69.36, 55.76, 43.47, 28.40. HRMS Calcd. For	$[\alpha]_{25}^{D}$ = 11.79 (*c* = 0.5, DCM)

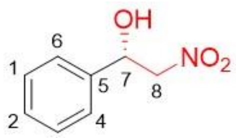
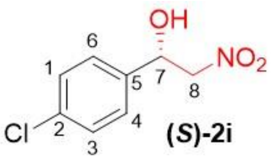
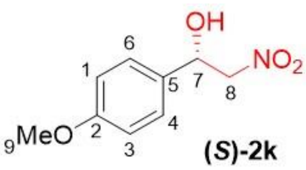
		$C_{15}H_{23}NNaO_5^+$[M+Na$^+$]: 320.1468. Found: 320.1466.	
 (*S*)-**S6** from SyADH-catalyzed reaction	42	^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm 7.01-6.90 (m, 4H, Ar-H), 5.31-5.30 (m, 1H, N-H), 4.15-4.10 (m, 1H, C_8-H), 4.08-4.05 (m, 1H, C_7-H), 4.00-3.96 (m, 1H, C_7-H), 3.88 (s, 3H, C_{10}-H), 3.53-3.47 (m, 1H, C_9-H), 3.34-3.28 (m, 1H, C_9-H), 1.47 (s, 9H, $C_{13, 14, 15}$-H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ/ppm 156.94, 149.78, 147.97, 122.22, 121.10, 115.02, 111.87, 79.60, 72.18, 69.36, 55.76, 43.47, 28.40. HRMS Calcd. For $C_{15}H_{23}NNaO_5^+$[M+Na$^+$]: 320.1468. Found: 320.1466.	$[\alpha]_{25}^{D}$ = -9.79 (*c* = 0.5, DCM)
 (*R*, *R*)-**S7** from YGL039w-catalyzed reaction	89	^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm 7.48-7.45 (m, 2H, Ar-H), 7.36-7.29 (m, 3H, Ar-H), 7.00-6.96 (m, 1H, Ar-H), 6.92-6.83 (m, 2H, Ar-H), 6.74-6.71 (m, 1H, Ar-H), 5.31-5.29 (m, 1H, C_8-H), 5.28-5.24 (m, 1H, N-H), 4.84 (s, 1H, C_{17}-H), 4.07-4.03 (m, 1H, C_7-H), 4.00-3.96 (m, 1H, C_7-H), 3.85 (s, 3H, C_{10}-H), 3.69-3.66 (m, 1H, C_9-H), 3.54-3.50 (m, 1H, C_9-H), 3.47 (s, 3H, C_{24}-H), 1.48 (s, 9H, $C_{13, 14, 15}$-H). ^{13}C NMR ($CDCl_3$, 100 MHz) 170.26, 156.05, 150.05, 147.64, 136.11, 128.68, 128.61, 127.07, 122.50, 120.93, 115.40, 112.10, 82.41, 79.34, 71.54, 69.24, 57.51, 55.73, 49.01, 41.24, 33.96, 28.44, 25.67, 25.01. HRMS Calcd. For $C_{24}H_{31}NNaO_7^+$[M+Na$^+$]: 468.1993. Found: 468.1990.	$[\alpha]_{25}^{D}$ = -3.4 (*c* = 0.5, DCM)

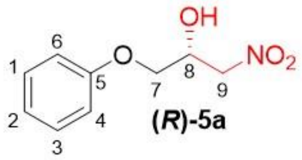
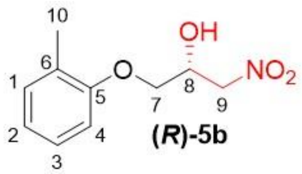
 (*S*, *R*)-**S7** from SyADH-catalyzed reaction	80	^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm 7.49-7.46 (m, 2H, Ar-H), 7.42-7.37 (m, 3H, Ar-H), 7.02-6.97 (m, 1H, Ar-H), 6.93-6.91 (m, 3H, Ar-H), 5.29-5.24 (m, 1H, N-H), 4.81 (s, 1H, C_{17}-H), 4.75-4.63 (m, 1H, C_8-H), 4.21-4.14 (m, 2H, C_7-H), 3.88 (s, 3H, C_{10}-H), 3.54-3.46 (m, 1H, C_9-H), 3.44 (s, 3H, C_{24}-H), 3.36-3.29 (m, 1H, C_9-H), 1.43 (s, 9H, $C_{13, 14, 15}$-H). ^{13}C NMR ($CDCl_3$, 100 MHz) 170.16, 155.76, 150.10, 147.83, 136.27, 128.92, 128.79, 127.18, 122.52, 120.97, 115.48, 112.24, 82.30, 79.37, 71.91, 69.35, 57.36, 55.82, 41.10, 28.17. HRMS Calcd. For $C_{24}H_{31}NNaO_7^+$[M+Na^+]: 468.1993. Found: 468.1991.	$[\alpha]_{25}^D$ = -43.77 (*c* = 0.5, DCM)

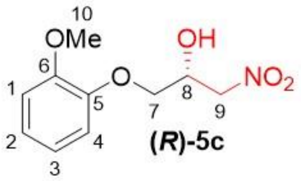
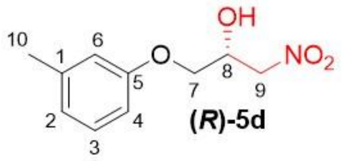
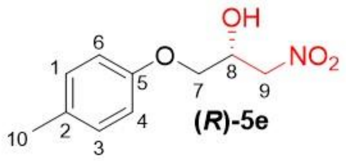
YGL039w, RasADH, and SyADH catalyzed reduction in preparative scale using cell-free extract (CFE)

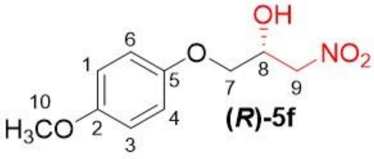
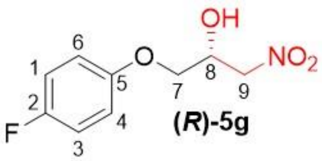
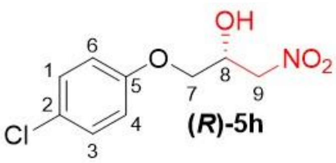
The preparative scale reaction was carried out with 250 mg ketone substrate, 1 g glucose, 50 mg $NADP^+$, 35 mL 15% (w/v) cell-free extract (CFE) of KRED, 10 mL 15% (w/v) CFE of GDH and 5 mL DMSO at 30 °C and 600 rpm for certain amounts of time (monitored by TLC). Silica gel was added to the reaction mixture and subjected to centrifugation. The supernatant was extracted with EtOAc. The organic layer was then washed with brine and dried with anhydrous Na_2SO_4, then filtered, and the filtrate was evaporated to dryness. The product was purified by flash chromatography (silica gel, petroleum ether: EtOAc = 8:1 for **2a**, **2i** and **2k**; dichloromethane for **5a** to **5j**). The ee of the products was determined using chiral HPLC. The absolute configuration was determined by comparing the sign of the optical rotation of the major enantiomer or the elution order in chiral HPLC with known data, or using the above-described Mosher's ester analysis.

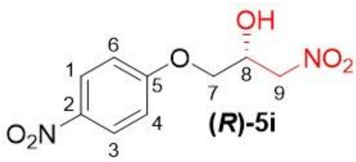
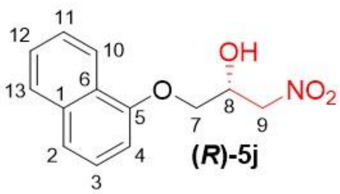
Table S12. Characterization of products from YGL039w catalyzed preparative scale reactions

Product	Isolated yield (%)	NMR and HRMS	Ee (%)	Optical rotation
 **(*S*)-2a**	44.3	^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.47-7.44 (m, 2H, Ar-H), 7.41-7.36 (m, 2H, Ar-H), 7.34-7.30 (m, 1H, Ar-H), 6.11-6.10 (d, 1H, *J* = 4.8 Hz, O-H), 5.30-5.26 (m, 1H, C_7-H), 4.88-4.83 (m, 1H, C_8-H), 4.60-4.54 (m, 1H, C_8-H).	97 (*S*)	$[\alpha]_{20}^{D}$ = 42.44 (*c* = 1, DCM) (Ref. $[\alpha]_{20}^{D}$ = -41.6 for (*R*)-isomer (*c* = 1, DCM))[1]
 **(*S*)-2i**	56	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.49-7.43 (m, 4H, Ar-H), 6.19-6.17 (d, 1H, *J* = 5.04 Hz, O-H), 5.31-5.26 (m, 1H, C_7-H), 4.88-4.84 (m, 1H, C_8-H), 4.61-4.55 (m, 1H, C_8-H).	95 (*S*)	$[\alpha]_{20}^{D}$ = 33.8 (*c* = 1, DCM) (Ref. $[\alpha]_{20}^{D}$ = -38.1 for (*R*)-isomer (*c* = 1, DCM))[2]
 **(*S*)-2k**	44	^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm 7.30-7.28 (m, 2H, Ar-H), 6.91-6.89 (m, 2H, Ar-H), 5.37-5.34 (m, 1H, C_7-H),	95 (*S*)	$[\alpha]_{25}^{D}$ = 40.4 (*c* = 1, DCM) (Ref. $[\alpha]_{25}^{D}$ = -

		4.60-4.53 (m, 1H, C_8-H), 4.47-4.43 (m, 1H, C_8-H), 3.80, (s, 3H, C_9-H).		41.6 for (*R*)-isomer (*c* = 1, DCM))[3]
 (*R*)-5a	42.1	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.33-7.28 (m, 2H, Ar-H), 6.99-6.95 (m, 3H, Ar-H), 5.87-5.83 (m, 1H, O-H), 4.89-4.83 (m, 1H, C_9-H), 4.61-4.54 (m, 1H, C_9-H), 4.53-4.47 (m, 1H, C_8-H), 4.07-3.93 (m, 2H, C_7-H) ^{13}C NMR (DMSO, 100 MHz) δ/ppm 130.32, 130.00, 121.40, 115.02, 114.90, 79.54, 69.47, 67.29. HRMS Calcd. For $C_9H_{11}NNaO_4^+$[M+Na$^+$]: 220.0580. Found: 220.0581.	97 (*R*)	$[\alpha]_{25}^{D}$ = 25.38 (*c* = 0.5, DCM)
 (*R*)-5b	57.9	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.18-7.14 (m, 2H, Ar-H), 6.93-6.85 (m, 2H, Ar-H), 5.86-5.84 (d, 1H, *J* = 5.68 Hz, O-H), 4.91-4.87 (m, 1H, C_9-H), 4.64-4.59 (m, 1H, C_9-H), 4.57-4.50 (m, 1H, C_8-H), 4.06-3.96 (m, 2H, C_7-H), 2.18 (s, 3H, C_{10}-H) ^{13}C NMR (DMSO, 100 MHz) δ/ppm 156.62, 130.92, 127.41, 126.43, 121.07, 111.80, 79.70, 69.61, 67.37, 16.35. HRMS Calcd. For $C_{10}H_{13}NNaO_4^+$[M+Na$^+$]: 234.0737. Found: 234.0733.	95 (*R*)	$[\alpha]_{25}^{D}$ = 24.98 (*c* = 0.5, DCM)

	50.4	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.00-6.87 (m, 4H, Ar-H), 5.83-5.82 (d, 1H, *J* = 5.64 Hz, O-H), 4.87-4.84 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.52-4.46 (m, 1H, C_8-H), 4.03-3.94 (m, 2H, C_7-H), 3.33 (s, 3H, C_{10}-H).	92 (*R*)	$[\alpha]_{28}^{D}$ = 10.19 (*c* = 0.5, DCM)
	48	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.20-7.16 (m, 1H, Ar-H), 6.79-6.73 (m, 3H, Ar-H), 5.85-5.83 (d, 1H, *J* = 5.68 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.05-3.94 (m, 2H, C_7-H), 2.29 (s, 3H, C_{10}-H).	88 (*R*)	$[\alpha]_{23}^{D}$ = 19.59 (*c* = 0.5, DCM)
	69	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.11-7.09 (m, 2H, Ar-H), 6.86-6.84 (m, 2H, Ar-H), 5.84-5.83 (d, 1H, *J* = 5.64 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.59-4.54 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.01-3.92 (m, 2H, C_7-H), 2.24 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 156.54, 130.32, 130.08, 114.90, 79.56, 69.61, 67.32, 20.55. HRMS Calcd. For $C_{10}H_{13}NNaO_4^+$[M+Na$^+$]: 234.0737. Found: 234.0730.	96 (*R*)	$[\alpha]_{25}^{D}$ = 22.18 (*c* = 0.5, DCM)

	65.5	^{1}H NMR (400 MHz, DMSO) δ/ppm 6.92-6.86 (m, 4H, Ar-H), 5.84-5.82 (d, 1H, *J* = 5.72 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.59-4.54 (m, 1H, C_9-H), 4.51-4.44 (m, 1H, C_8-H), 3.99-3.90 (m, 2H, C_7-H), 3.71 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 154.12, 152.65, 116.05, 115.08, 79.58, 70.19, 67.35, 55.82. HRMS Calcd. For $C_{10}H_{13}NNaO_5^+$[M+Na$^+$]: 250.0686. Found: 250.0687.	96 (*R*)	$[\alpha]_{25}^{D}$ = 17.99 (*c* = 0.5, DCM)
	63.5	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.17-7.10 (m, 2H, Ar-H), 7.01-6.96 (m, 2H, Ar-H), 5.87-5.85 (d, 1H, *J* = 5.72 Hz, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.60-4.55 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.03-3.95 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 157.16 (d, *J* = 234.69 Hz), 155.00 (d, *J* = 1.96 Hz), 116.44, 116.28 (d, *J* = 13.84 Hz), 79.48, 70.21, 67.24. HRMS Calcd. For $C_9H_{10}FNNaO_4^+$[M+Na$^+$]: 238.0486. Found: 238.0485.	96 (*R*)	$[\alpha]_{25}^{D}$ = 15.79 (*c* = 0.5, DCM)
	65	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.37-7.33 (m, 2H, Ar-H), 7.01-6.97 (m, 2H, Ar-H), 5.88-5.87 (d, 1H, *J* = 5.68 Hz, O-H), 4.88-	93 (*R*)	$[\alpha]_{25}^{D}$ = 15.79 (*c* = 0.5, DCM)

		4.84 (m, 1H, C_9-H), 4.60-4.55 (m, 1H, C_9-H), 4.52-4.46 (m, 1H, C_8-H), 4.05-3.98 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 157.53, 129.75, 125.10, 116.84, 79.42, 69.94, 67.17. HRMS Calcd. For $C_9H_{10}ClNNaO_4^+$[M+Na$^+$]: 254.0191. Found: 254.0192.		
 **(*R*)-5i**	48	^{1}H NMR (400 MHz, DMSO) δ/ppm 8.25-8.21 (m, 2H, Ar-H), 7.21-7.16 (m, 2H, Ar-H), 5.96-5.95 (d, 1H, *J* = 5.56 Hz, O-H), 4.90-4.87 (m, 1H, C_9-H), 4.64-4.57 (m, 1H, C_9-H), 4.56-4.51 (m, 1H, C_8-H), 4.19-4.18 (d, 2H, *J* = 5.04 Hz, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 163.95, 126.37, 115.64, 79.24, 70.43, 67.00. HRMS Calcd. For $C_9H_{11}N_2O_6^+$[M+H$^+$]: 243.0612. Found: 243.0616.	32 (*R*)	$[\alpha]_{25}^{D}$ = 8.79 (*c* = 0.5, DCM)
 **(*R*)-5j**	72.6	^{1}H NMR (400 MHz, DMSO) δ/ppm 8.27-8.25 (m, 1H, Ar-H), 7.90-7.87 (m, 1H, Ar-H), 7.57-7.50 (m, 3H, Ar-H), 7.45-7.41 (m, 1H, Ar-H), 6.99-6.96 (m, 1H, Ar-H), 5.98-5.97 (d, 1H, *J* = 5.52 Hz, O-H), 5.03-5.00 (m, 1H, C_9-H), 4.76-4.71 (m, 1H, C_9-H), 4.70-4.64 (m, 1H, C_8-H), 4.25-4.16 (m, 2H,	94 (*S*)	$[\alpha]_{28}^{D}$ = 19.78 (*c* = 0.5, DCM)

		C_7-H).		

Table S13. Characterization of products from RasADH catalyzed preparative scale reactions

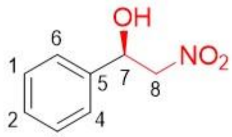
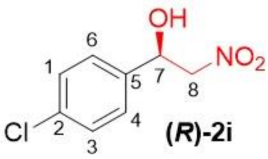
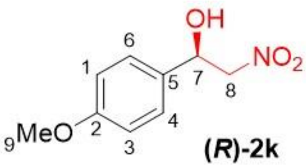
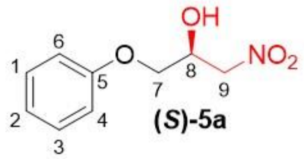
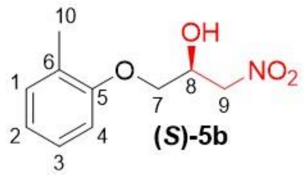
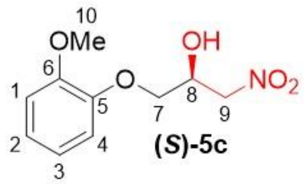
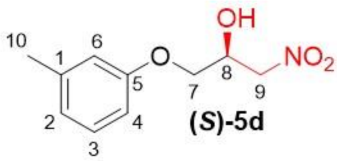
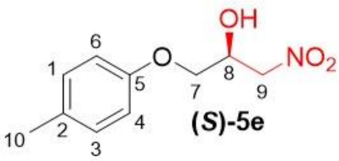
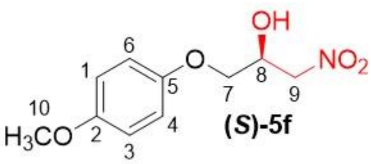
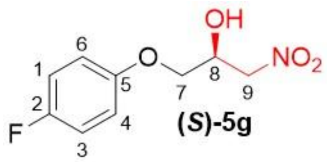
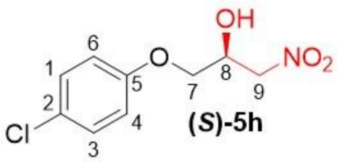
Product	Isolated yield (%)	^{1}H NMR data	Ee (%)	Optical rotation
 (*R*)-2a	80.2	^{1}H NMR (DMSO, 400 MHz) δ/ppm 7.46-7.44 (m, 2H, Ar-H), 7.41-7.37 (m, 2H, Ar-H), 7.34-7.30 (m, 1H, Ar-H), 6.10-6.08 (d, 1H, *J* = 4.8 Hz, O-H), 5.30-5.26 (m, 1H, C_7-H), 4.88-4.83 (m, 1H, C_8-H), 4.60-4.54 (m, 1H, C_8-H).	95 (*R*)	$[\alpha]_{20}^{D}$ = -35.2 (*c* = 1, DCM) (Ref. $[\alpha]_{20}^{D}$ = -41.6 (*c* = 1, DCM))[1]
 (*R*)-2i	67.5	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.49-7.43 (m, 4H, Ar-H), 6.19-6.17 (d, 1H, *J* = 5.04 Hz, O-H), 5.31-5.25 (m, 1H, C_7-H), 4.88-4.84 (m, 1H, C_8-H), 4.61-4.55 (m, 1H, C_8-H).	96 (*R*)	$[\alpha]_{20}^{D}$ = -34.7 (*c* = 1, DCM) (Ref. $[\alpha]_{20}^{D}$ = -38.1 (*c* = 1, DCM))[2]
 (*R*)-2k	76.6	^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.29 (m, 2H, Ar-H), 6.91-6.89 (m, 2H, Ar-H), 5.37-5.34 (m, 1H, C_7-H), 4.60-4.53 (m, 1H, C_8-H), 4.47-4.43 (m, 1H, C_8-H), 3.81, (s, 3H, C_9-H).	95 (*R*)	$[\alpha]_{25}^{D}$ = -33.3 (*c* = 1, DCM) (Ref. $[\alpha]_{25}^{D}$ = -41.6 (*c* = 1, DCM))[3]

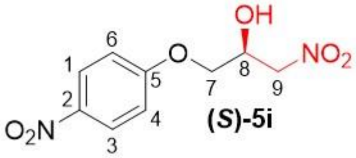
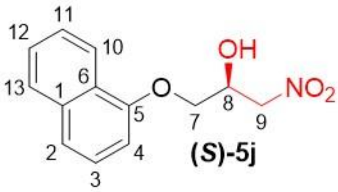
Table S14. Characterization of products from SyADH catalyzed preparative scale reactions

Product	Isolated yield (%)	NMR and HRMS	Ee (%)	Optical rotation

 (*S*)-5a	47	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.33-7.29 (m, 2H, Ar-H), 6.98-6.95 (m, 3H, Ar-H), 5.89-5.88 (d, 1H, *J* = 5.68 Hz, O-H), 4.89-4.85 (m, 1H, C_9-H), 4.61-4.56 (m, 1H, C_9-H), 4.54-4.47 (m, 1H, C_8-H), 4.05-3.97 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.60, 130.01, 121.40, 115.00, 79.54, 69.44, 67.28. HRMS Calcd. For $C_9H_{11}NNaO_4^+$[M+Na$^+$]: 220.0580. Found: 220.0575.	96 (*S*)	$[\alpha]_{25}^{D}$ = -22.38 (*c* = 0.5, DCM)
 (*S*)-5b	49	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.18-7.14 (m, 2H, Ar-H), 6.93-6.85 (m, 2H, Ar-H), 5.86-5.84 (d, 1H, *J* = 5.68 Hz, O-H), 4.91-4.87 (m, 1H, C_9-H), 4.64-4.59 (m, 1H, C_9-H), 4.57-4.50 (m, 1H, C_8-H), 4.06-3.96 (m, 2H, C_7-H), 2.18 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.60, 156.62, 130.92, 127.42, 126.43, 121.07, 111.80, 79.70, 69.61, 67.37, 16.35. HRMS Calcd. For $C_{10}H_{13}NNaO_4^+$[M+Na$^+$]: 234.0737. Found: 234.0739.	35 (*S*)	$[\alpha]_{25}^{D}$ = -8.99 (*c* = 0.5, DCM)
 (*S*)-5c	44	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.01-6.87 (m, 4H, Ar-H), 5.86-5.85 (d, 1H, *J* = 5.68 Hz, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.61-4.55 (m, 1H, C_9-H), 4.53-4.46 (m, 1H, C_8-H), 4.03-3.94 (m, 2H, C_7-H),	99 (*S*)	$[\alpha]_{25}^{D}$ = -7.39 (*c* = 0.5, DCM)

		3.78 (s, 3H, C_{10}-H).		
 (S)-5d	66	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.20-7.16 (m, 2H, Ar-H), 6.79-6.74 (m, 2H, Ar-H), 5.85-5.84 (d, 1H, *J* = 5.68 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.03-3.94 (m, 2H, C_7-H), 2.29 (s, 3H, C_{10}-H).	97 (*S*)	$[\alpha]_{25}^{D}$ = -22.58 (*c* = 0.5, DCM)
 (S)-5e	67	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.11-7.09 (m, 2H, Ar-H), 6.90-6.83 (m, 2H, Ar-H), 5.85-5.84 (d, 1H, *J* = 5.68 Hz, O-H), 4.87-4.83 (m, 1H, C_9-H), 4.60-4.54 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.01-3.92 (m, 2H, C_7-H), 2.24 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.63, 156.53, 130.32, 130.08, 114.89, 79.56, 69.60, 67.31, 20.55. HRMS Calcd. For $C_{10}H_{13}NNaO_4^+$[M+Na$^+$]: 234.0737. Found: 234.0734.	99 (*S*)	$[\alpha]_{25}^{D}$ = -22.18 (*c* = 0.5, DCM)
 (S)-5f	42	^{1}H NMR (400 MHz, DMSO) δ/ppm 6.92-6.86 (m, 4H, Ar-H), 5.84-5.83 (d, 1H, *J* = 5.72 Hz, O-H), 4.87-4.84 (m, 1H, C_9-H), 4.59-4.53 (m, 1H, C_9-H), 4.51-4.44 (m, 1H, C_8-H), 3.99-3.90 (m, 2H, C_7-H), 3.71 (s, 3H, C_{10}-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.63, 154.11, 152.65, 116.04, 115.08, 79.58, 70.18, 67.35, 55.82. HRMS	99 (*S*)	$[\alpha]_{25}^{D}$ = -21.78 (*c* = 0.5, DCM)

		Calcd. For $C_{10}H_{13}NNaO_5^+$[M+Na+]: 250.0686. Found: 250.0672.		
 (S)-5g	82	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.16-7.11 (m, 2H, Ar-H), 7.00-6.96 (m, 2H, Ar-H), 5.89-5.87 (d, 1H, *J* = 5.68 Hz, O-H), 4.88-4.84 (m, 1H, C_9-H), 4.60-4.55 (m, 1H, C_9-H), 4.52-4.45 (m, 1H, C_8-H), 4.03-3.95 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.63, 157.15 (d, *J* = 234.52 Hz), 154.98 (d, *J* = 2 Hz), 116.43 (d, *J* = 4.93 Hz), 116.27 (d, *J* = 9.86 Hz), 79.48, 70.17, 67.24. HRMS Calcd. For $C_9H_{10}FNNaO_4^+$[M+Na+]: 238.0486. Found: 238.0481.	97 (*S*)	$[\alpha]_{25}^{D}$ = -18.39 (*c* = 0.5, DCM)
 (S)-5h	90	^{1}H NMR (400 MHz, DMSO) δ/ppm 7.40-7.36 (m, 2H, Ar-H), 7.04-7.00 (m, 2H, Ar-H), 5.91-5.90 (d, 1H, *J* = 5.68 Hz, O-H), 4.90-4.87 (m, 1H, C_9-H), 4.63-4.58 (m, 1H, C_9-H), 4.56-4.49 (m, 1H, C_8-H), 4.08-4.01 (m, 2H, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 158.63, 157.56, 129.77, 125.15, 116.88, 79.45, 69.98, 67.21. HRMS Calcd. For $C_9H_{10}ClNNaO_4^+$[M+Na+]: 254.0191. Found: 254.0186.	99 (*S*)	$[\alpha]_{25}^{D}$ = -21.78 (*c* = 0.5, DCM)

 (*S*)-5i	62	^{1}H NMR (400 MHz, DMSO) δ/ppm 8.25-8.20 (m, 2H, Ar-H), 7.21-7.16 (m, 2H, Ar-H), 5.97-5.95 (d, 1H, *J* = 5.52 Hz, O-H), 4.90-4.87 (m, 1H, C_9-H), 4.64-4.58 (m, 1H, C_9-H), 4.56-4.51 (m, 1H, C_8-H), 4.19-4.18 (d, 2H, *J* = 4.96 Hz, C_7-H). ^{13}C NMR (DMSO, 100 MHz) δ/ppm 163.95, 141.56, 126.36, 115.62, 79.24, 70.43, 67.00. HRMS Calcd. For $C_9H_{10}N_2NaO_6^+$[M+Na$^+$]: 265.0431. Found: 265.0426.	99 (*S*)	$[\alpha]_{25}^{D}$ = -22.58 (*c* = 0.5, DCM)
 (*S*)-5j	74	^{1}H NMR (400 MHz, DMSO) δ/ppm 8.28-8.25 (m, 1H, Ar-H), 7.90-7.87 (m, 1H, Ar-H), 7.57-7.50 (m, 3H, Ar-H), 6.99-6.96 (m, 1H, Ar-H), 6.00-5.98 (d, 1H, *J* = 5.52 Hz, O-H), 5.04-5.00 (m, 1H, C_9-H), 4.76-4.71 (m, 1H, C_9-H), 4.70-4.65 (m, 1H, C_8-H), 4.25-4.17 (m, 2H, C_7-H).	84 (*S*)	$[\alpha]_{25}^{D}$ = -17.59 (*c* = 0.5, DCM)

References

[1] D. Qin, W. Lai, D. Hu, Z. Chen, A. Wu, Y. Ruan, Z. Zhou and H. Chen, *Chem. Eur. J.* 2012, **18**, 10515-10518.

[2] B. V. S. Reddy and J. George, *Tetrahedron: Asymmetry*, 2011, **22**, 1169-1175.

[3] H. Maheswaran, K. L. Prasanth, G. G. Krishna, K. Ravikumar, B. Sridharb and M. L. Kantam, *Chem. Commun.* 2006, **39**, 4066-4068.

Cell-free extract of KRED catalyzed reduction of 1k at elevated substrate concentrations

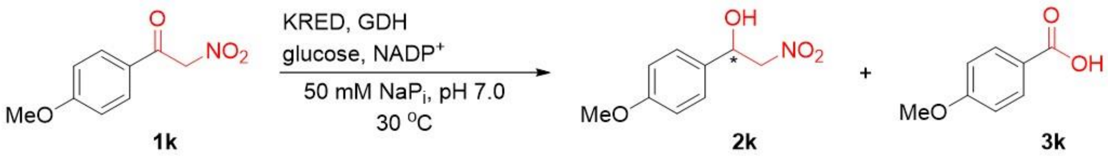


Table S15. YGL039w and RasADH catalyzed reduction of 1k at elevated substrate concentrations

		YGL039w[a]			RasADH[b]		
Entry	Substrate loadings (g/L)	**1k** [%]	**2k** [%]	**3k** [%]	**1k** [%]	**2k** [%]	**3k** [%]
1	10	6	89	5	0	>99	0
2	20	28	68	4	27	71	2
3	50	75	21	4	82	16	2

The biotransformation was carried out with appropriate amounts of **1k** and glucose (the weight of glucose is 4 times of that of **1k**), 5 mg $NADP^+$, 3.5 mL 15% (w/v) cell-free extract (CFE) of KREDs in 50 mM NaP_i (pH 7.0), 1 mL 15% (w/v) CFE of GDH in 50 mM NaP_i (pH 7.0) and 0.5 mL DMSO at 30 °C. [a] Reaction time was 4h. [b] Reaction time was 2h.

Table S16. YGL039w and RasADH catalyzed reduction of ketone 1k at elevated substrate concentrations in the presence of other organic solvents

		YGL039w			RasADH		
Entry	Organic solvent (10%, v/v)	**1k** [%]	**2k** [%]	**3k** [%]	**1k** [%]	**2k** [%]	**3k** [%]
1	N.A.[a]	86	6	8	78	15	7

2	Ethyl acetate	79	7	14	73	18	9
3	Et_2O	72	11	17	36	48	16
4	EtOH	69	16	15	45	40	15
5	Methyl *tert*-butyl ether (MTBE)	23	30	47	35	47	18
6	diethylene glycol dimethyl ether (DGDE)	61	23	16	48	39	13
7	Dioxane	58	22	20	41	45	14
8	cyclohexane	91	2	7	64	24	12
9	acetone	75	12	13	62	28	10
10	THF	56	31	13	56	32	12
11	MeOH	77	12	11	78	15	7
12	Dichloromethane	>99	0	0	81	14	5
13	DMF	63	22	15	64	26	10
14	toluene	87	4	9	72	21	7

15	*i*-PrOH	52	23	25	51	35	14
16	CCl_4	90	2	8	78	16	6
17	hexane	91	3	6	76	17	7

The biotransformation was carried out with 0.1 g **1k**, 0.04 g glucose, 2 mg $NADP^+$, 1.24 mL 15% (w/v) CFE of KREDs in 50 mM NaP_i (pH 7.0), 0.36 mL 15% (w/v) CFE of GDH in 50 mM NaP_i (pH 7.0), 0.2 mL DMSO and 0.2 mL of appropriate organic solvents at 30 °C for 3 h.
[a] N.A. stands for not applicable, meaning no organic solvent other than DMSO was added.

***E coli.* whole-cell coexpressing RasADH and GDH catalyzed reduction of 1k at elevated substrate concentrations**

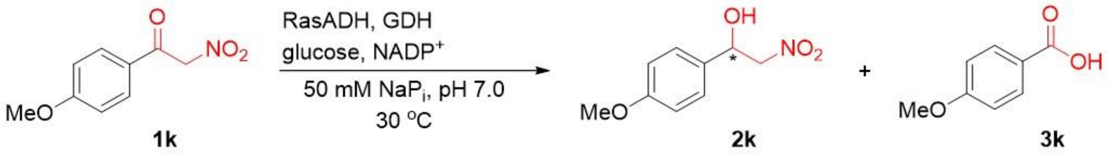


Table S17. Whole cells of *E coli.* strain coexpressing RasADH and GDH catalyzed reduction of ketone 1k at elevated substrate concentrations

Entry	Substrate loading (g/L)	Reaction time (h)	Organic solvent (v/v)	**1k** [%]	**2k** [%]	**3k** [%]
1	50	5	*N.A.*[a]	24	54	22
2	75	5	*N.A.*	50	40	10
3	100	5	*N.A.*	56	29	15
4	50	3	DGDE (20%)	4	80	16
5	50	3	Dioxane (20%)	2	79	19
6	50	3	Et_2O (20%)	15	70	15
7	50	3	Acetone (20%)	4	76	20
8	50	3	EtOH (20%)	2	75	23
9	50	3	*i*-PrOH (20%)	5	73	22
10	50	3	MTBE (20%)	17	70	13
11	50	3	THF (20%)	34	53	13
12	50	3	Acetone (50%)	7	79	14
13	50	3	DGDE (50%)	8	78	14
14	**50**	**3**	**Dioxane (50%)**	**0**	**86**	**14**
15	75	3	Dioxane (50%)	17	58	25
16	75	3	Dioxane (50%)	6	66	28

The biotransformation was carried out with appropriate amounts of **1k** and glucose (the weight of glucose is 4 times of that of **1k**), 2 mg $NADP^+$, 0.6 g of appropriate *E coli*. whole-cells (for entries 1 to 14, *E coli*. strain constructed via two gene-two plasmid method; for entries 15 and 16, *E coli*. strains constructed via two gene-one plasmid method, with plasmids pRSF-duet-RasADH (MCS1)-GDH (MCS2) and pRSF-duet-GDH (MCS1)-RasADH (MCS2), respectively), 0.2 mL DMSO, appropriate amount of other organic solvents and 50 mM NaP_i (pH 7.0) at 30 °C for appropriate hours. [a] *N.A.* stands for not applicable, meaning no organic solvent other than DMSO was added.

Product purification:

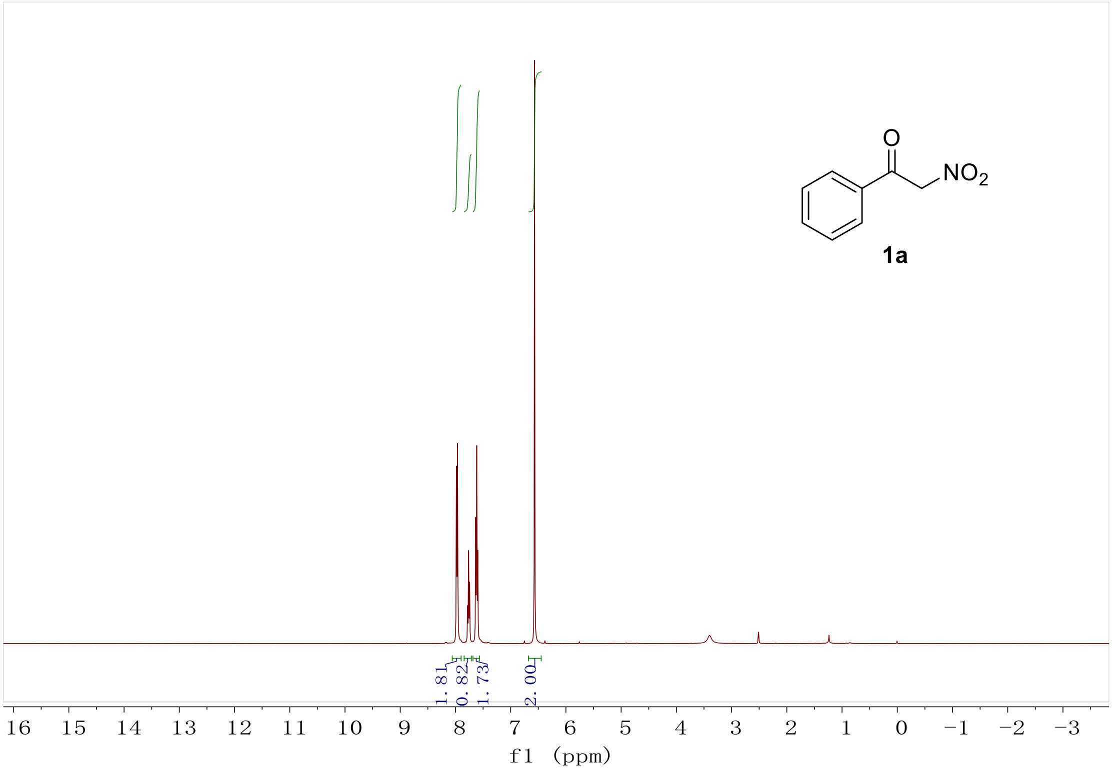
After 3h (entry 14), the reaction mixture was subjected to centrifugation and the supernatant was extracted with EtOAc. The organic layer was then washed with brine and dried with anhydrous Na_2SO_4, then filtered, and the filtrate was evaporated to dryness. The product **2k** was purified by flash chromatography (silica gel, petroleum ether: EtOAc = 8:1).

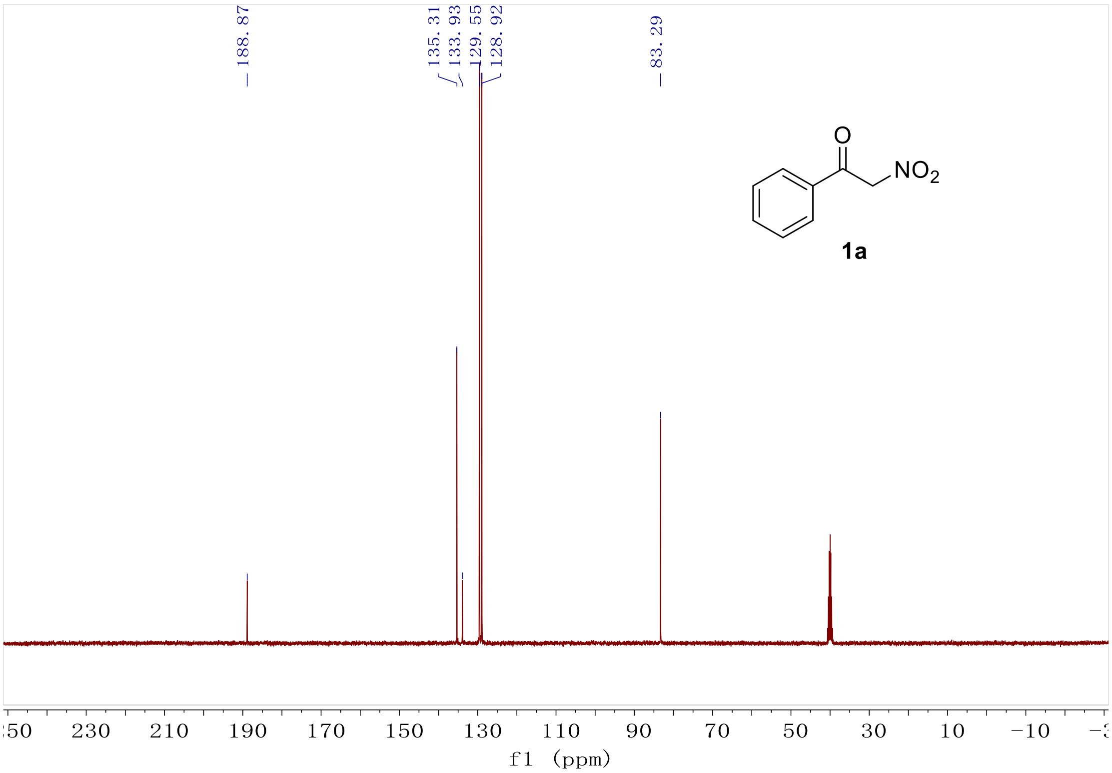
Table S18. List of oligonucleotides used in this study

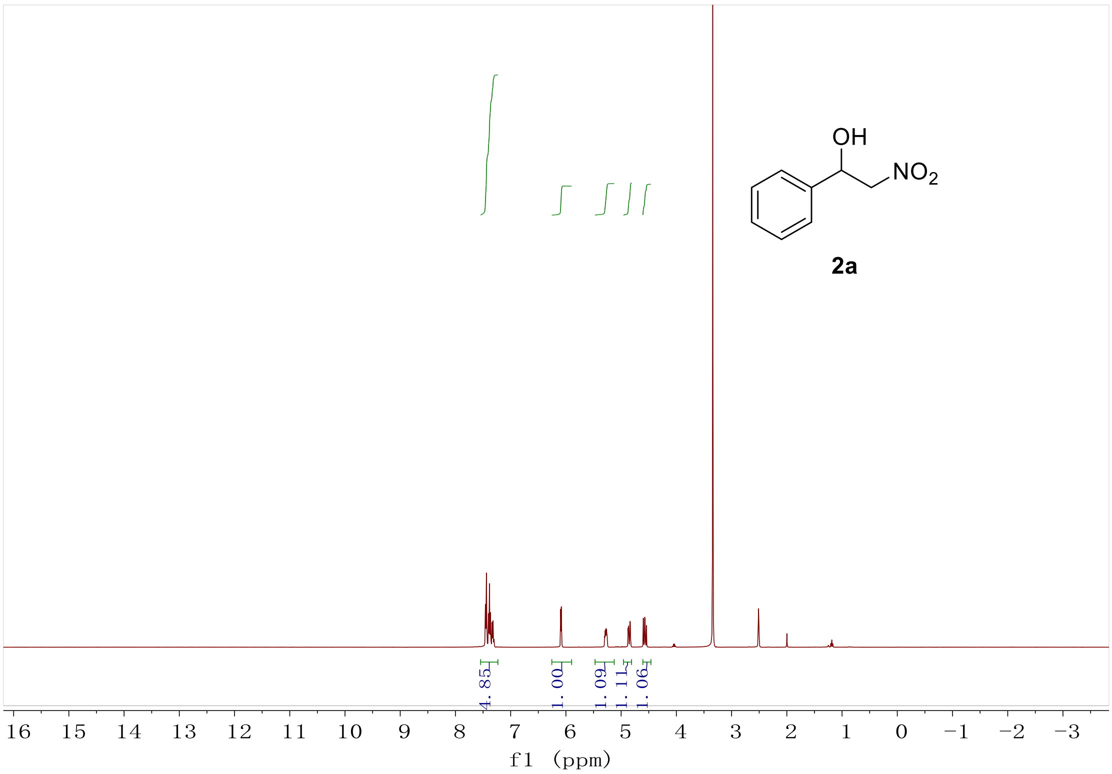
Name	Sequence (5'→3')[a]
pET28a-NdeI-YDR541c_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGTCTAATACAGTTCTAGTTTCT
pET28a-XhoI-YDR541c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCATAATCTGTTCTCCTTCTTC
pET28a-NdeI-YGL157w_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGACTACTGATACCACTGTTTTC
pET28a-XhoI-YGL157w_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTTAGGCTTCATTTGAACTTCT
pET28a-NdeI-YPL113c_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGATTACTTCAATTGACATAGCAG
pET28a-XhoI-YPL113c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCAGTTGAGCACATACTTACCAT
pET28a-NdeI-YHR104w_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGTCTTCACTGGTTACTCTTAAT
pET28a-XhoI-YHR104w_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCAGGCAAAAGTGGGGAATTTAC
pET28a-NdeI-YNL274c_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGAGTAAGAAACCAATTGTTTTG
pET28a-XhoI-YNL274c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCAAACTAATGGCTTAGATTCAT
pET28a-NdeI-YDR368w_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGCCTGCTACGTTAAAGAATTCT
pET28a-XhoI-YDR368w_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCATTGGAAAATTGGGAAGGAT
pET28a-NdeI-YGL039w_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGACTACTGAAAAAACCGTTG
pET28a-XhoI-YGL039w_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTTAGCTTTTACTTTGAACTTCTAGT
pET28a-NdeI-YNL331c_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGACTGACTTGTTTAAACCTCT
pET28a-XhoI-YNL331c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGCTAATTGTCAAAAGCTATCCTGGC
pET28b-NcoI-Ymr226c_fw	TTTAACTTTAAGAAGGAGATATACCATGTCCCAAGGTAGAAAAGCTGCAG
pET28b-XhoI-Ymr226c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTgATCCACGGAAGATATGATGAGGT
pET28b-NcoI-YOL151w_fw	ACTTTAAGAAGGAGATATACCATGTCAGTTTTCGTTTCAGGTGCT
pET28b-XhoI-YOL151w_rc	GTGGTGGTGGTGGTGGTGCTCGAGTATTCTGCCCTCAAATTTTAA AAT

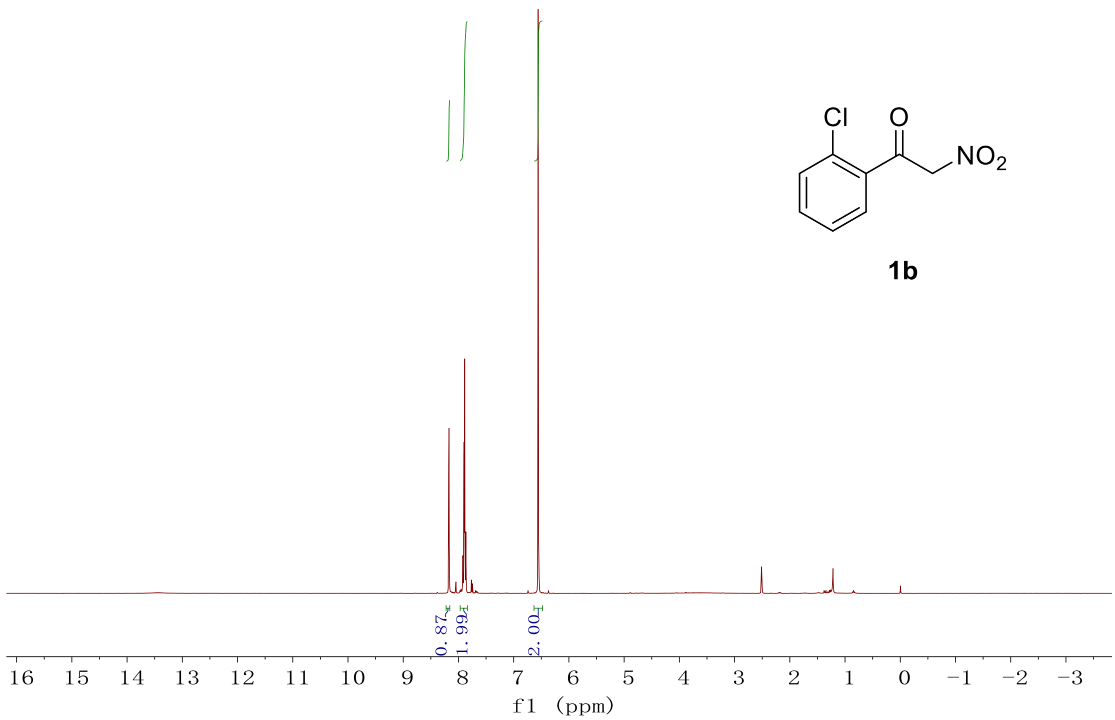
pET28a-NdeI-YAL060w_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGAGAG CTTTGGCATATTTCAAG
pET28a-XhoI-YAL060w_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTTACTTCA TTTCACCGTGATTGT
pET28b-NcoI-YOR120w_fw	ACTTTAAGAAGGAGATATACCATGCCTGCTACT TTACATGATTCT
pET28b-XhoI-YOR120w_rc	GTGGTGGTGGTGGTGGTGCTCGAGCTTGAATAC TTCGAAAGGAGACCAAT
pET28a-NdeI-YGL185c_fw	CGGCCTGGTGCCGCGCGGCAGCCATATGTGCG ATTCTCCTGCAACGACT
pET28a-XhoI-YGL185c_rc	AGTGGTGGTGGTGGTGGTGCTCGAGTCAAACT ACACGGGAGAAATGCT
pACYC-NcoI-GDH(1)-fw	TTTAACTTTAATAAGGAGATATACCATGGCAACT GAACAGAAAGCCATTGT
pACYC-EcoRI-GDH(2)-rc	CTGCAGGCGCGCCGAGCTCGAATTCTCACTGC CACTTTATCACCGTCTTTAT
pRSF-NcoI-RasADH(1)-fw	TTTAACTTTAATAAGGAGATATACCATGTACCGT TTACTGAATAAAACCG
pRSF-EcoRI-RasADH(1)-rc	CTGCAGGCGCGCCGAGCTCGAATTCTTAAACTT GGGTTAAACCGCCAT
pRSF-NdeI-RasADH(1)-GDH(2)-fw	TTAAGTATAAGAAGGAGATATACATAtggcaACTG AACAGAAAGCCATTGT
pRSF-XhoI-RasADH(1)-GDH(2)-rc	CAGCGGTTTCTTTACCAGACTCGAGTCACTGCC ACTTTATCACCGTC
pRSF-NcoI-GDH(1)-fw	TTTAACTTTAATAAGGAGATATACCATGGCAA CTGAACAGAAAGCCATTGT
pRSF-EcoRI-GDH(1)-rc	CTGCAGGCGCGCCGAGCTCGAATTCTCACTGC CACTTTATCACCGTCTTTAT
pRSF-NdeI-GDH(1)-RasADH(2)-fw	AGTATAAGAAGGAGATATACATATGTACCGTTTA CTGAATAAAACCGCCGT
pRSF-XhoI-GDH(1)-RasADH(2)-rc	CAGCGGTTTCTTTACCAGACTCGAGTTAAACTT GGGTTAAACCGCCAT

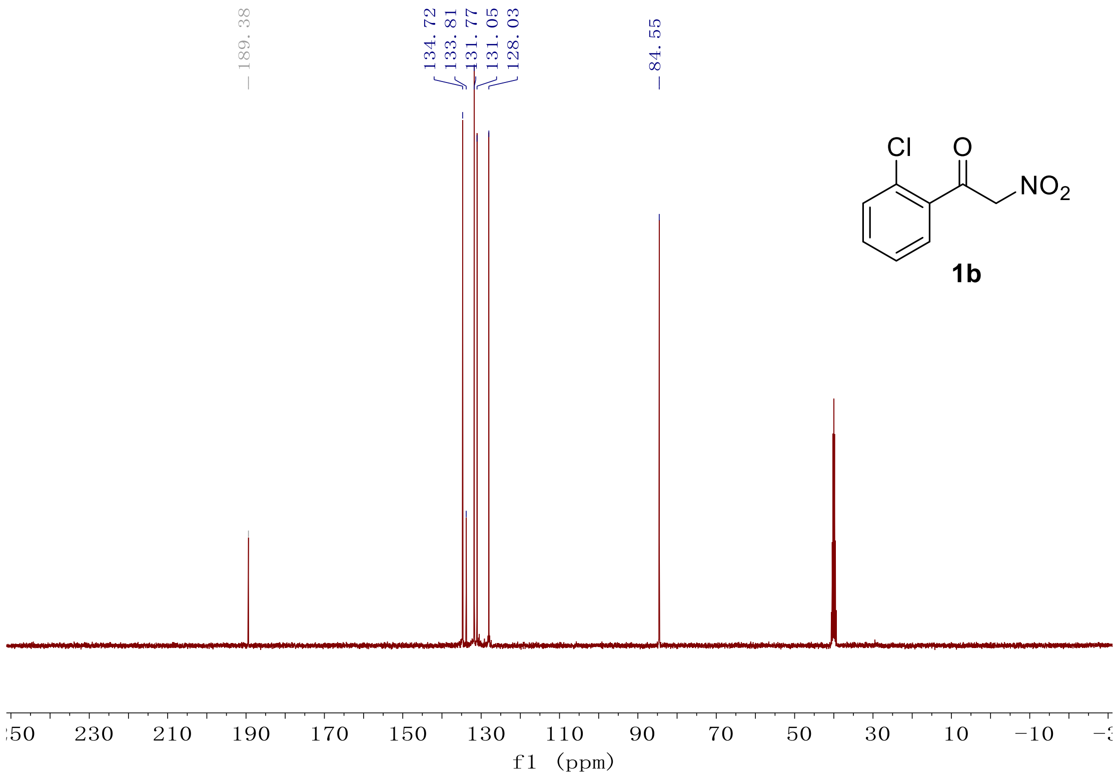
[a]Nucleotides colored in red indicate cleavage sites

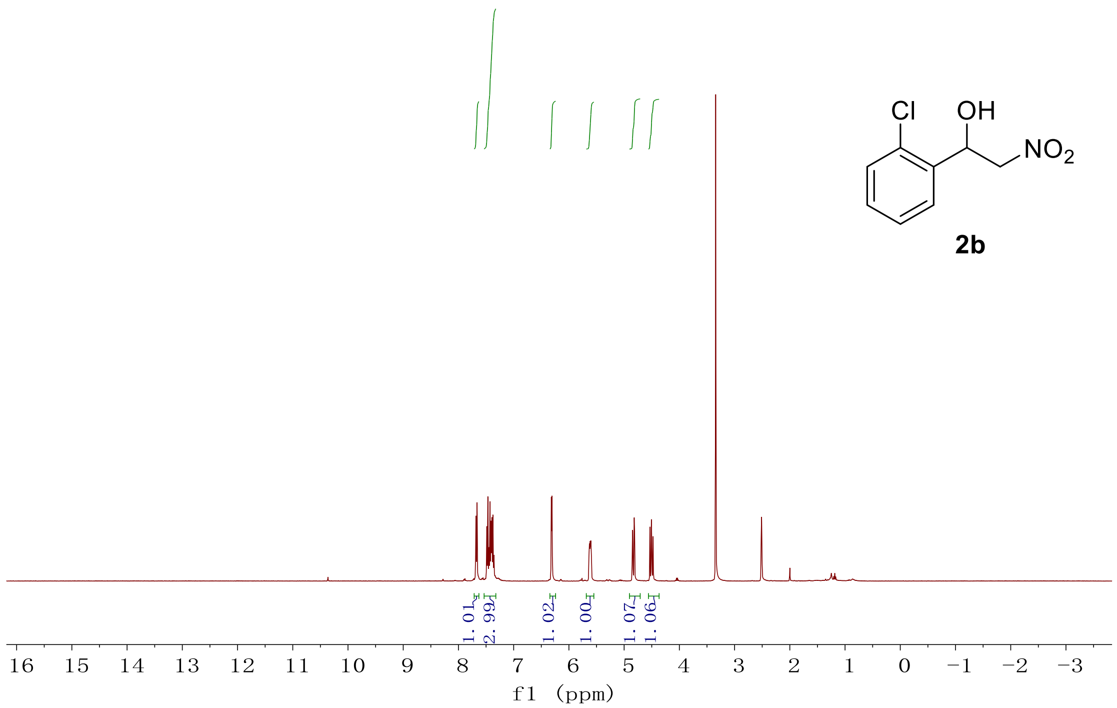

1.81
0.82
1.73
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO2
1a

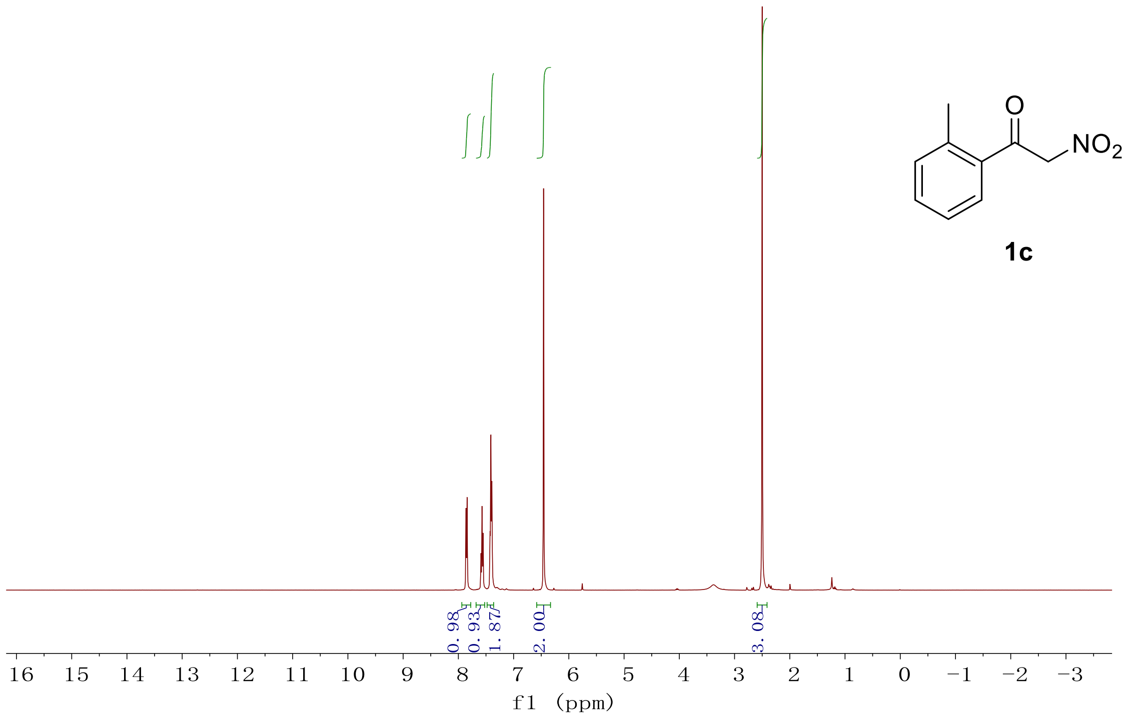

188.87
135.31
133.93
129.55
128.92
83.29
O
NO2
1a
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OH
NO2
2a
4.85
1.00
1.09
1.11
1.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

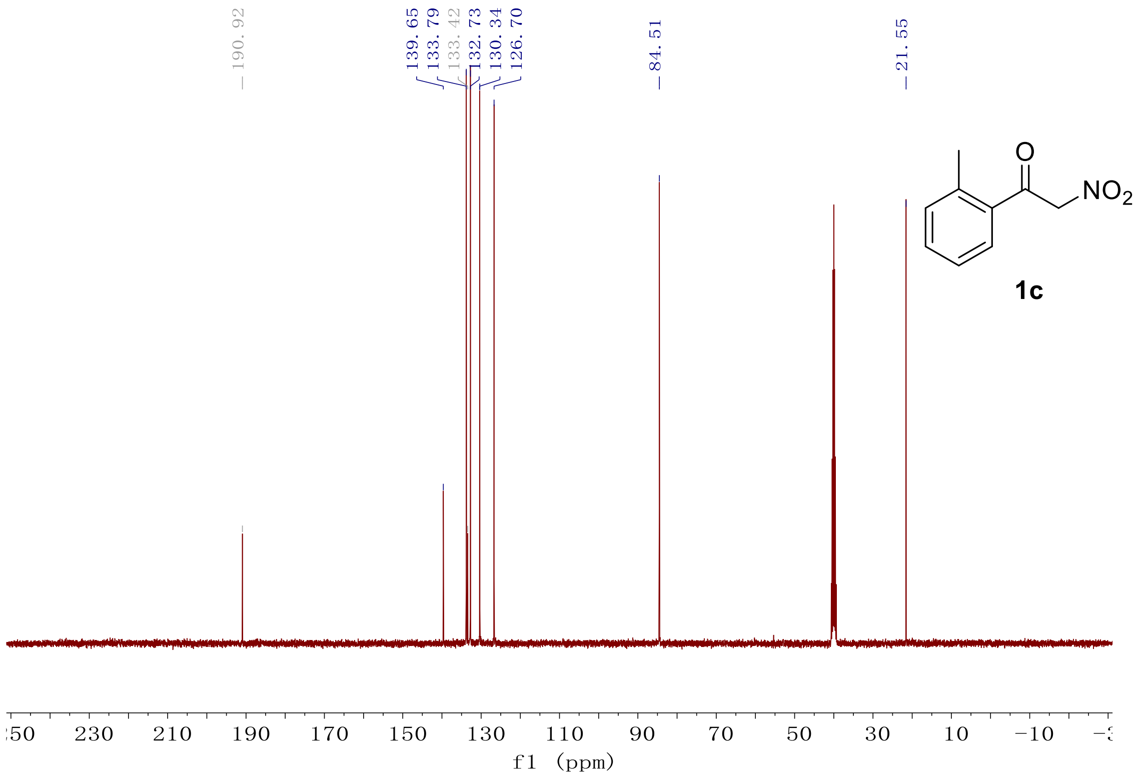

0.87
1.99
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
Cl
O
NO2
1b


189.38
134.72
133.81
131.77
131.05
128.03
84.55
Cl
O
NO2
1b
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

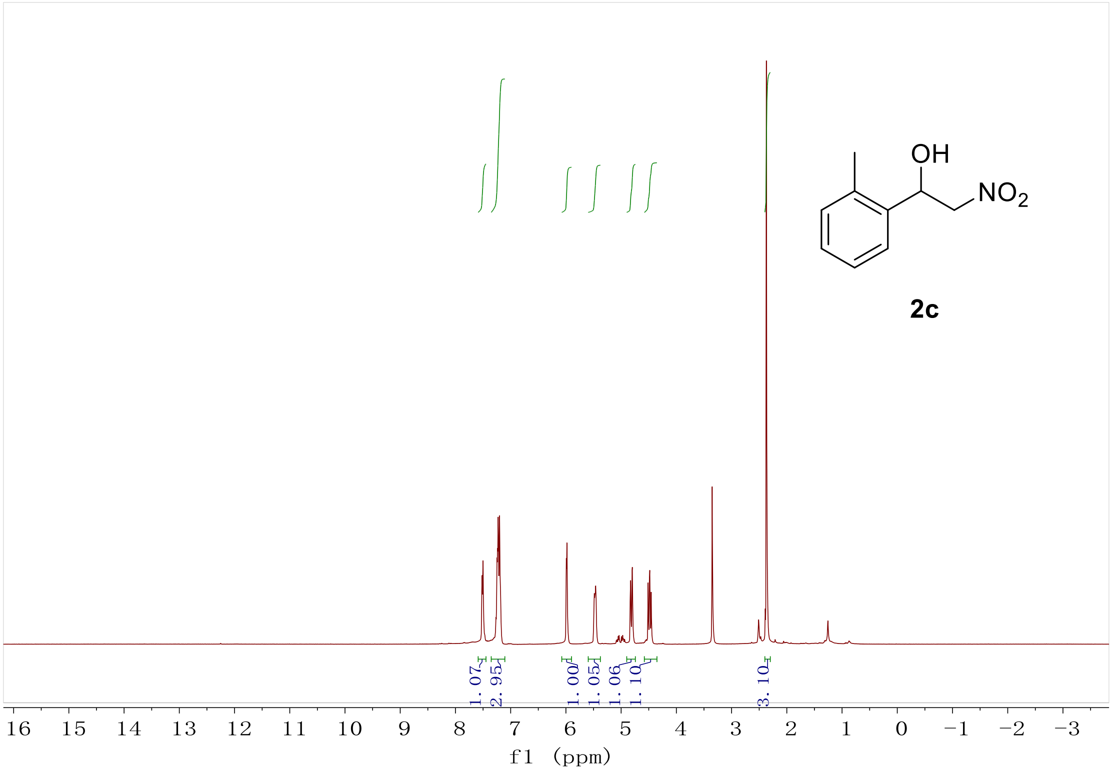

Cl
OH
NO2
2b
1.01
2.99
1.02
1.00
1.07
1.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



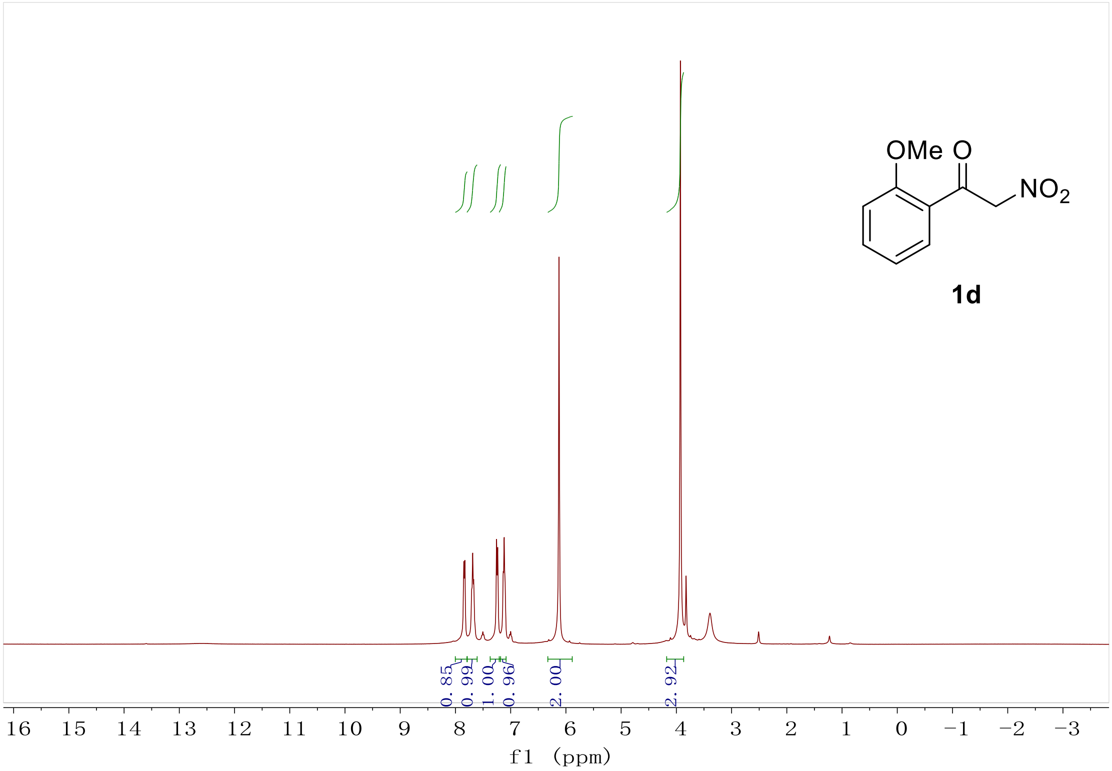
NO2
1c
0.98
0.93
1.87
2.00
3.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

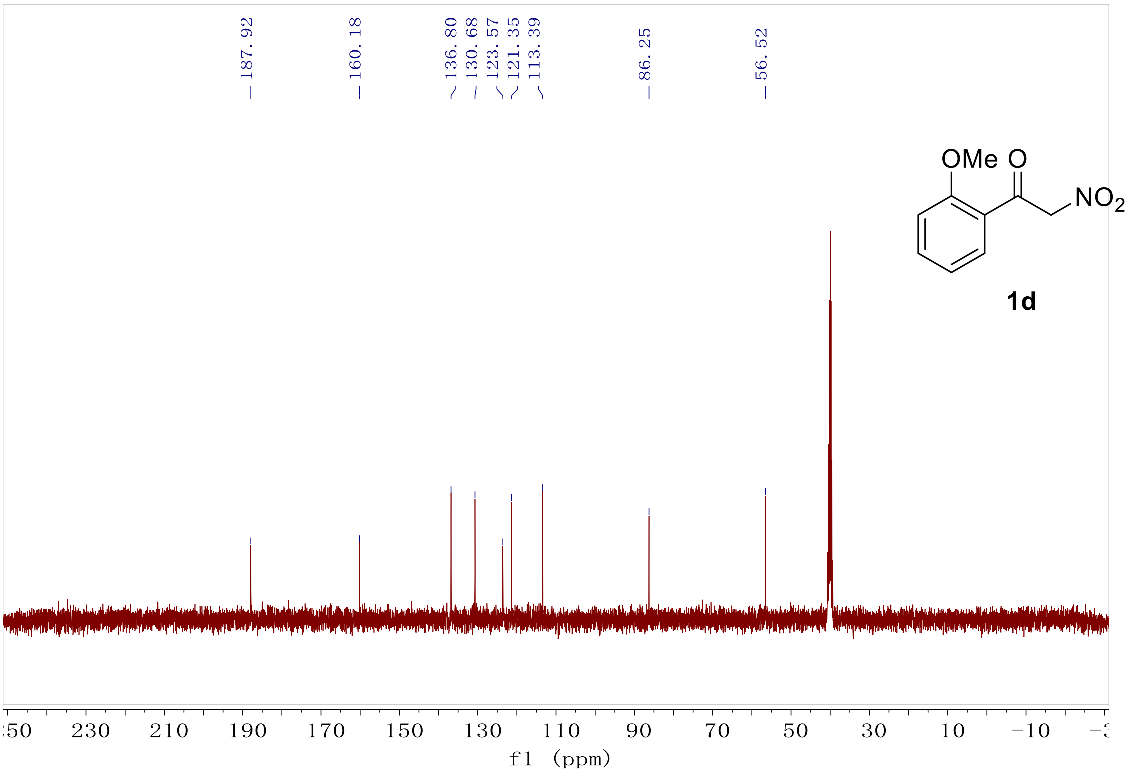


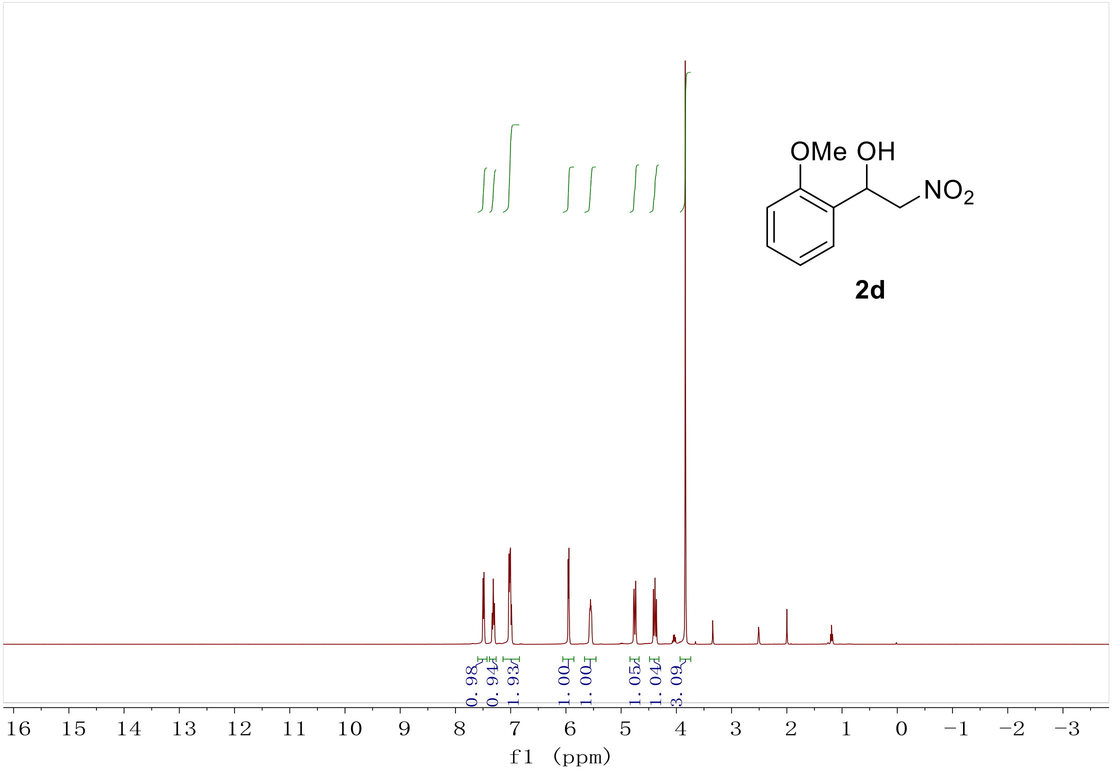
190.92
139.65
133.79
133.42
132.73
130.34
126.70
84.51
21.55
NO2
1c
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OH
NO2
1.07
2.95
1.00
1.05
1.06
1.10
3.10
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

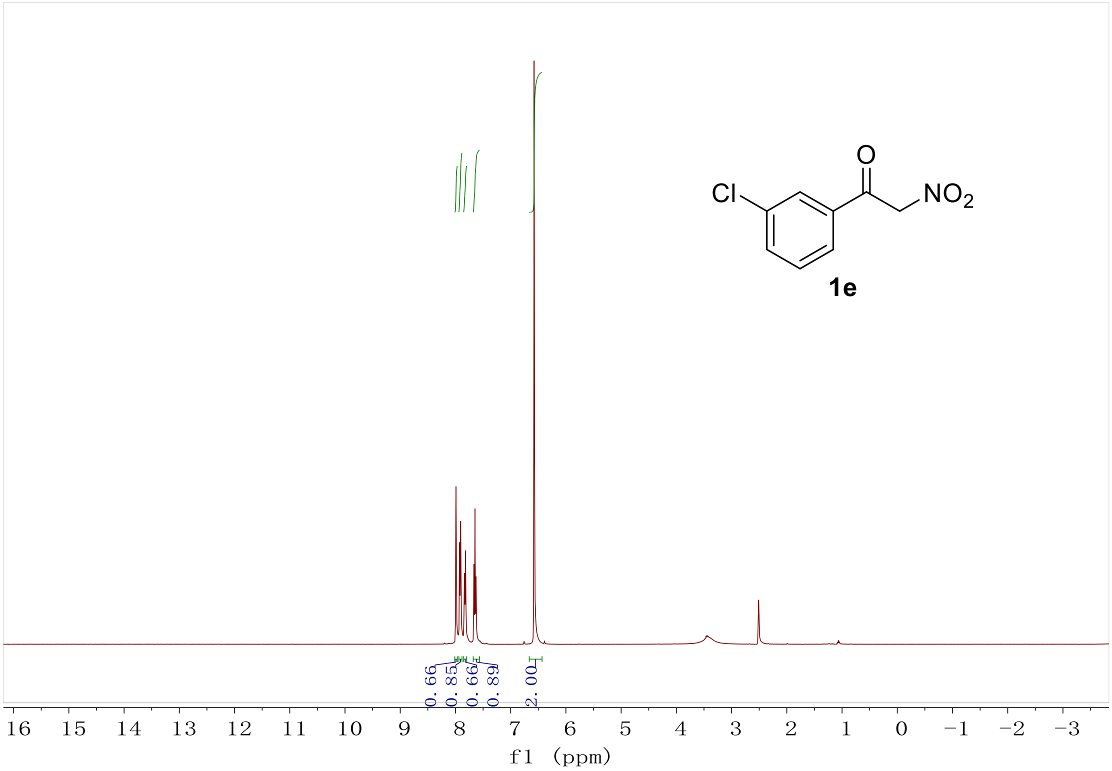
2c


OMe O
NO2
1d
0.85
0.99
1.00
0.96
2.00
2.92
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

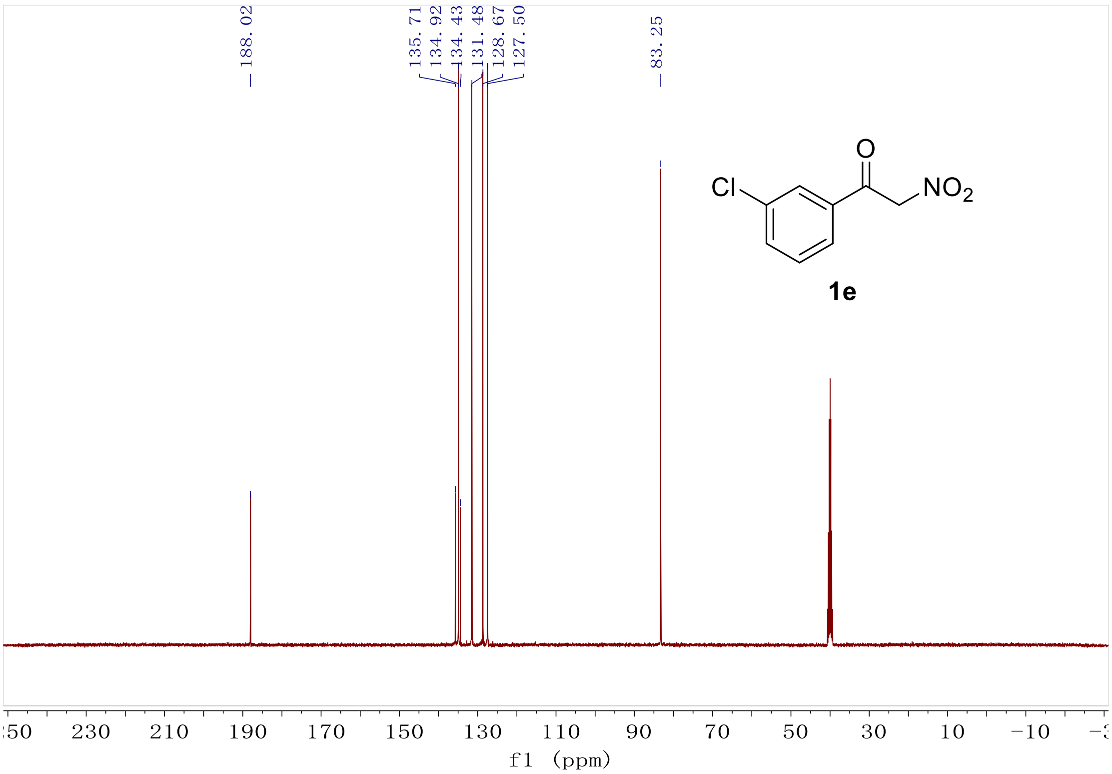

187.92
160.18
136.80
130.68
123.57
121.35
113.39
86.25
56.52
OMe O
NO2
1d
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OMe OH
NO2
0.98
0.94
1.93
1.00
1.00
1.05
1.04
3.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

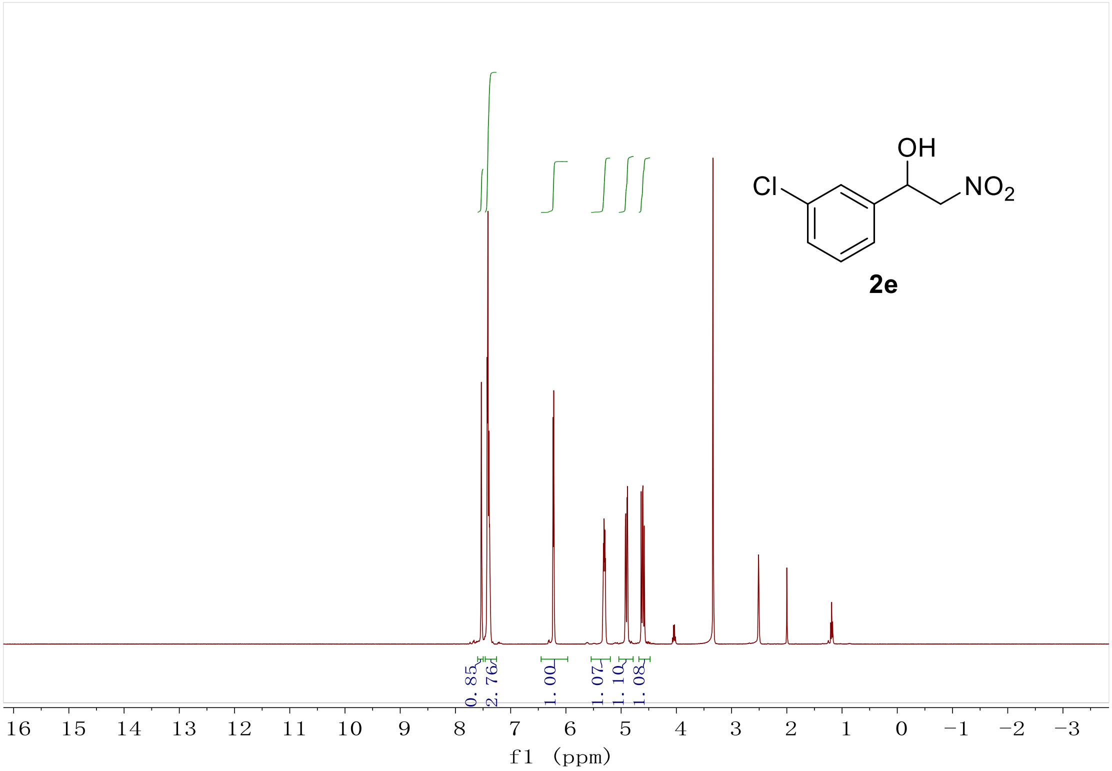
2d

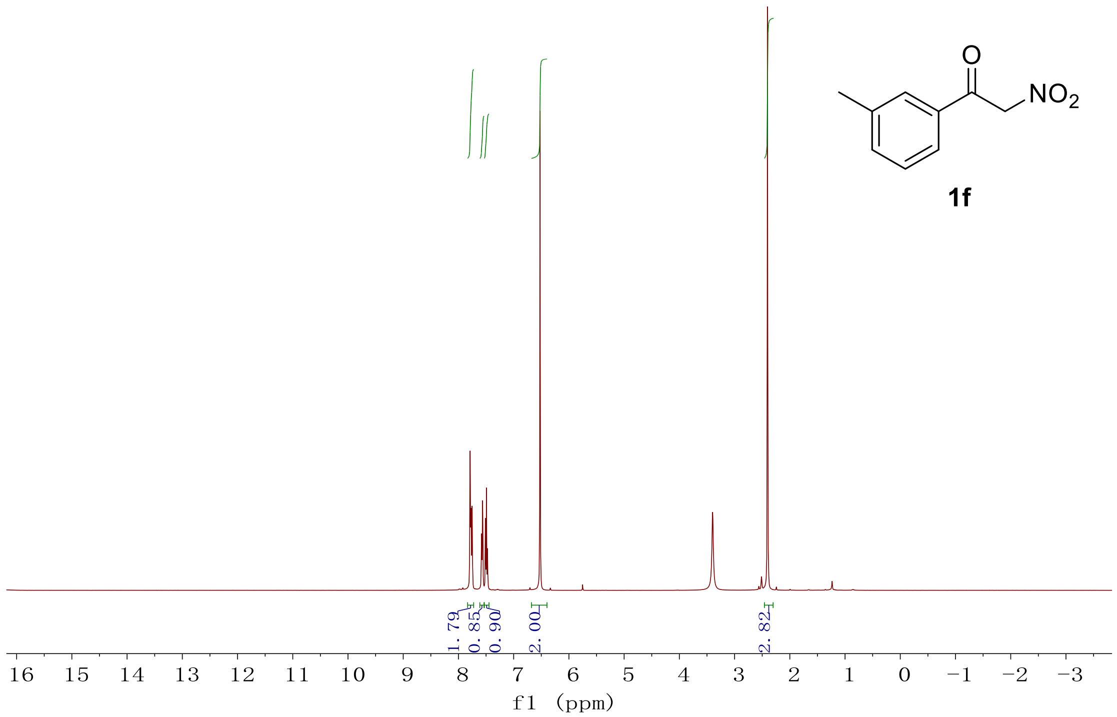

Cl
O
NO2
0.66
0.85
0.66
0.89
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

1e

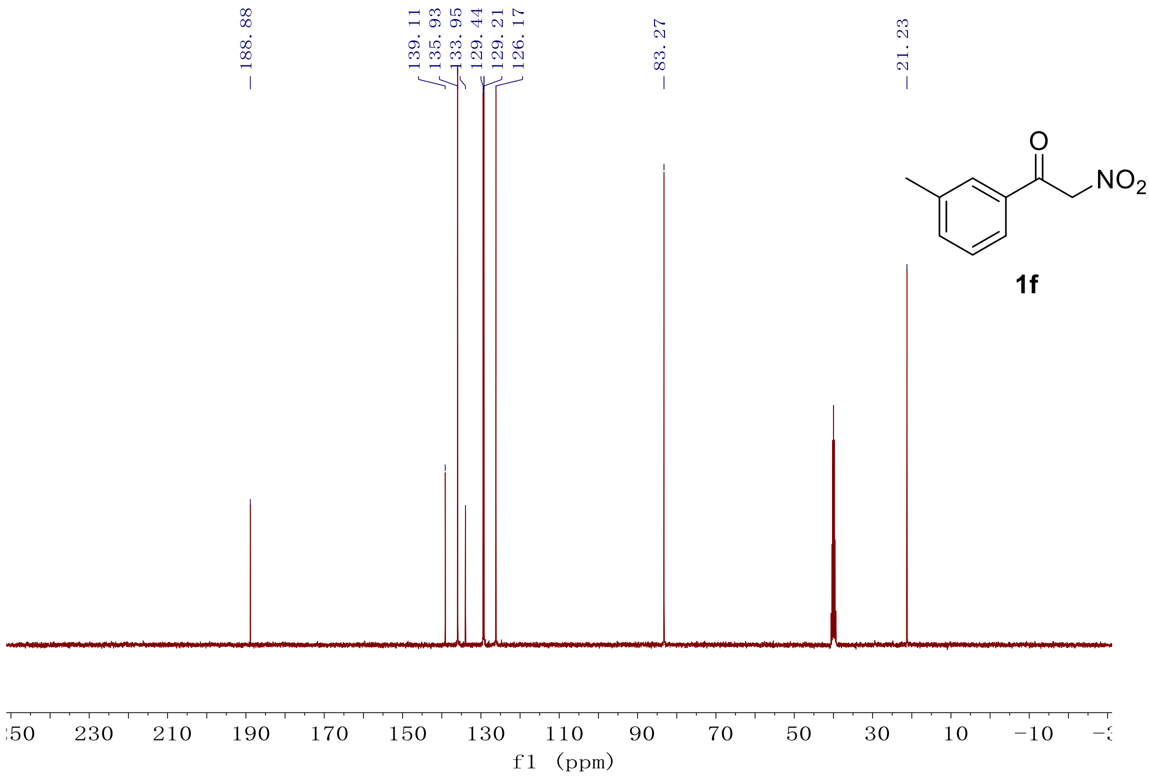

188.02
135.71
134.92
134.43
131.48
128.67
127.50
83.25
Cl
O
NO2
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

1e

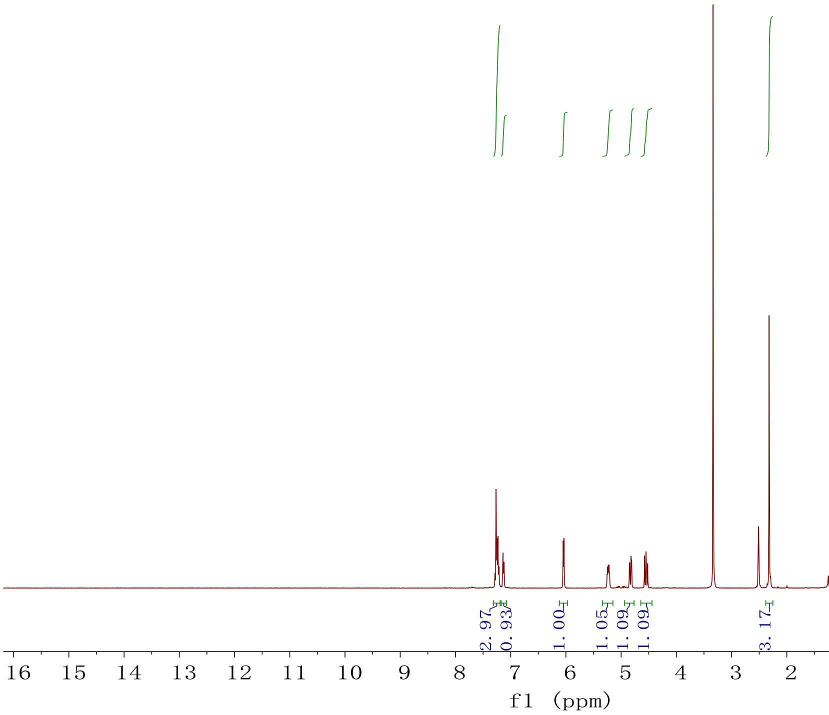

OH
Cl
NO2
2e
0.85
2.76
1.00
1.07
1.10
1.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

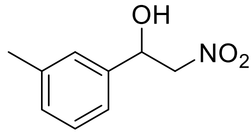


O
NO2
1f
1.79
0.85
0.90
2.00
2.82
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

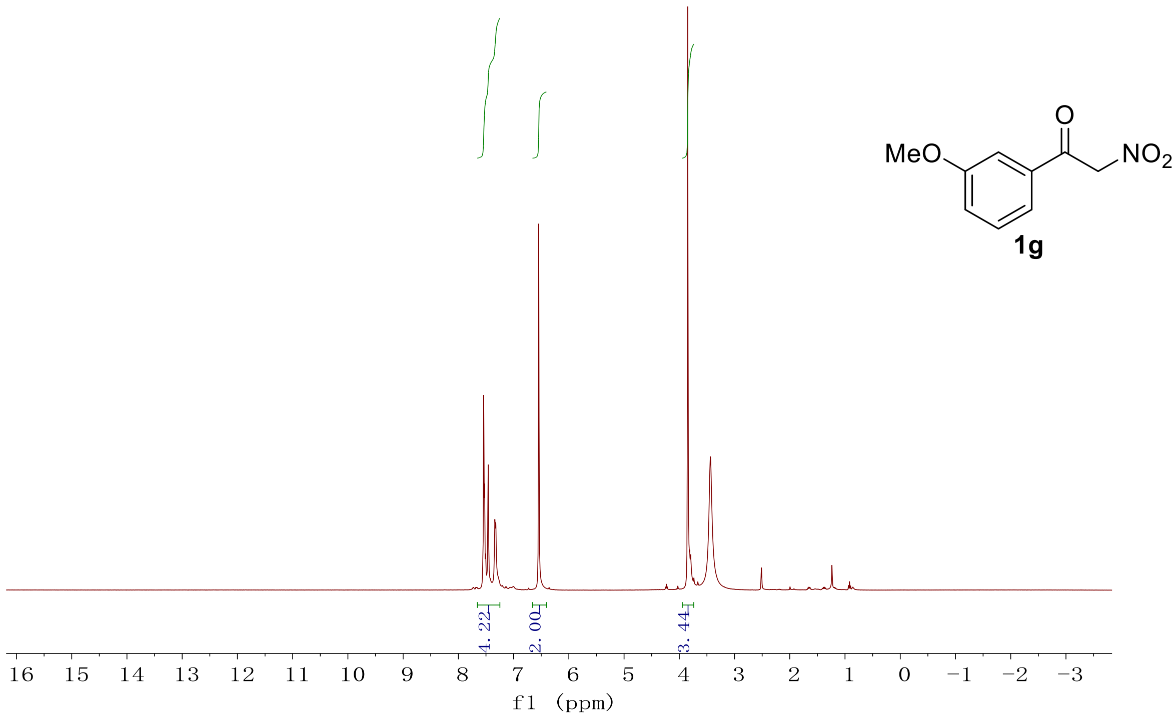


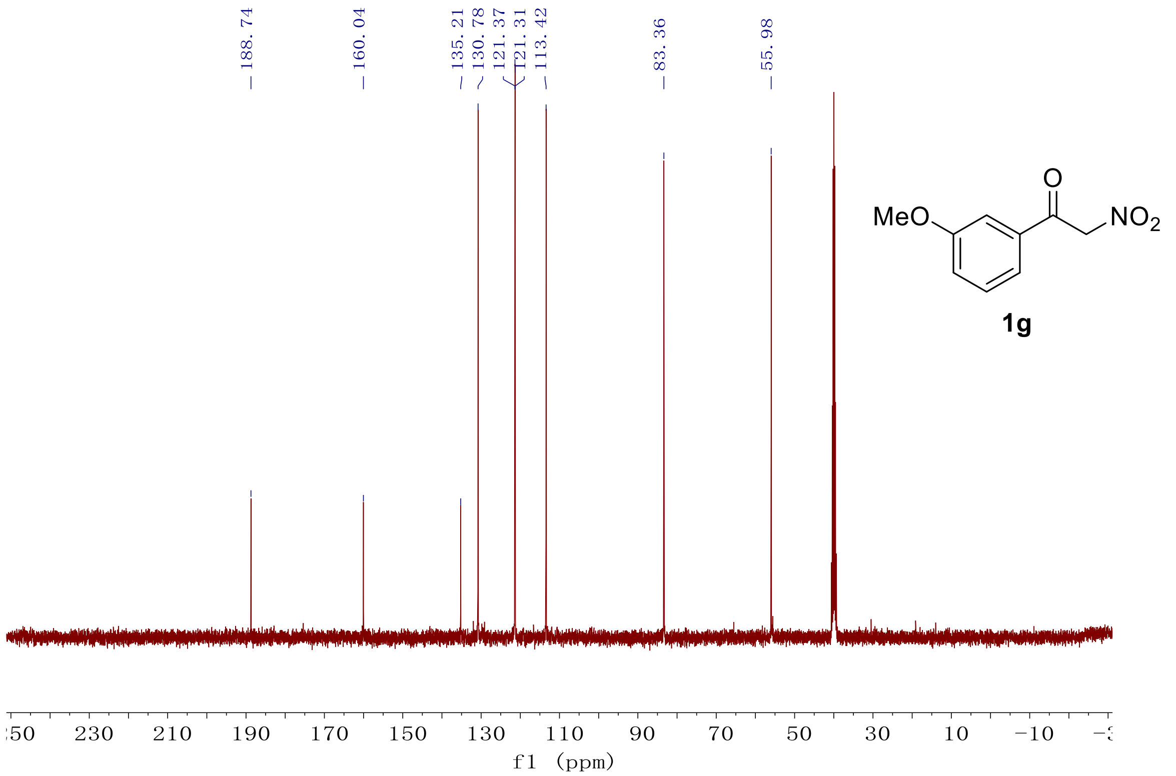
188.88
139.11
135.93
133.95
129.44
129.21
126.17
83.27
21.23
O
NO2
1f
250 230 210 190 170 150 130 110 90 70 50 30 10 −10 −30
f1 (ppm)

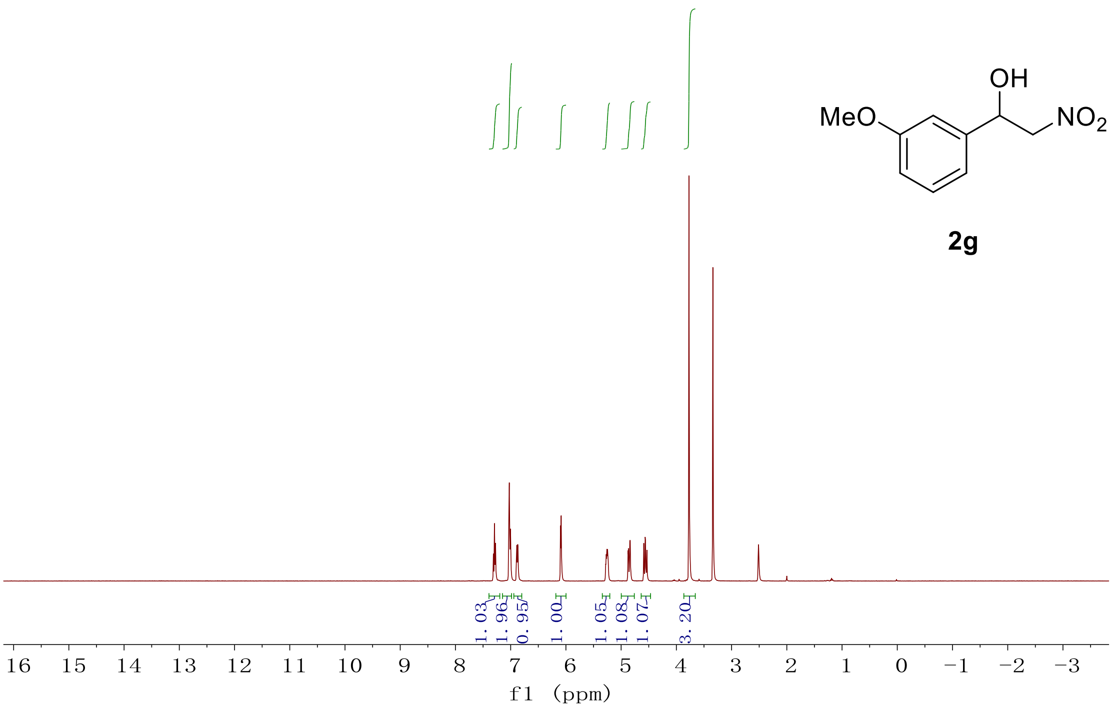

2.97
0.93
1.00
1.05
1.09
1.09
3.17
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


OH
NO2

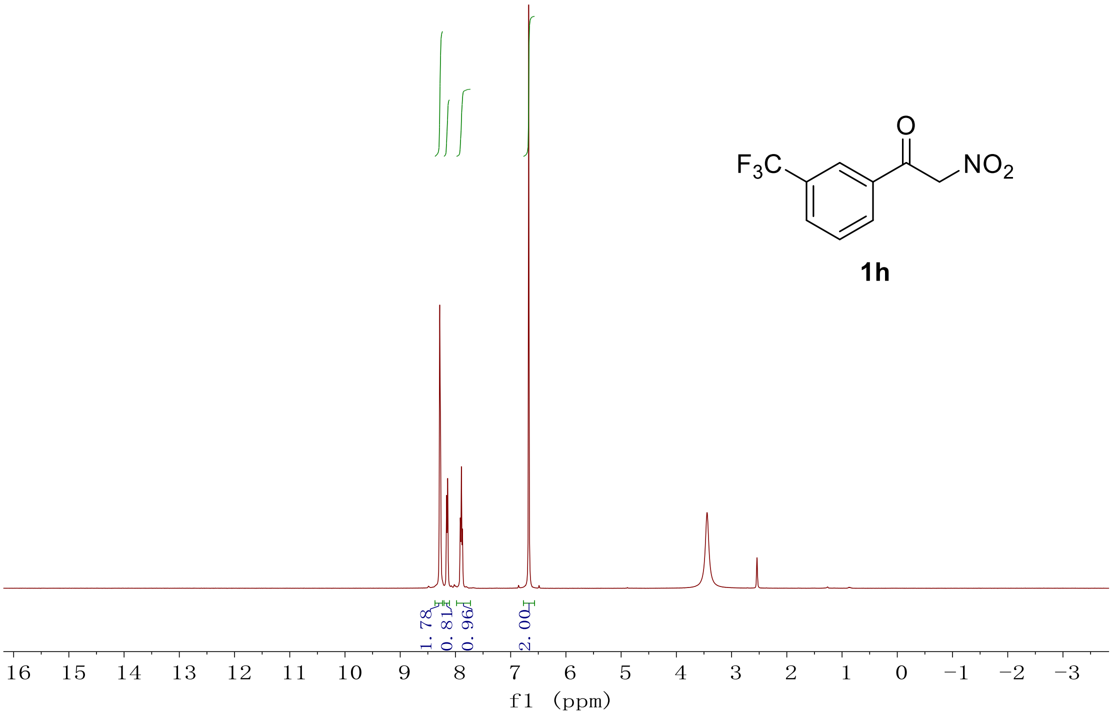
2f


MeO
O
NO2
1g
4.22
2.00
3.44
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

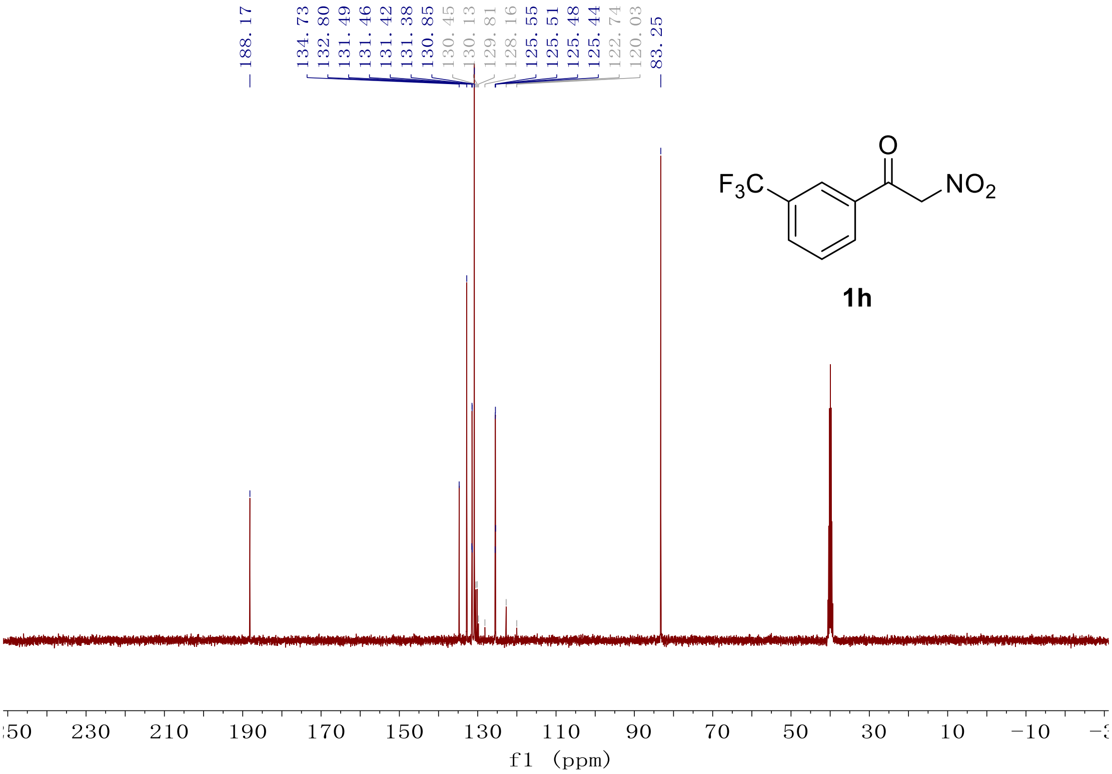

188.74
160.04
135.21
130.78
121.37
121.31
113.42
83.36
55.98
MeO
O
NO2
1g
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)



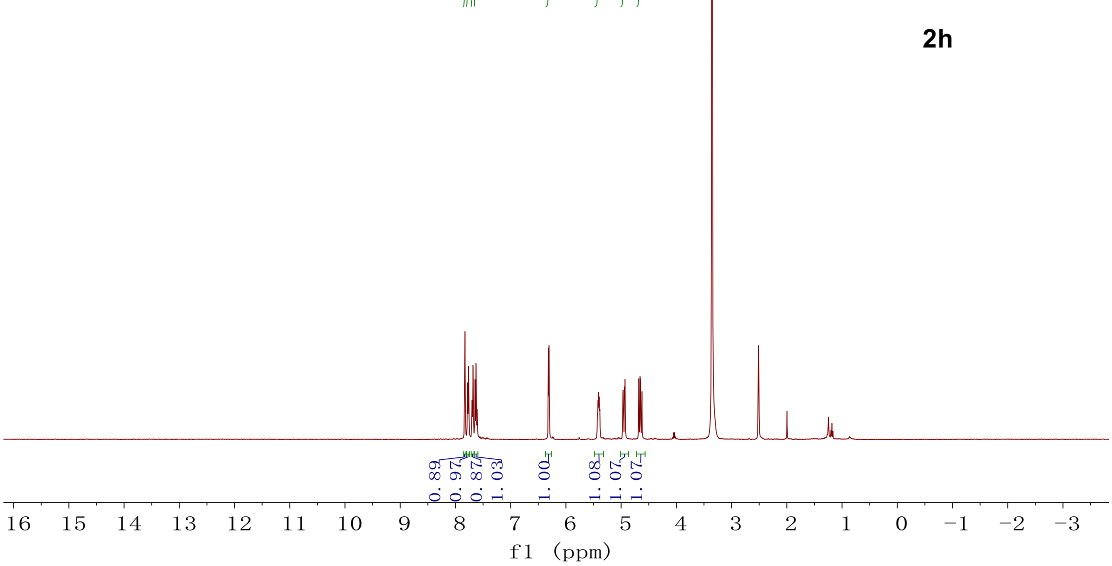
2g

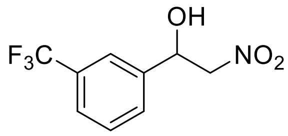


F3C
O
NO2
1h
1.78
0.81
0.96
2.00
f1 (ppm)

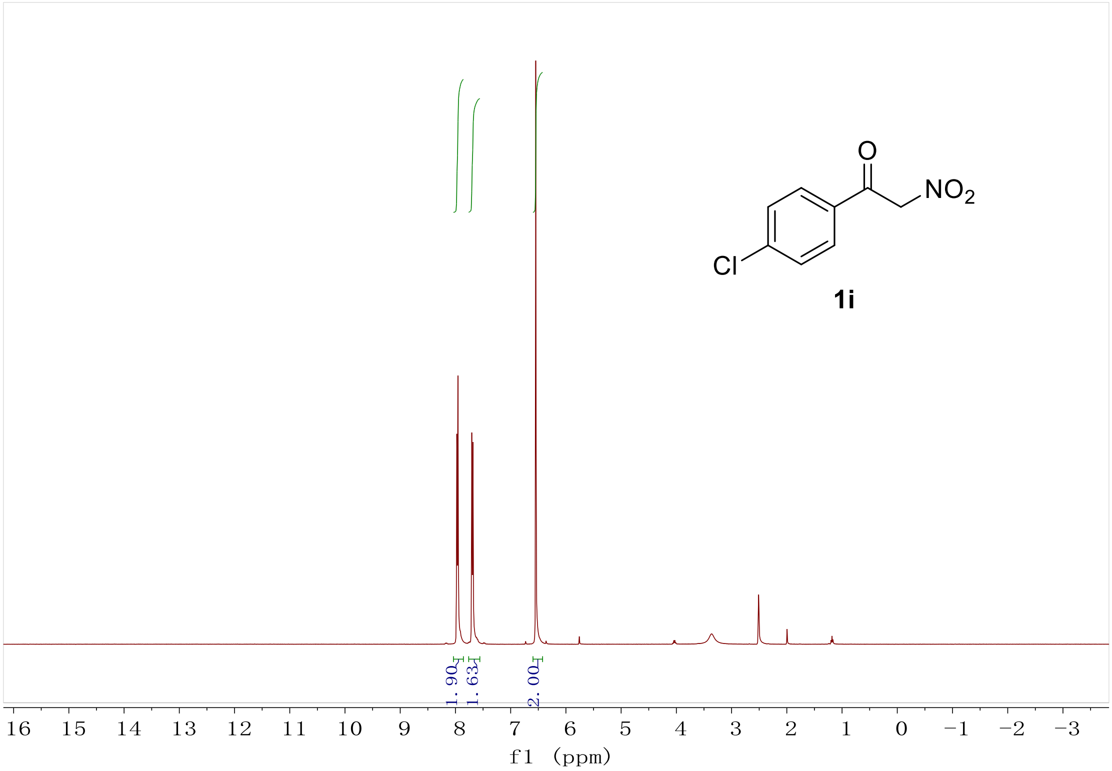


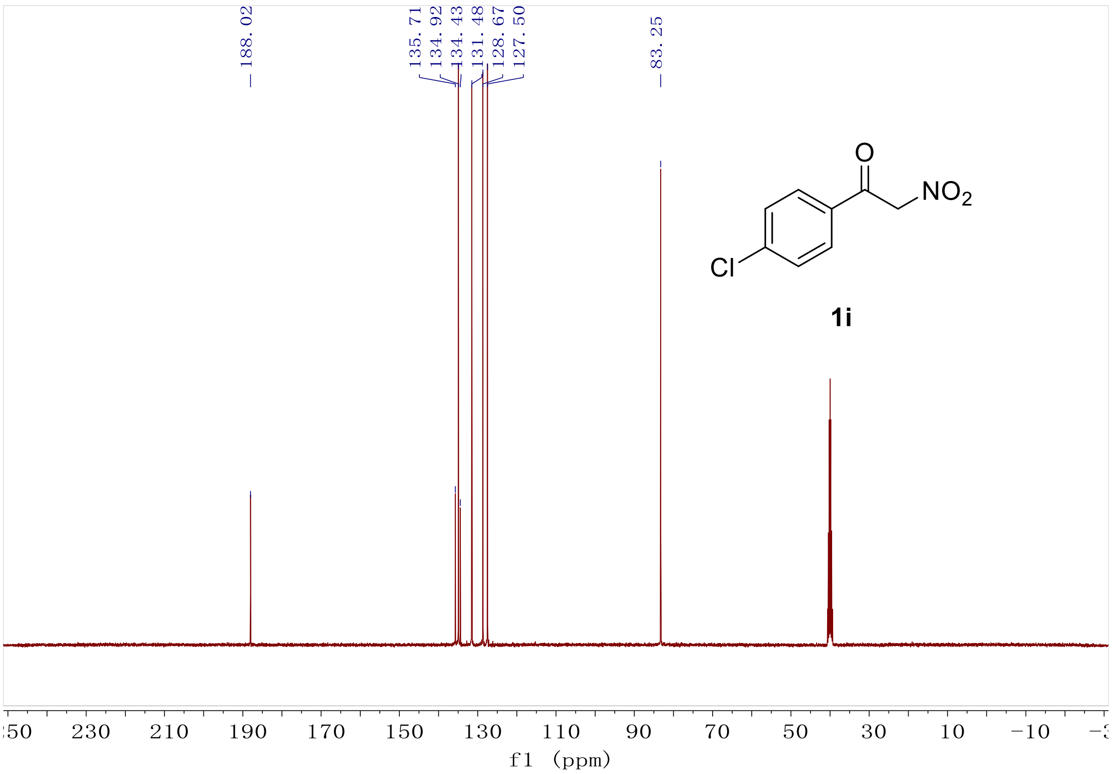
188.17
134.73
132.80
131.49
131.46
131.42
131.38
130.85
130.45
130.13
129.81
128.16
125.55
125.51
125.48
125.44
122.74
120.03
83.25
F3C
O
NO2
1h
f1 (ppm)

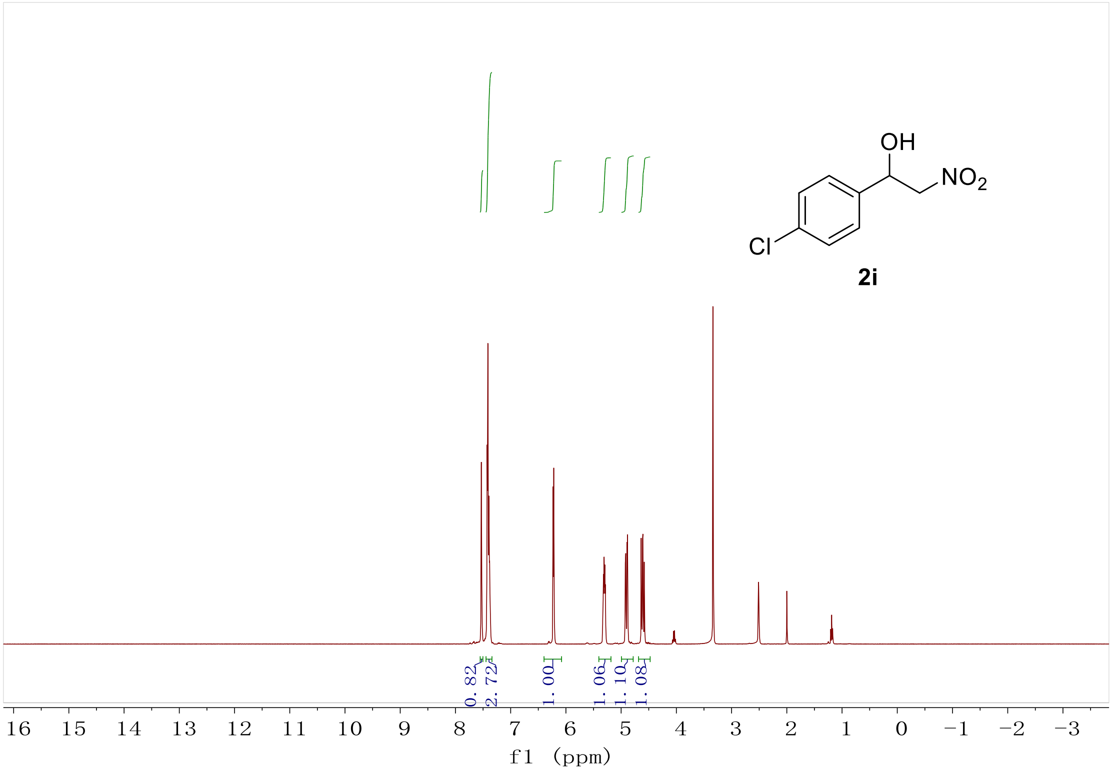

0.89
0.97
0.87
1.03
1.00
1.08
1.07
1.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

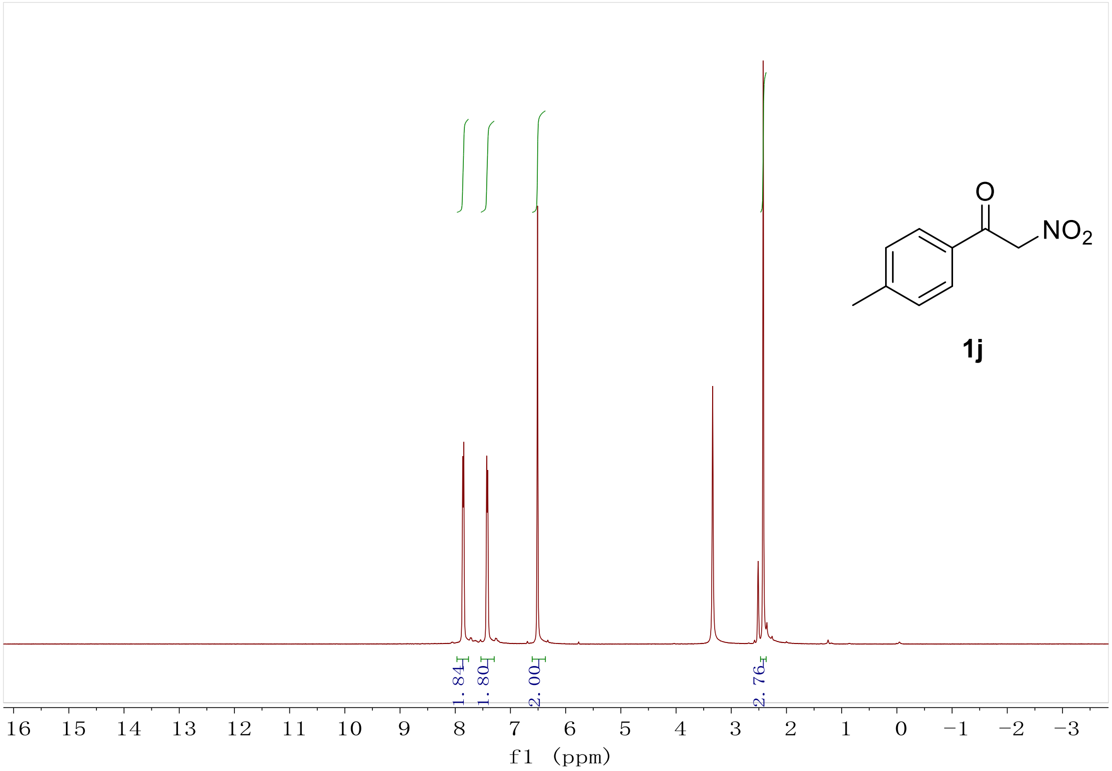

OH
F_3C
NO_2

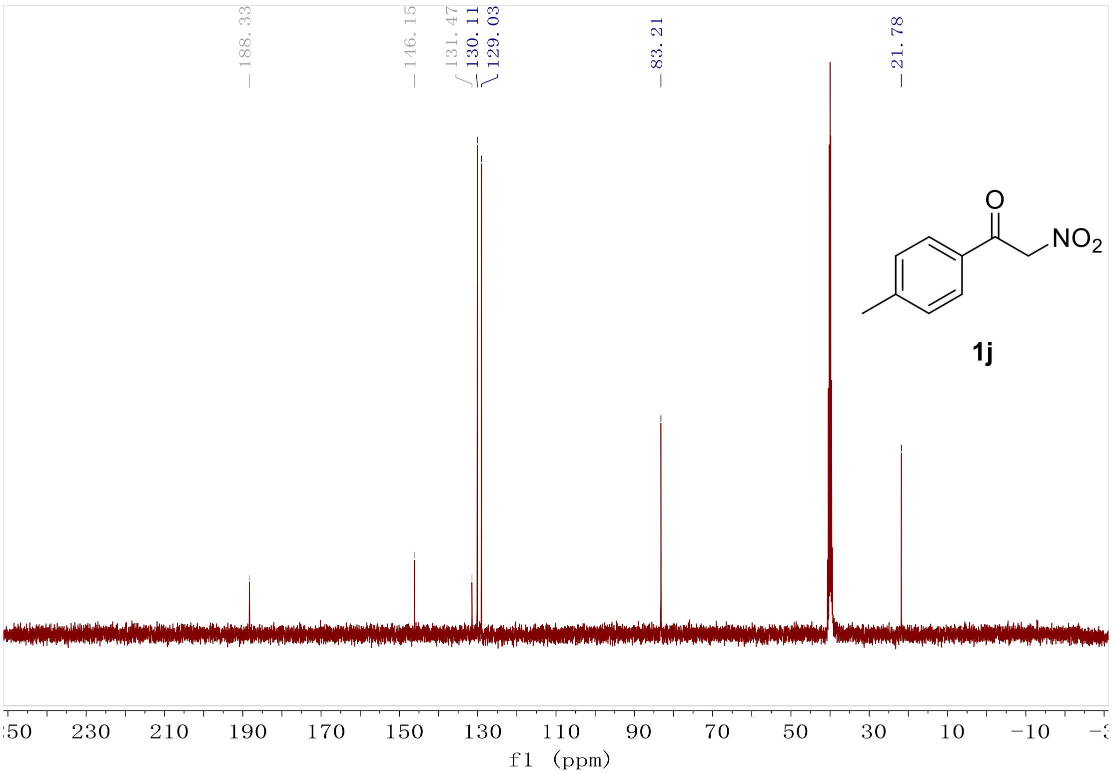
2h

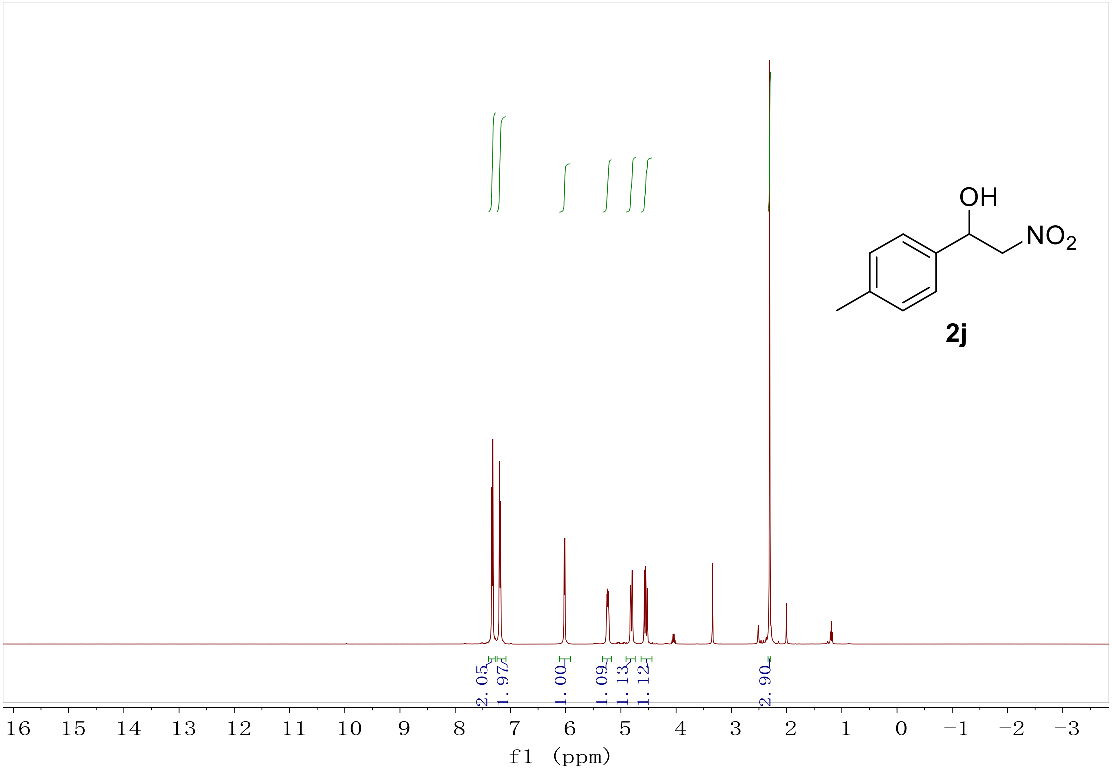

1.90
1.63
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO_2
Cl
1i


188.02
135.71
134.92
134.43
131.48
128.67
127.50
83.25
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)
O
NO_2
Cl
1i

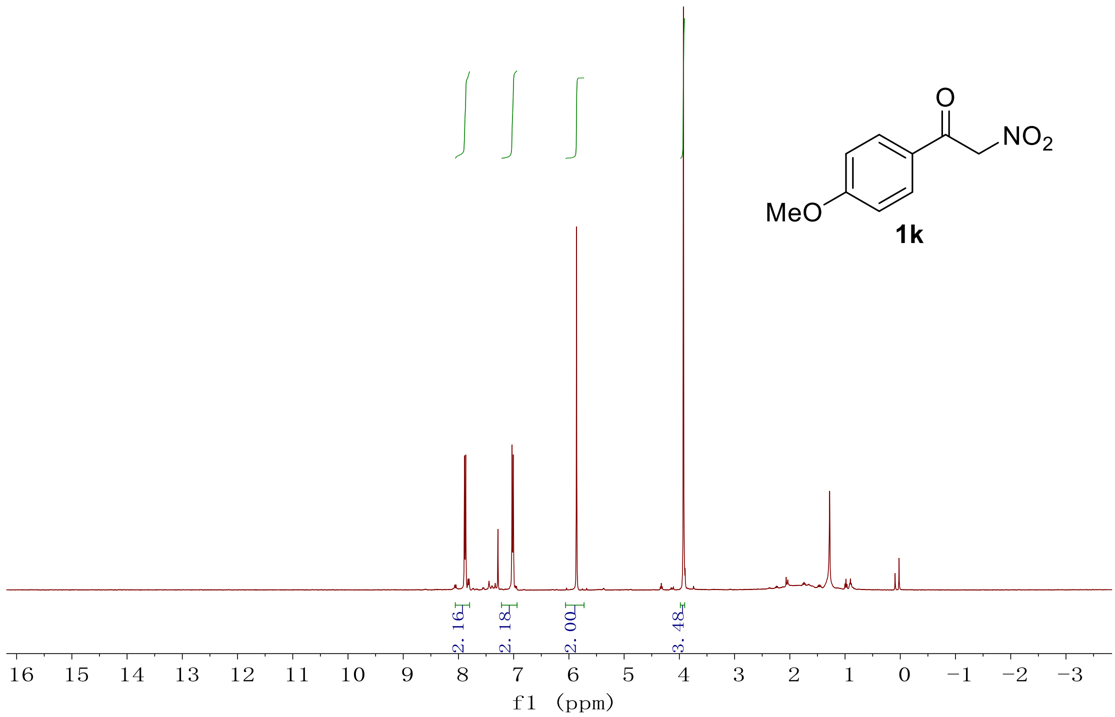

OH
NO2
Cl
2i
0.82
2.72
1.00
1.06
1.10
1.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


1.84
1.80
2.00
2.76
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO2
1j

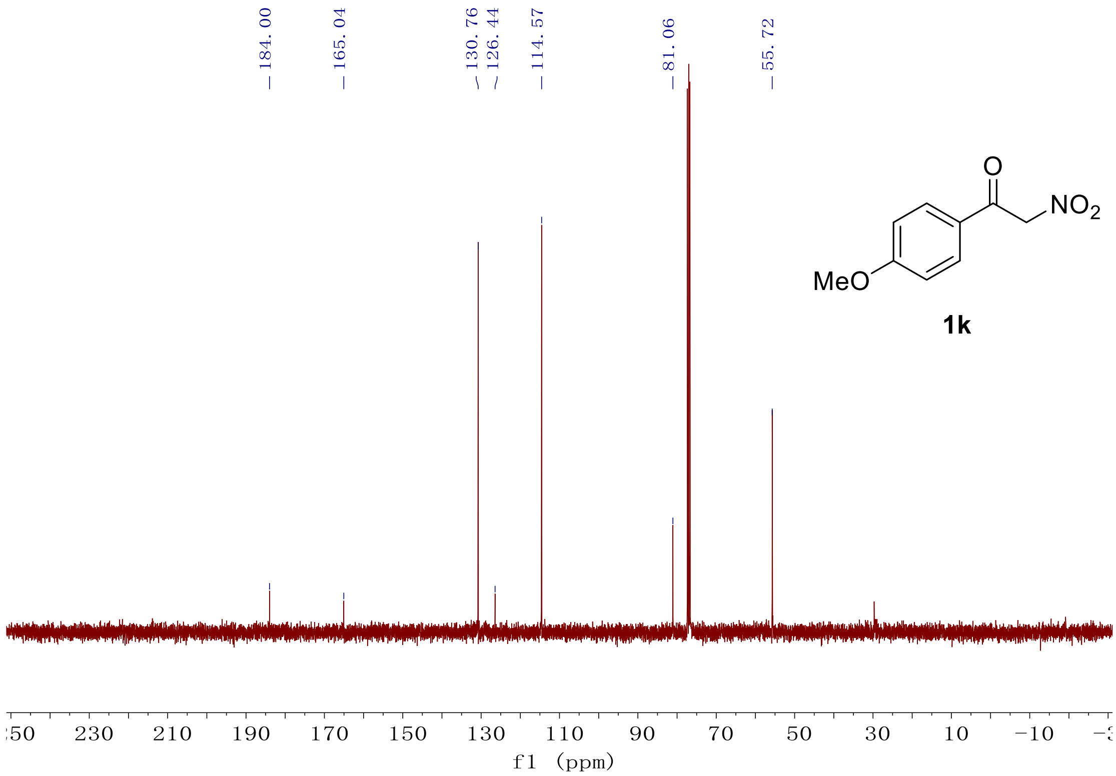

188.33
146.15
131.47
130.11
129.03
83.21
21.78
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)
O
NO2
1j



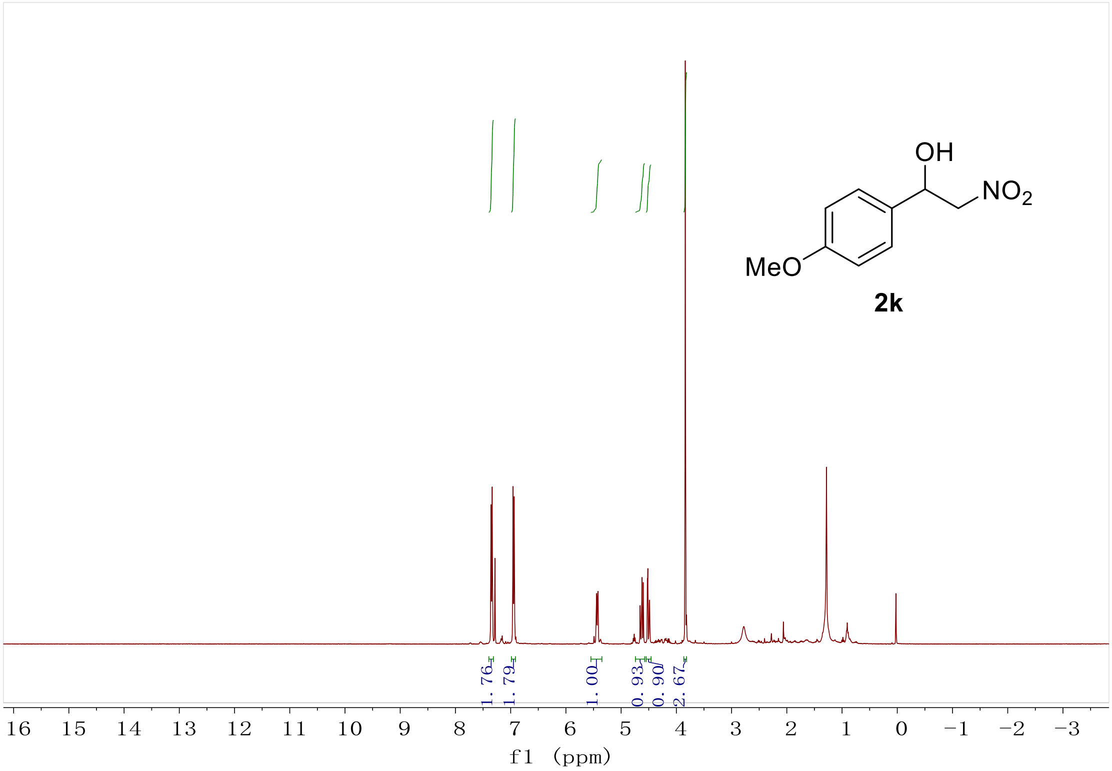
OH
NO_2
2j
2.05
1.97
1.00
1.09
1.13
1.12
2.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

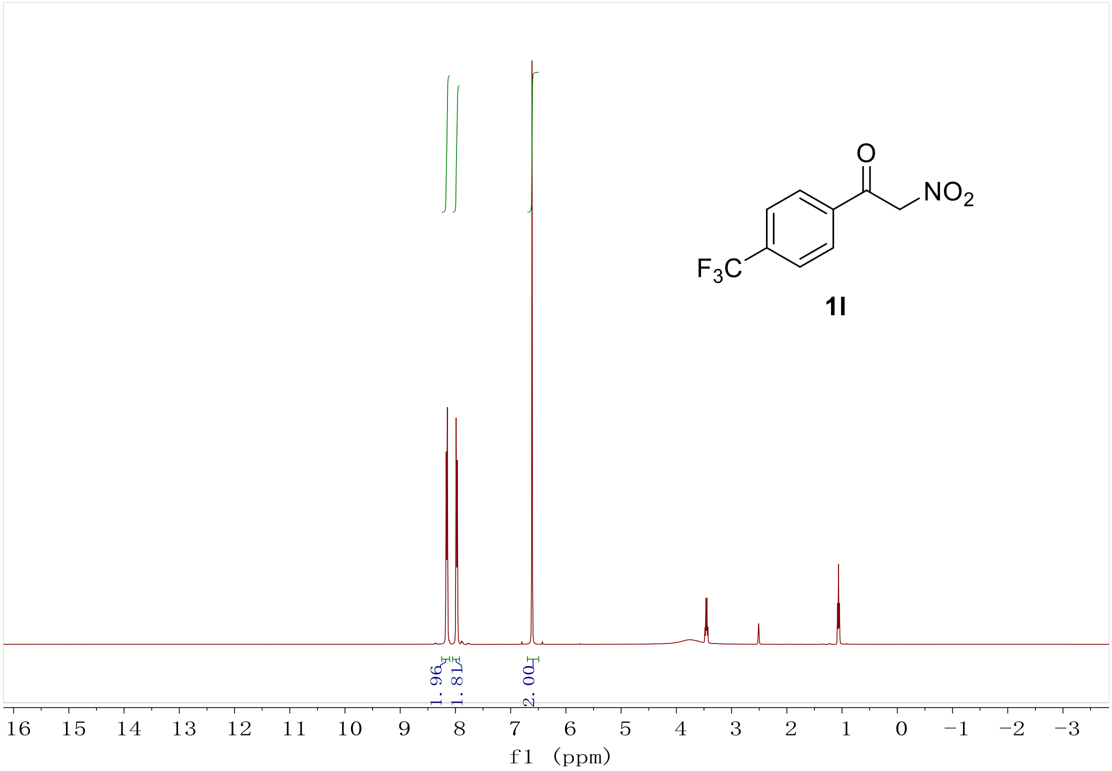


O
NO2
MeO
1k
2.16
2.18
2.00
3.48
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

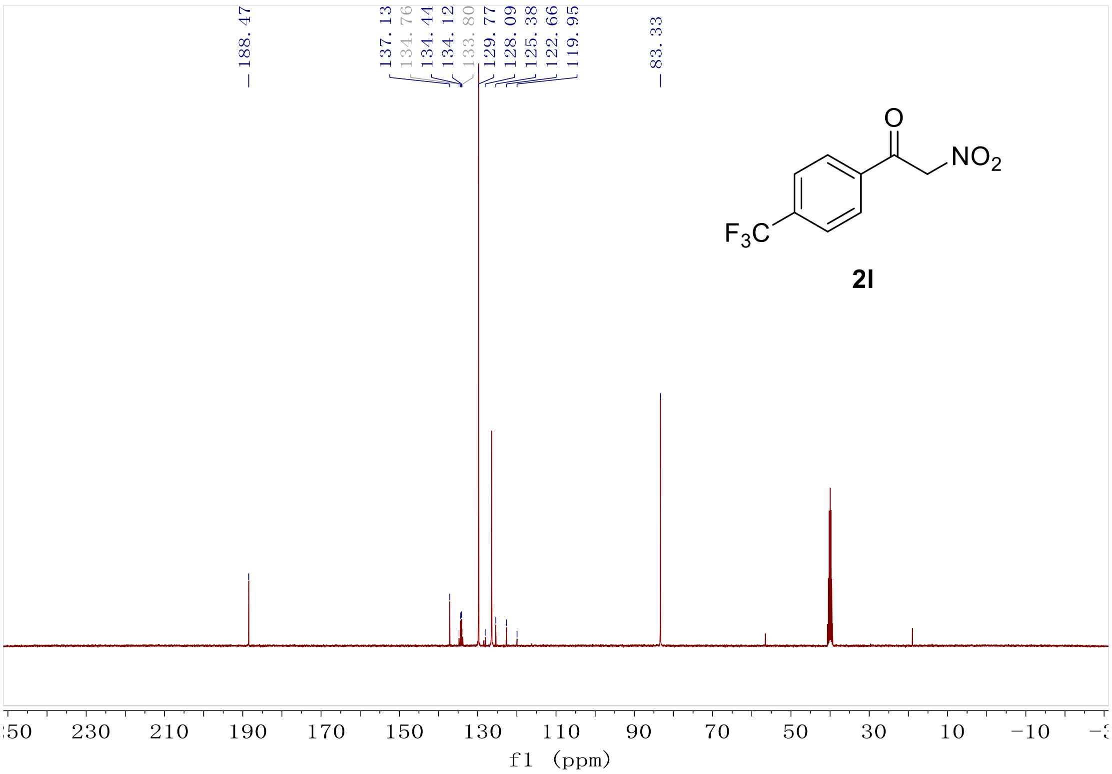


184.00
165.04
130.76
126.44
114.57
81.06
55.72
O
NO2
MeO
1k
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

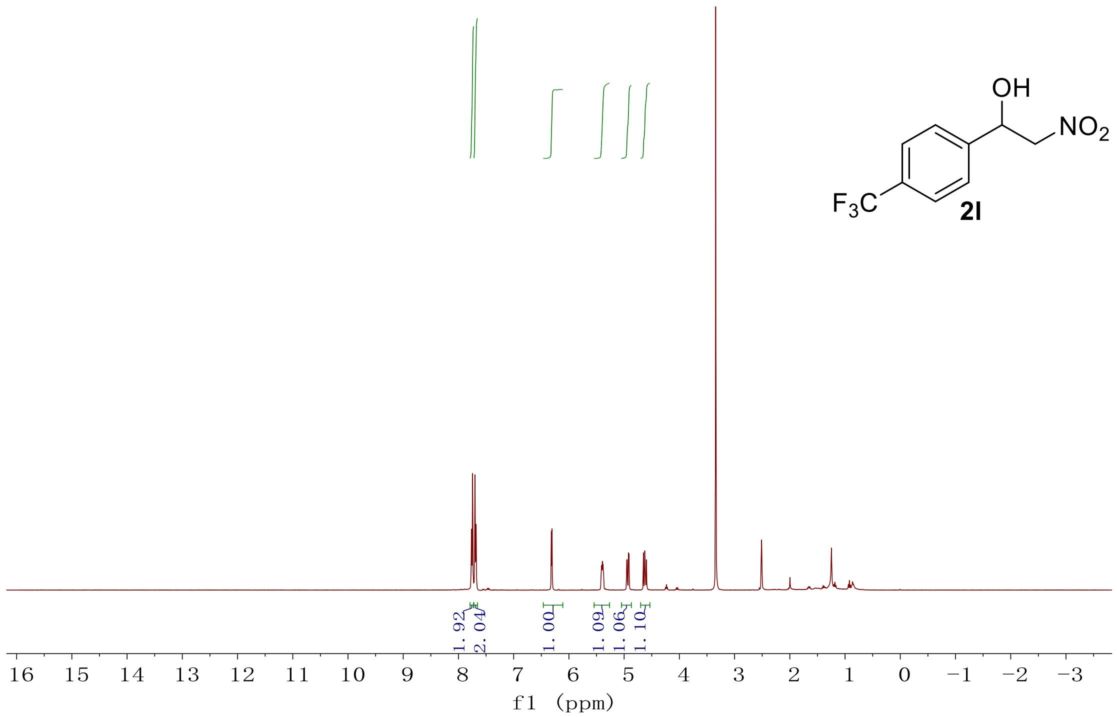

OH
NO2
MeO
2k
1.76
1.79
1.00
0.93
0.90
2.67
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

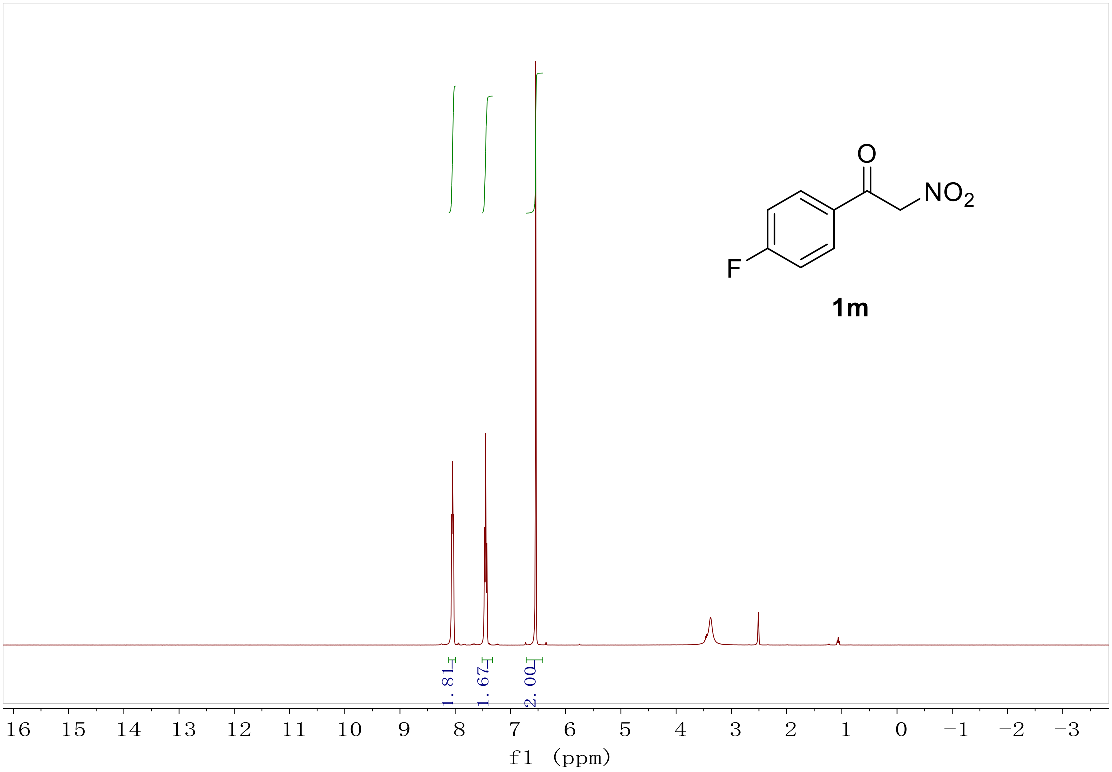


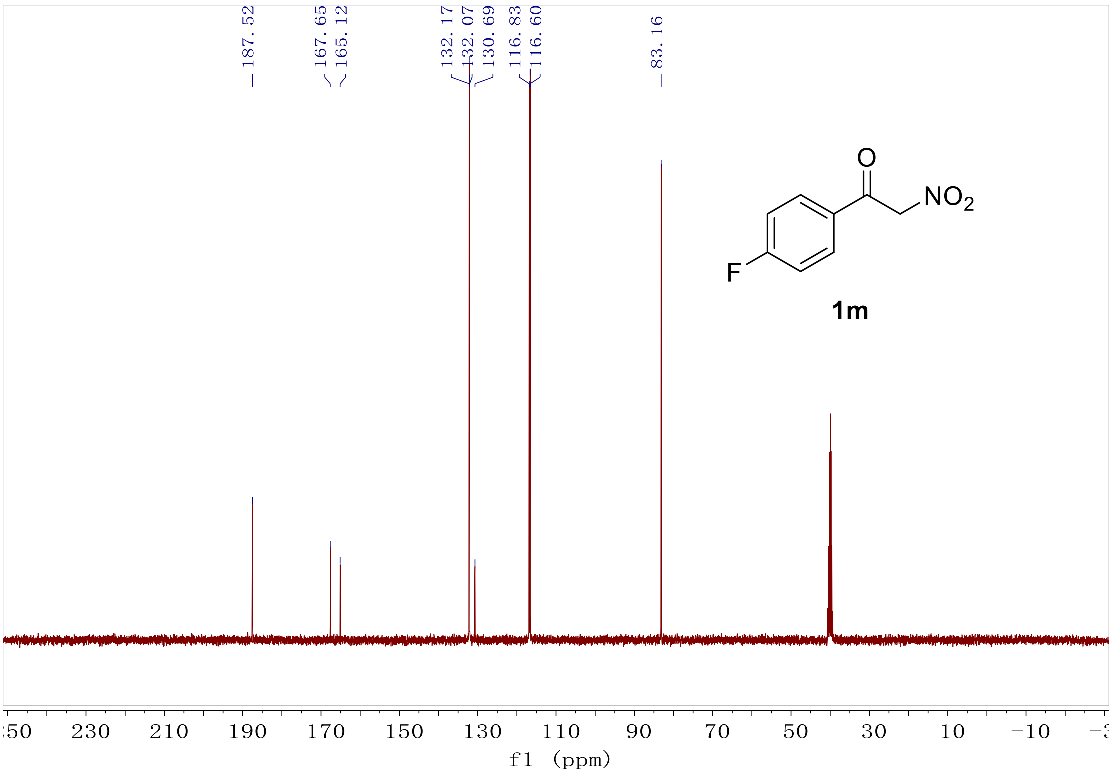
F3C
NO2
O
1l
1.96
1.81
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

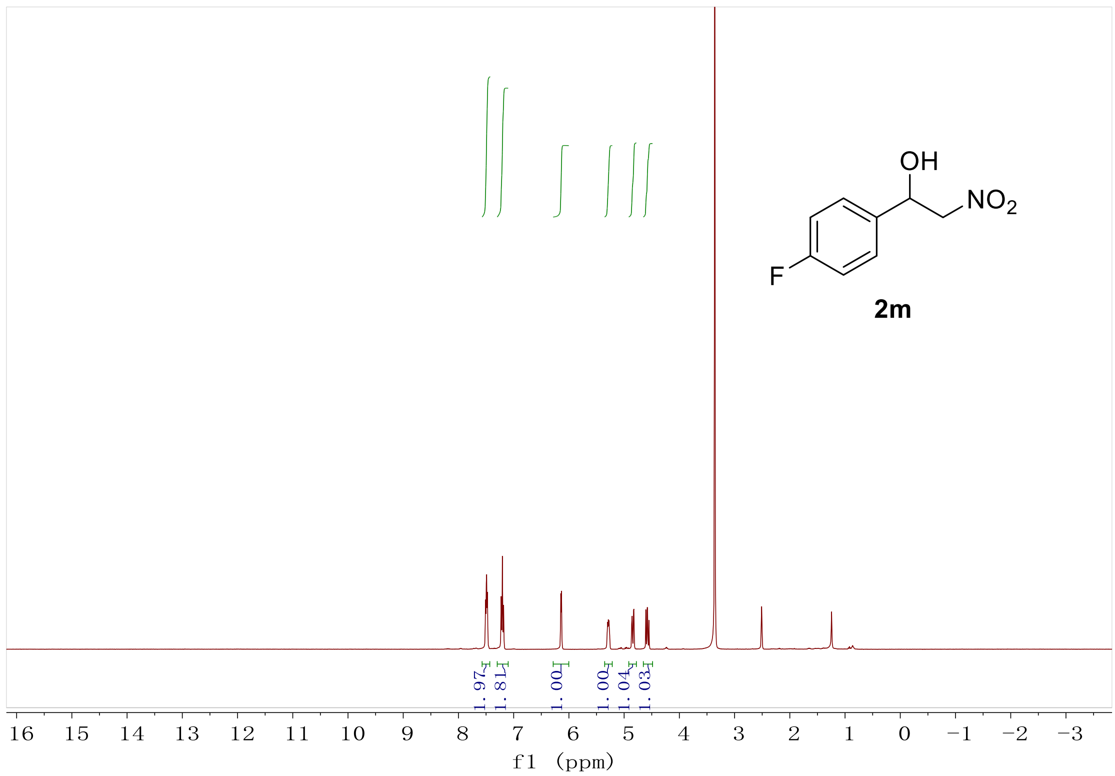


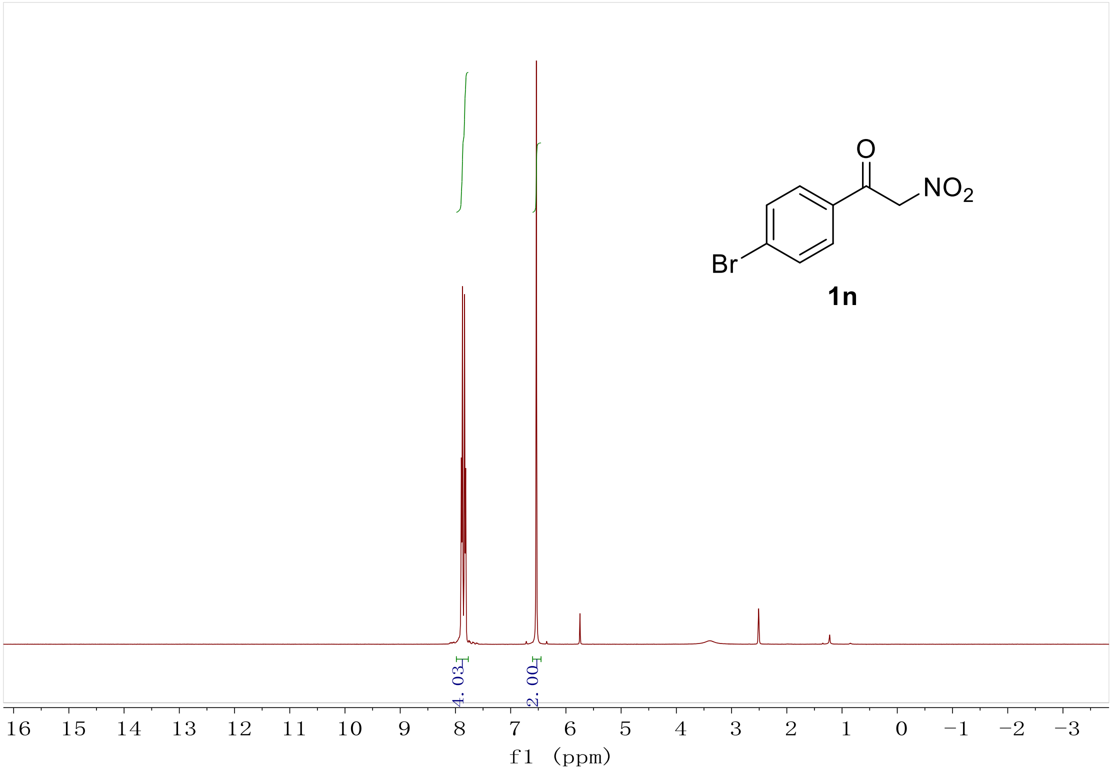
188.47
137.13
134.76
134.44
134.12
133.80
129.77
128.09
125.38
122.66
119.95
83.33
F3C
NO2
O
2l
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

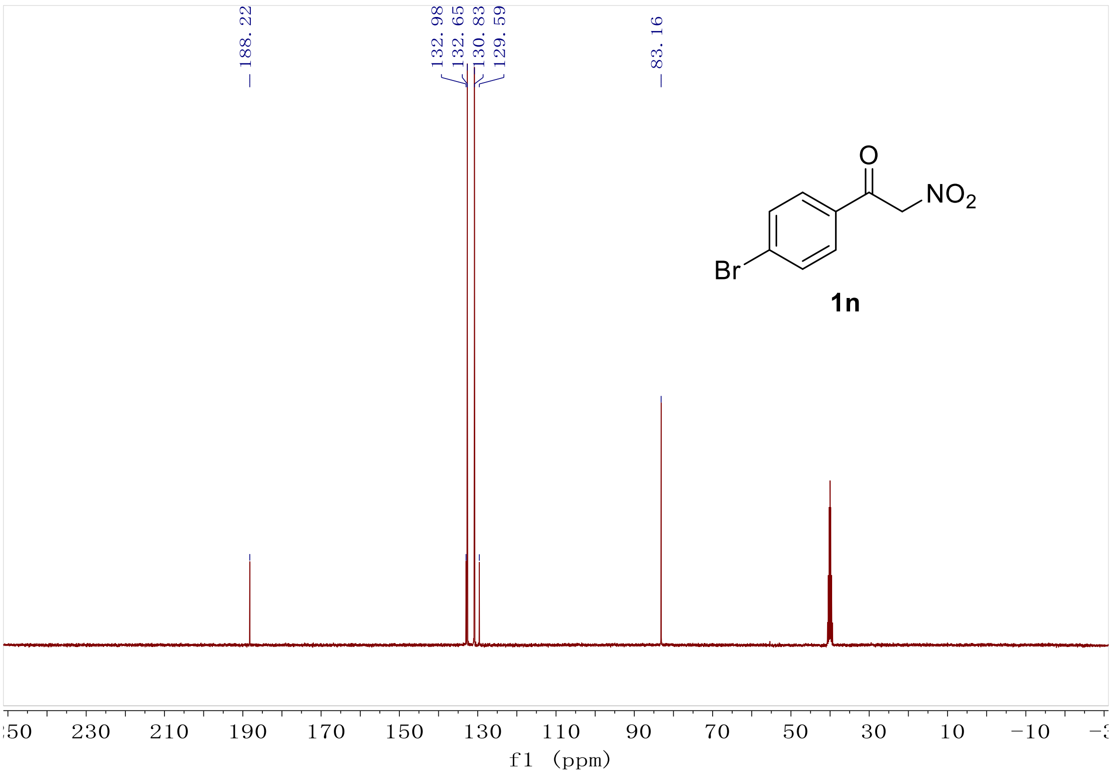

OH
NO2
F3C
2l
1.92
2.04
1.00
1.09
1.06
1.10
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

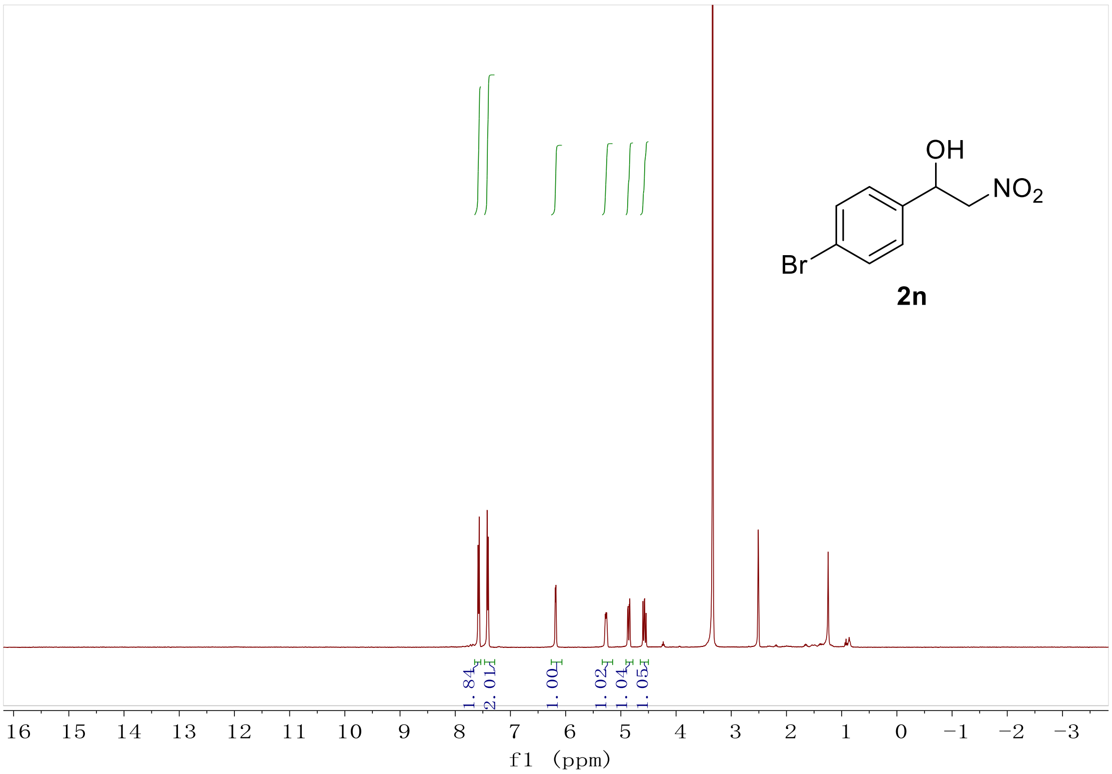

1.81
1.67
2.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)
O
NO2
F
1m

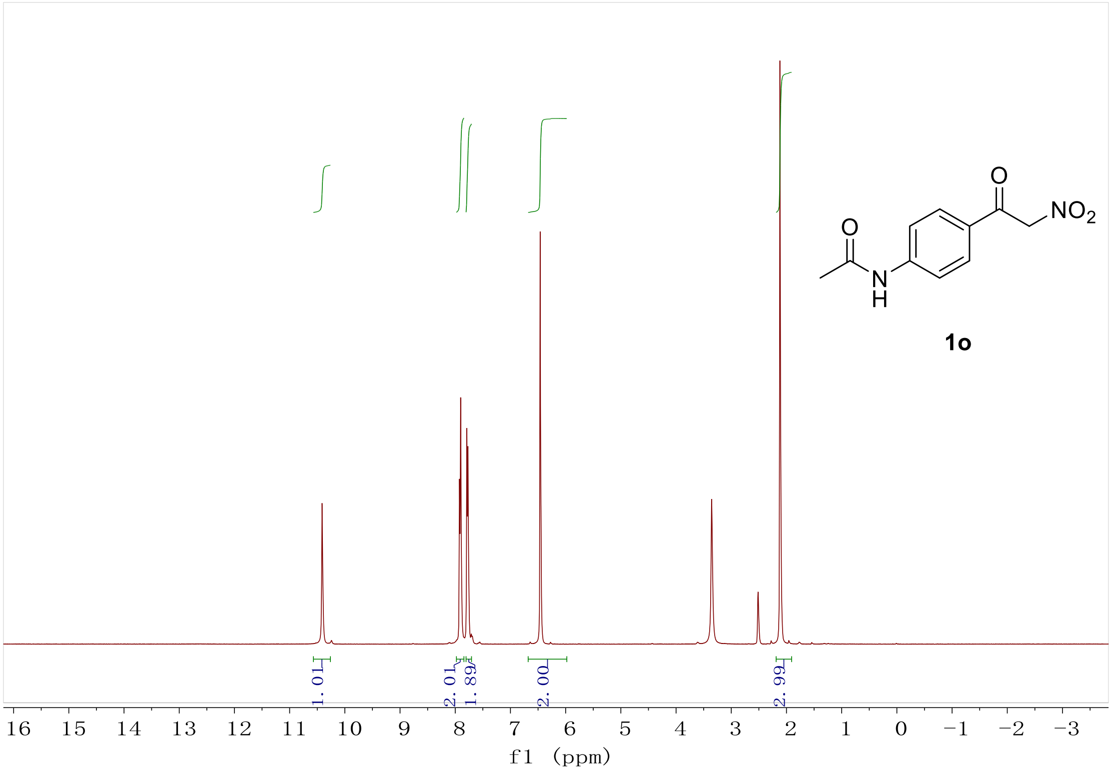

187.52
167.65
165.12
132.17
132.07
130.69
116.83
116.60
83.16
O
NO2
F
1m
230
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)

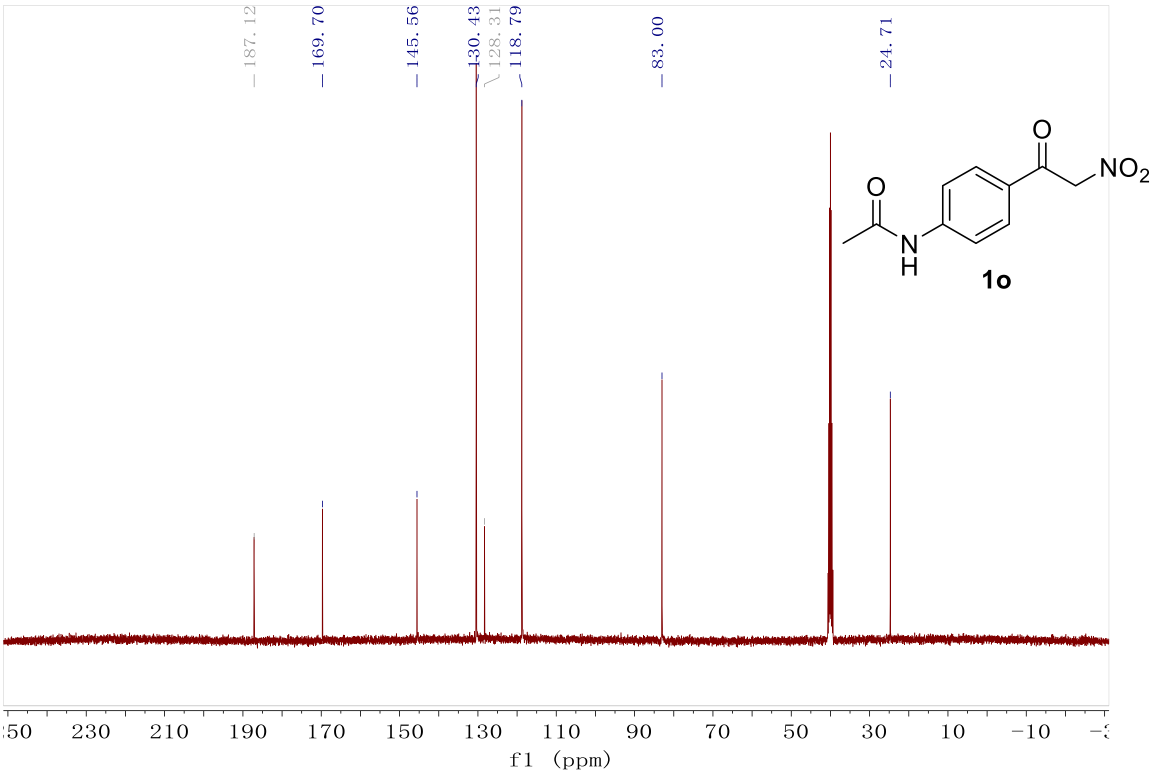

OH
NO_2
F
2m
1.97
1.81
1.00
1.00
1.04
1.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

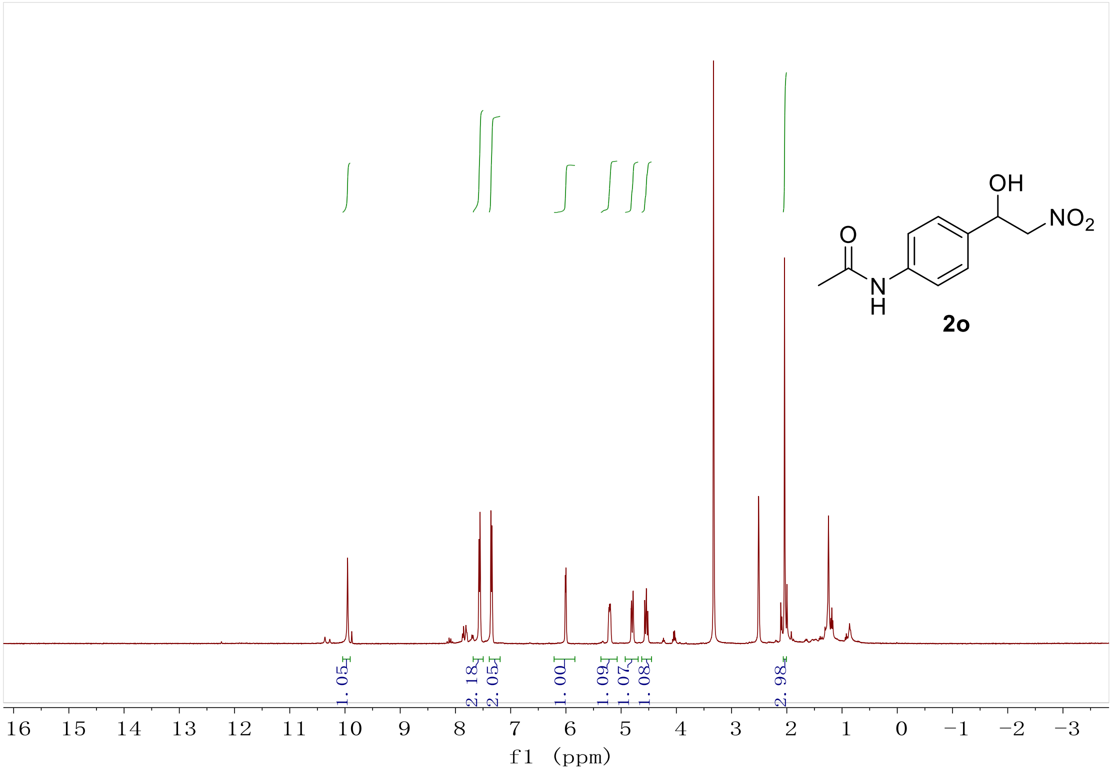

O
NO2
Br
1n
4.03
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


188.22
132.98
132.65
130.83
129.59
83.16
O
NO2
Br
1n
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OH
NO2
Br
2n
1.84
2.01
1.00
1.02
1.04
1.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

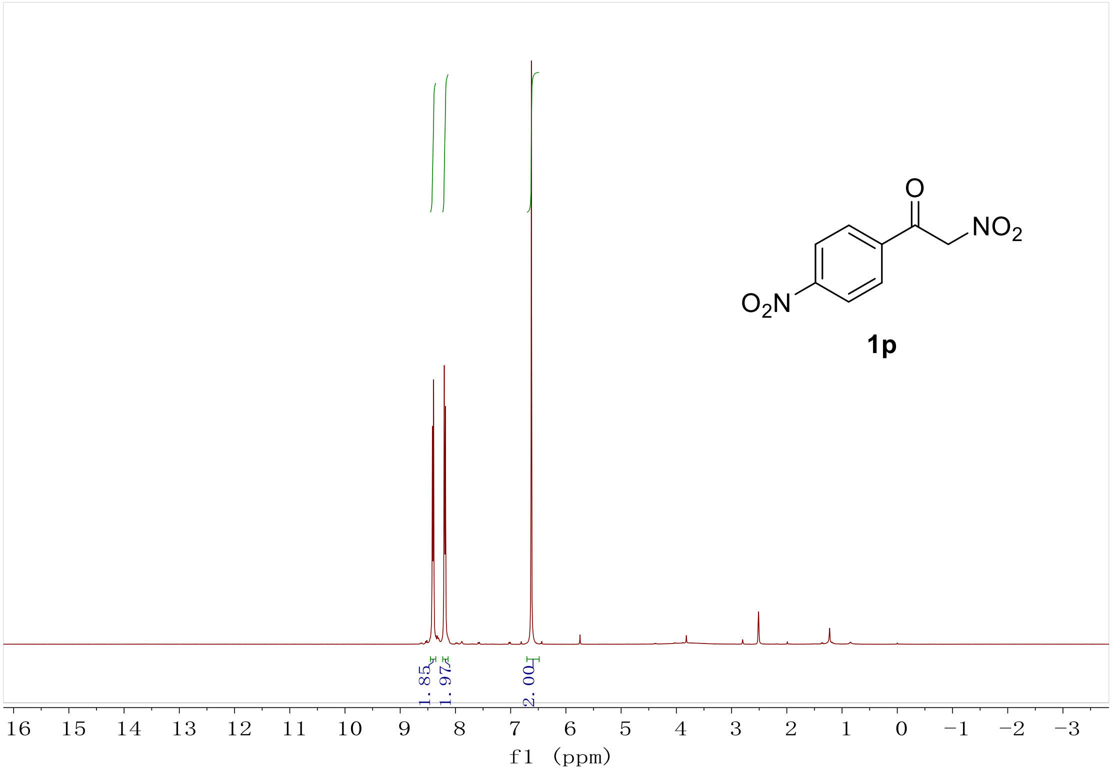

1.01
2.01
1.89
2.00
2.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO2
O
N
H
1o


187.12
169.70
145.56
130.43
128.31
118.79
83.00
24.71
O
NO2
O
N
H
1o
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

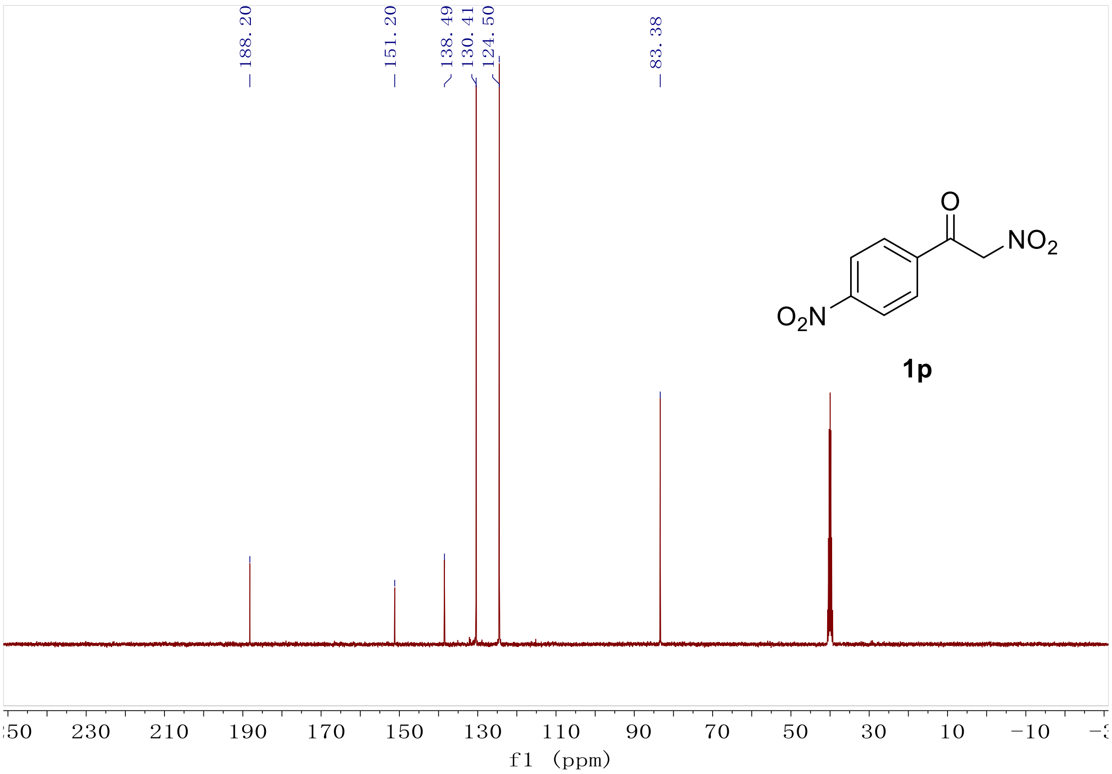


1.05
2.18
2.05
1.00
1.09
1.07
1.08
2.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
OH
NO_2
O
N
H

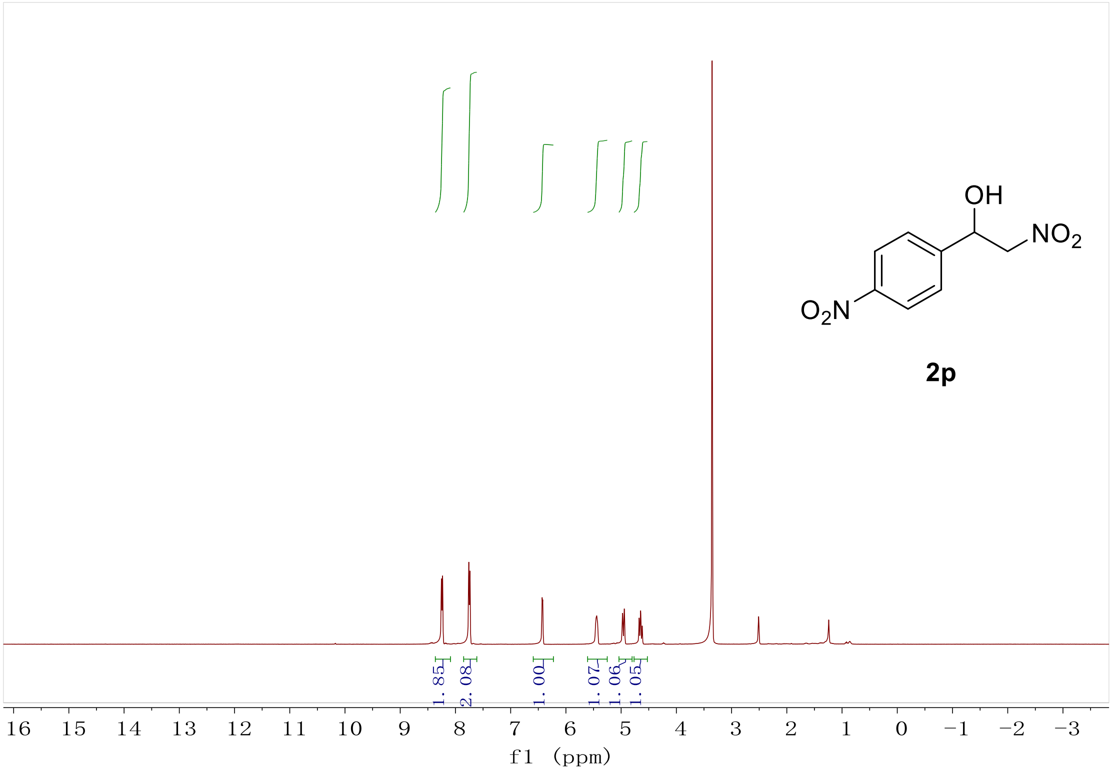
2o

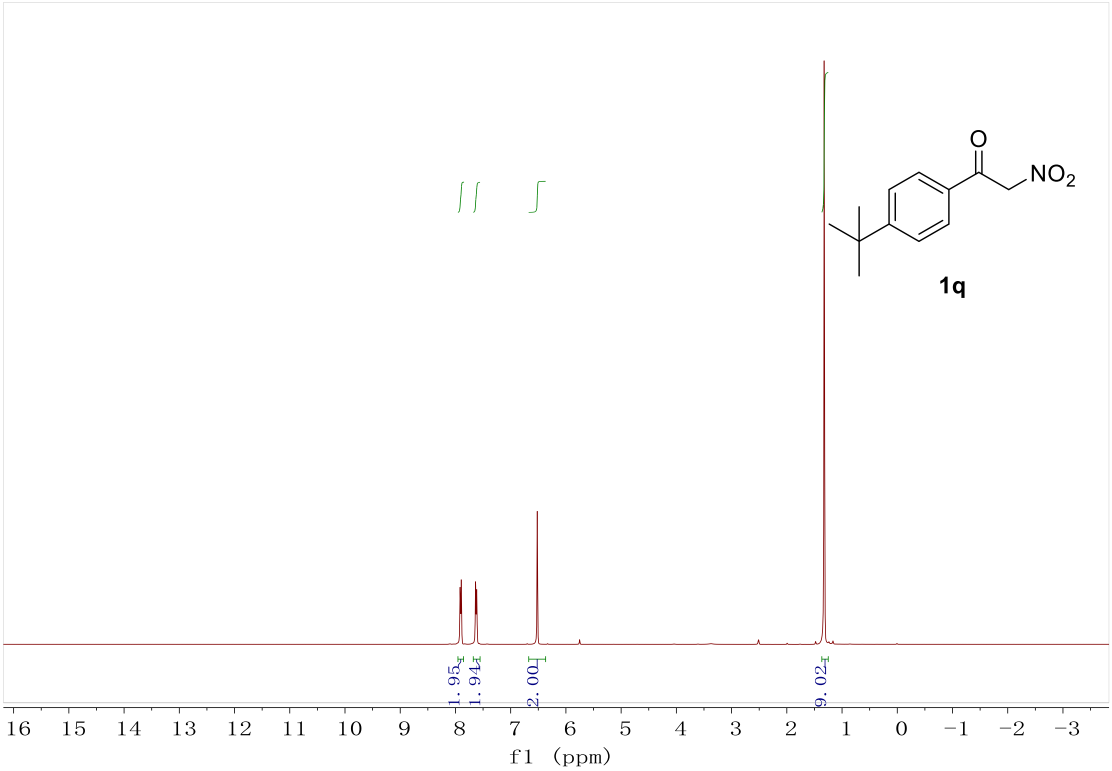


1.85
1.97
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO2
O2N
1p

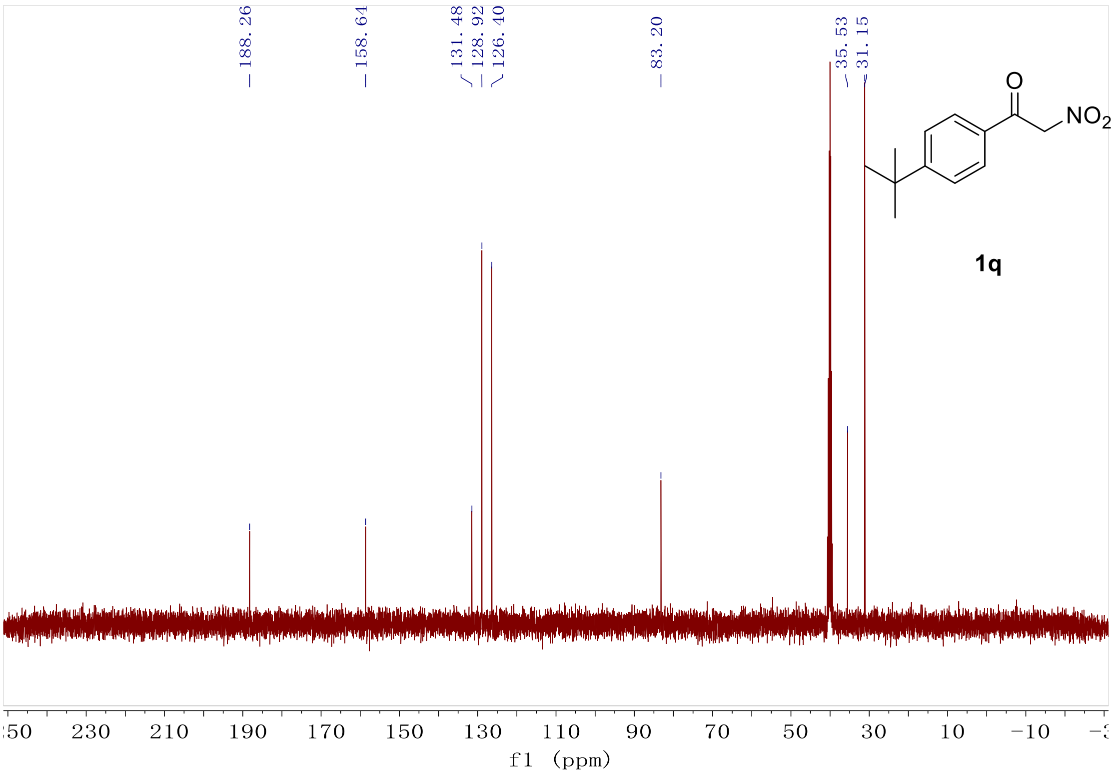


188.20
151.20
138.49
130.41
124.50
83.38
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)
O
NO2
O2N
1p

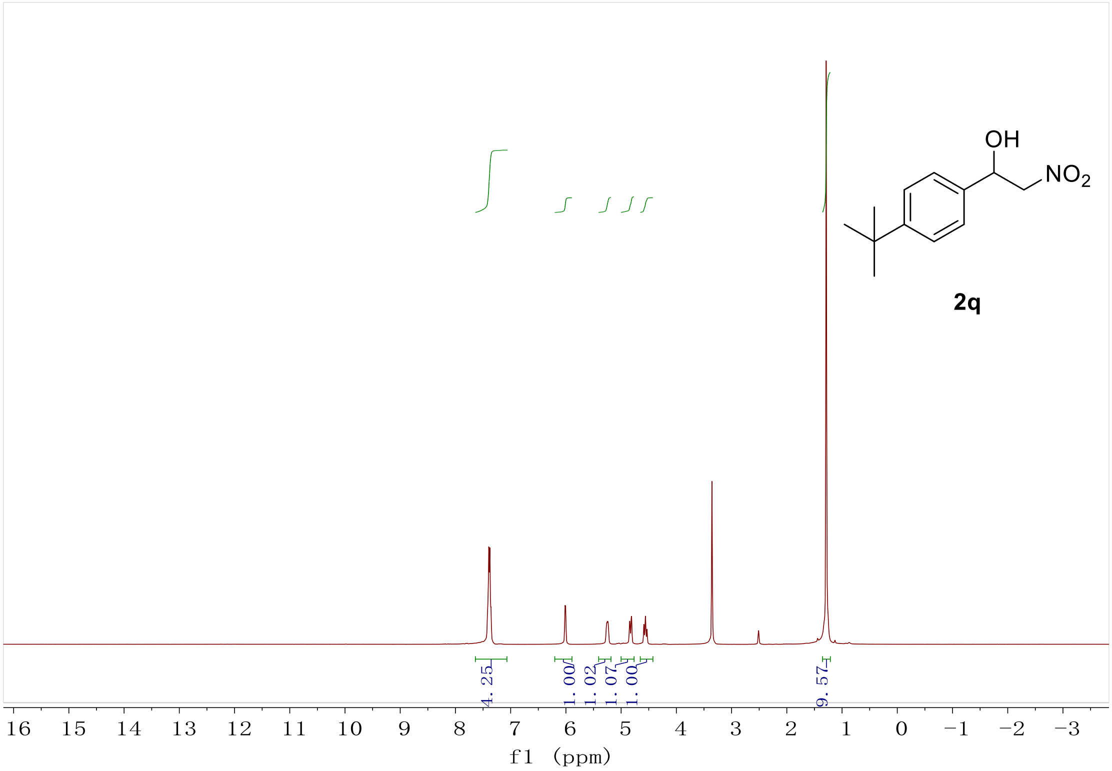

OH
NO_2
O_2N
2p
1.85
2.08
1.00
1.07
1.06
1.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



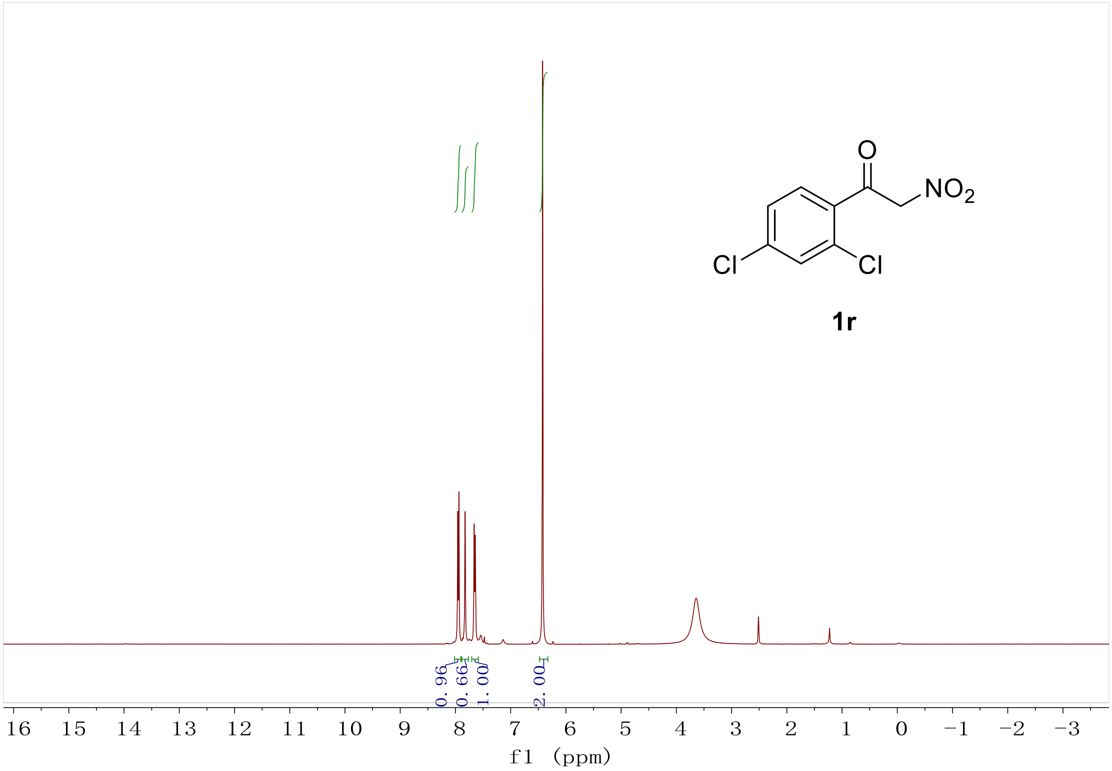
O
NO2
1q
1.95
1.94
2.00
9.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



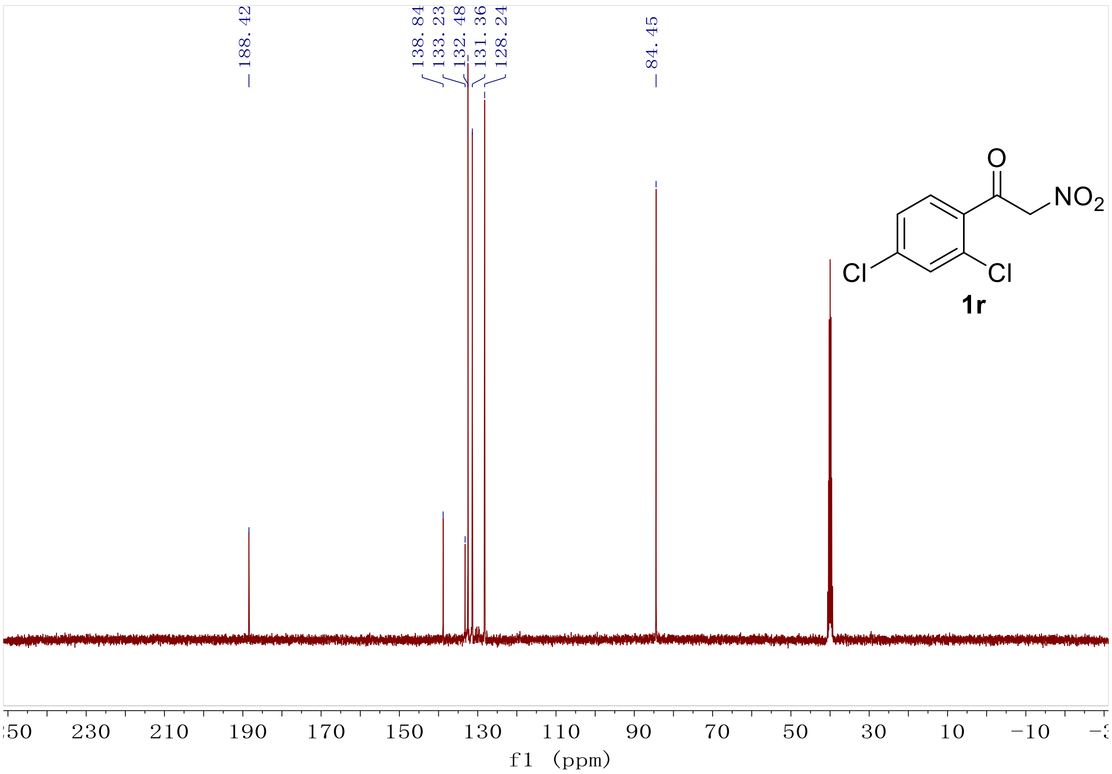
188.26
158.64
131.48
128.92
126.40
83.20
35.53
31.15
O
NO2
1q
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)



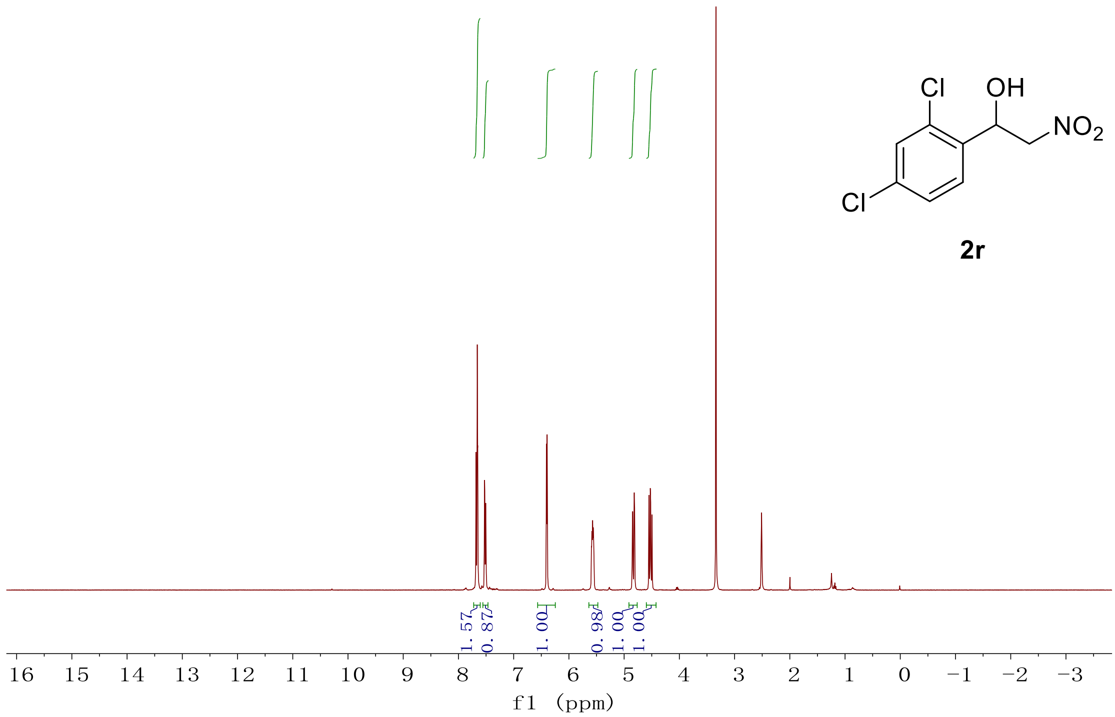
4.25
1.00
1.02
1.07
1.00
9.57
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)
OH
NO2
2q



O
NO2
Cl
Cl
1r
0.96
0.66
1.00
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

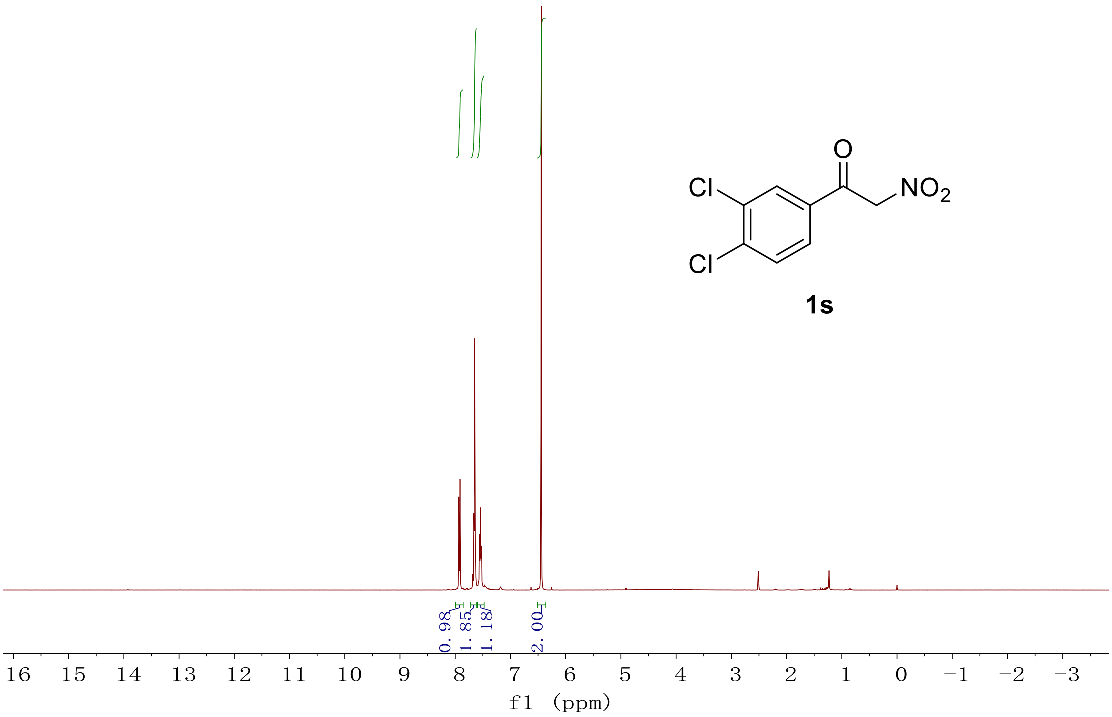


188.42
138.84
133.23
132.48
131.36
128.24
84.45
O
NO2
Cl
Cl
1r
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

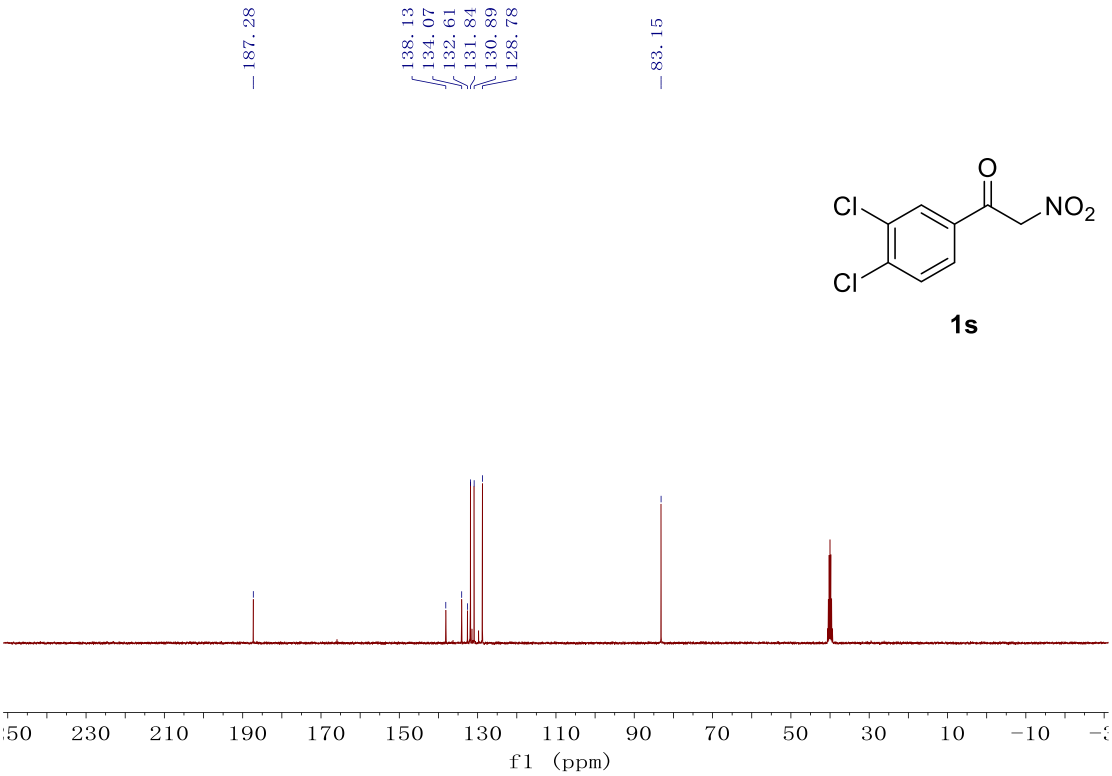


1.57
0.87
1.00
0.98
1.00
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
Cl
OH
NO2
Cl

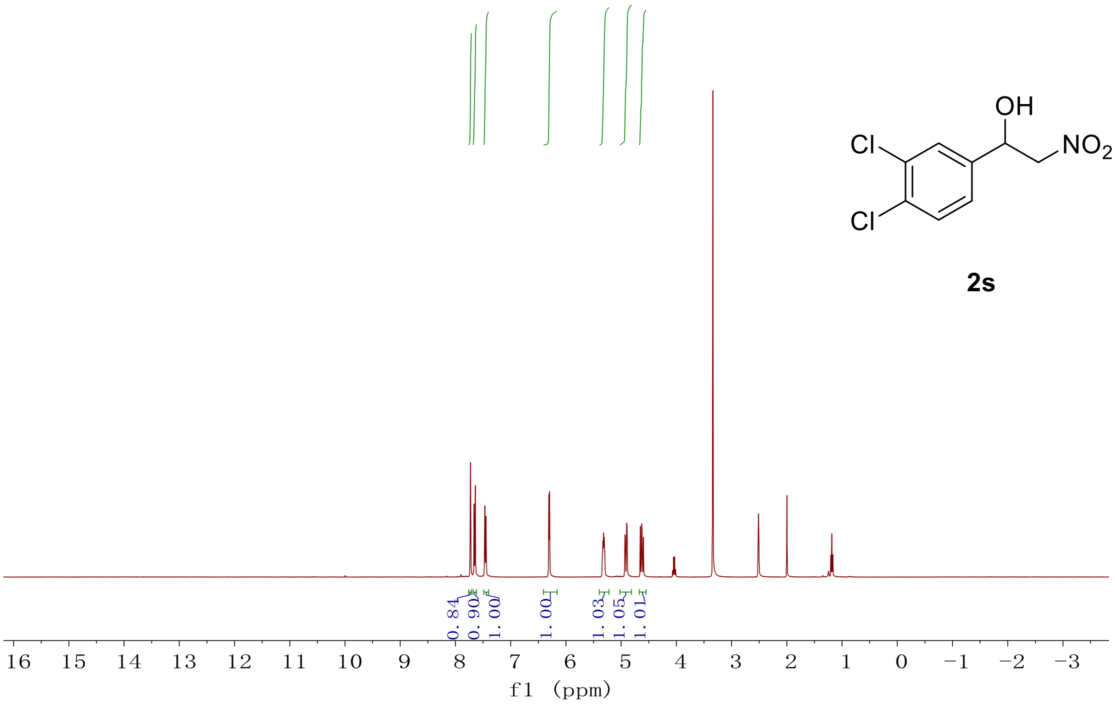
2r



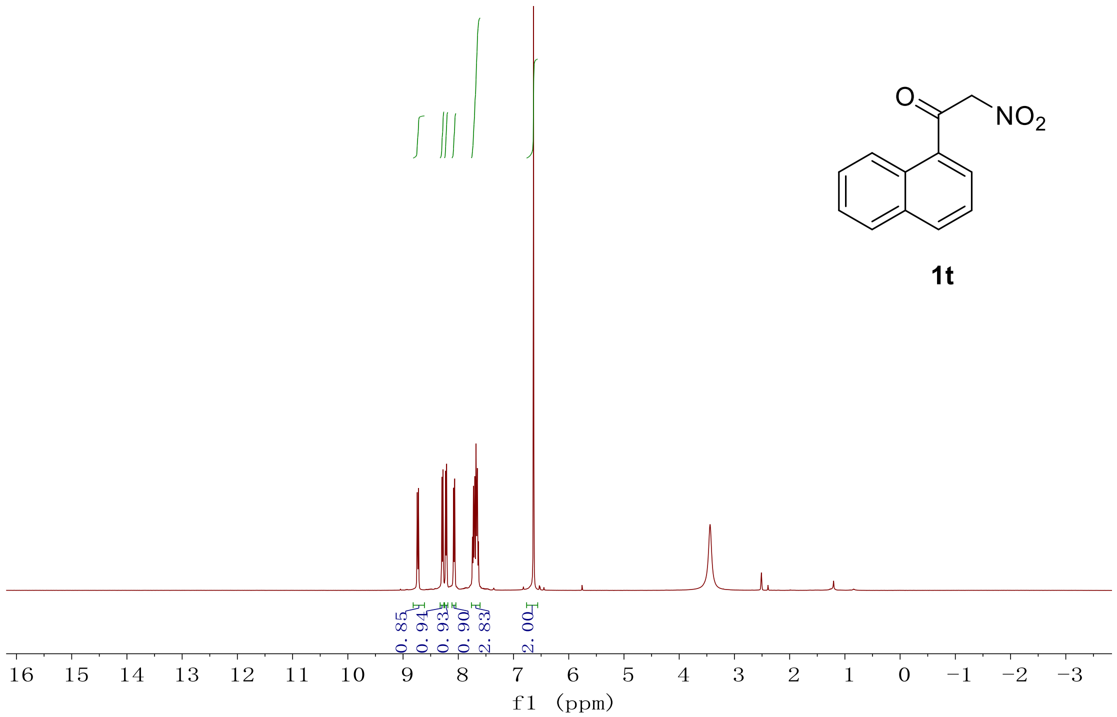
Cl
Cl
O
NO_2
1s
0.98
1.85
1.18
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

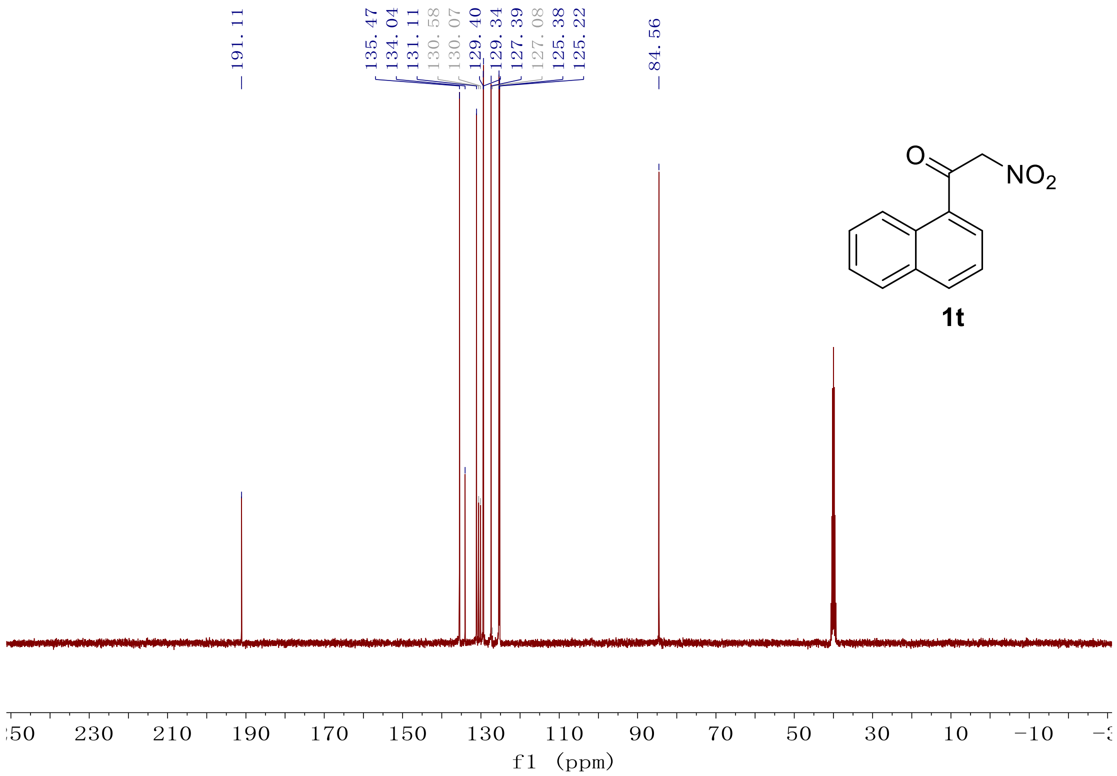


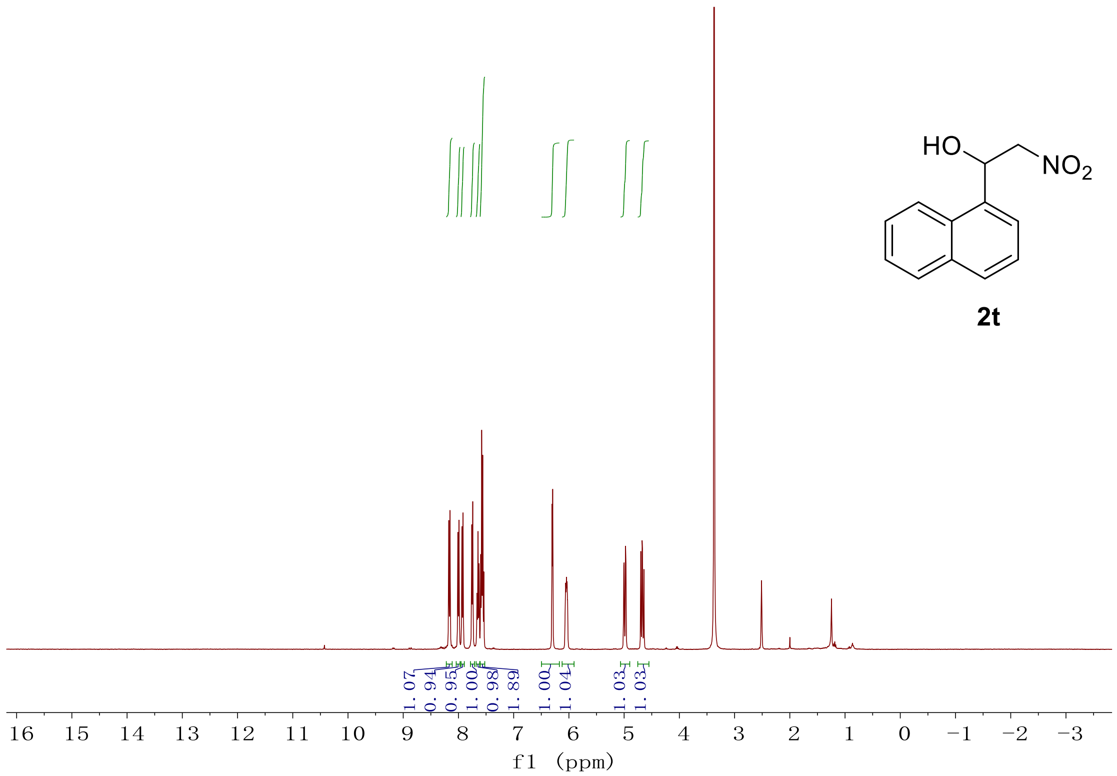
187.28
138.13
134.07
132.61
131.84
130.89
128.78
83.15
Cl
Cl
O
NO_2
1s
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


0.84
0.90
1.00
1.00
1.03
1.05
1.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
OH
Cl
NO2
Cl

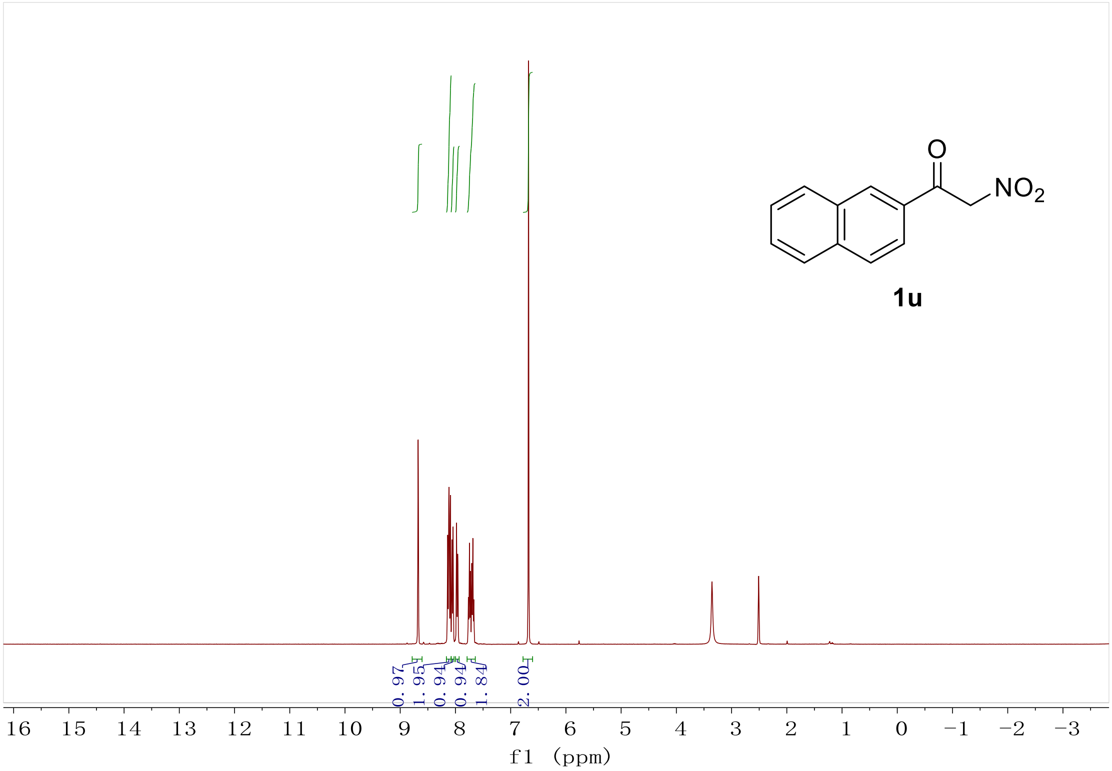
2s


O
NO2
1t
0.85
0.94
0.93
0.90
2.83
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

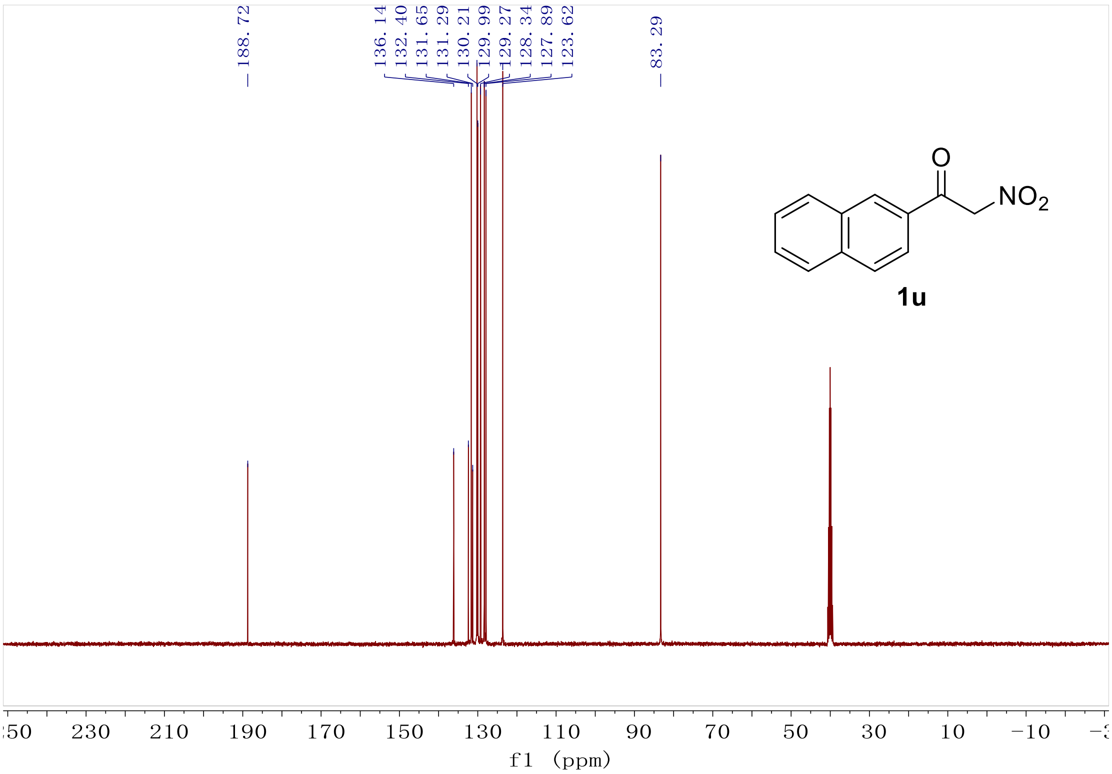

191.11
135.47
134.04
131.11
130.58
130.07
129.40
129.34
127.39
127.08
125.38
125.22
84.56
O
NO2
1t
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


1.07
0.94
0.95
1.00
0.98
1.89
1.00
1.04
1.03
1.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
HO
NO2

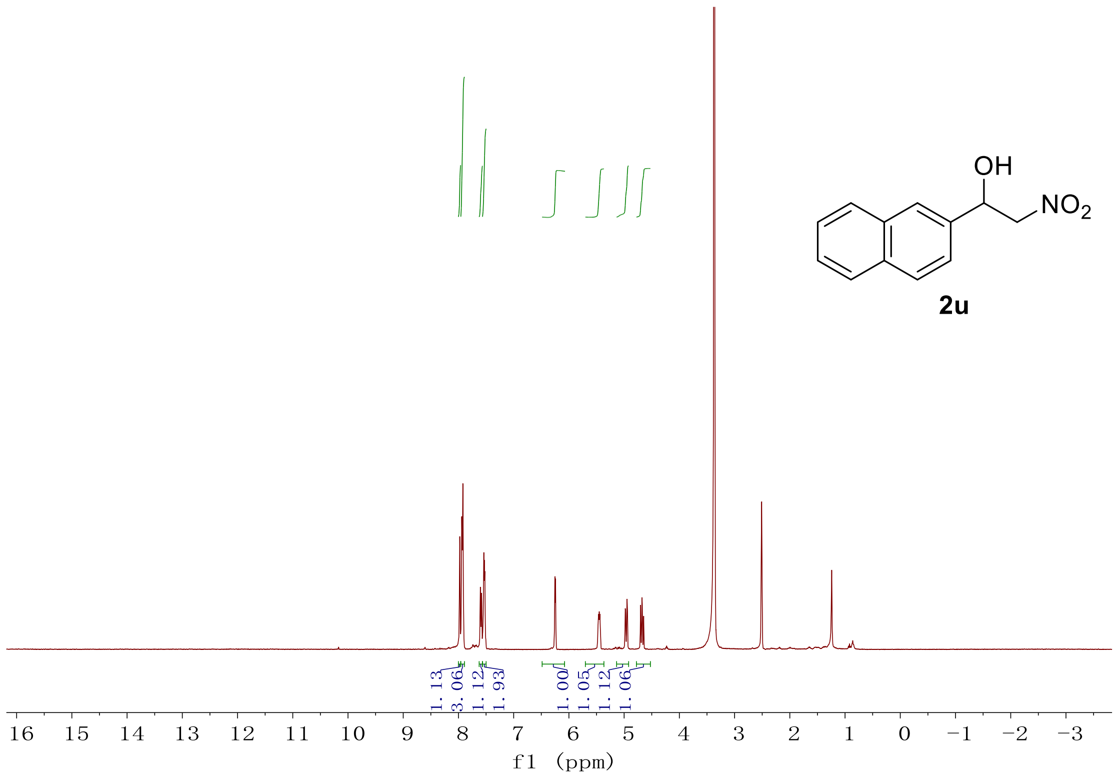
2t



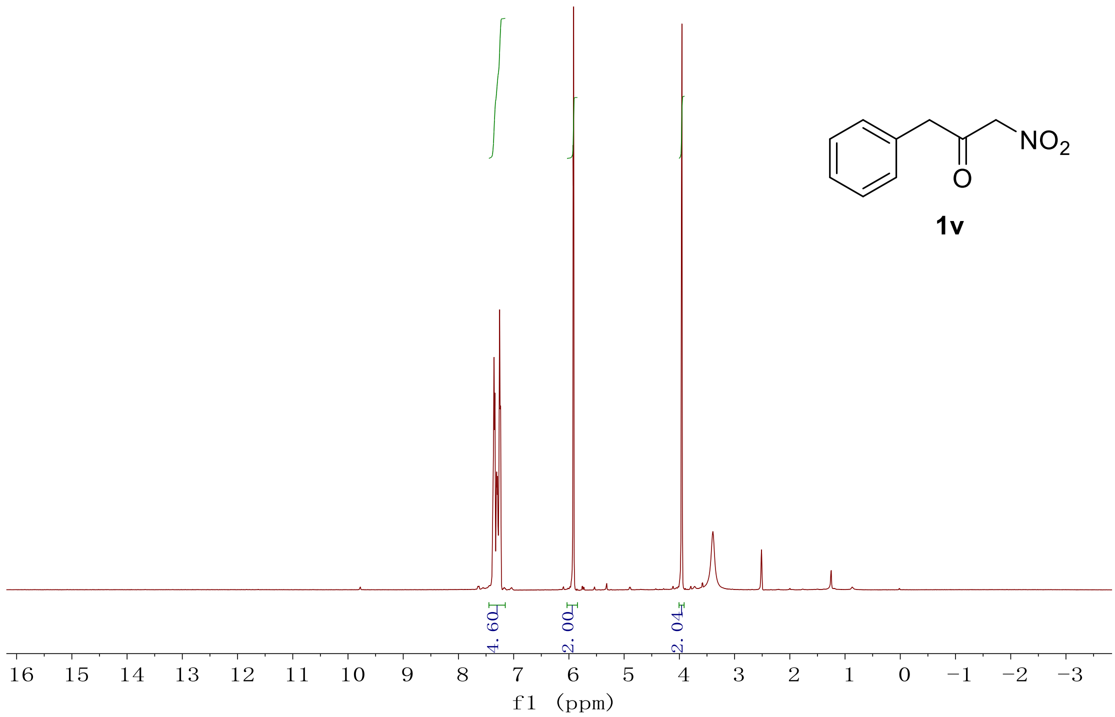
0.97
1.95
0.94
0.94
1.84
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
O
NO2
1u



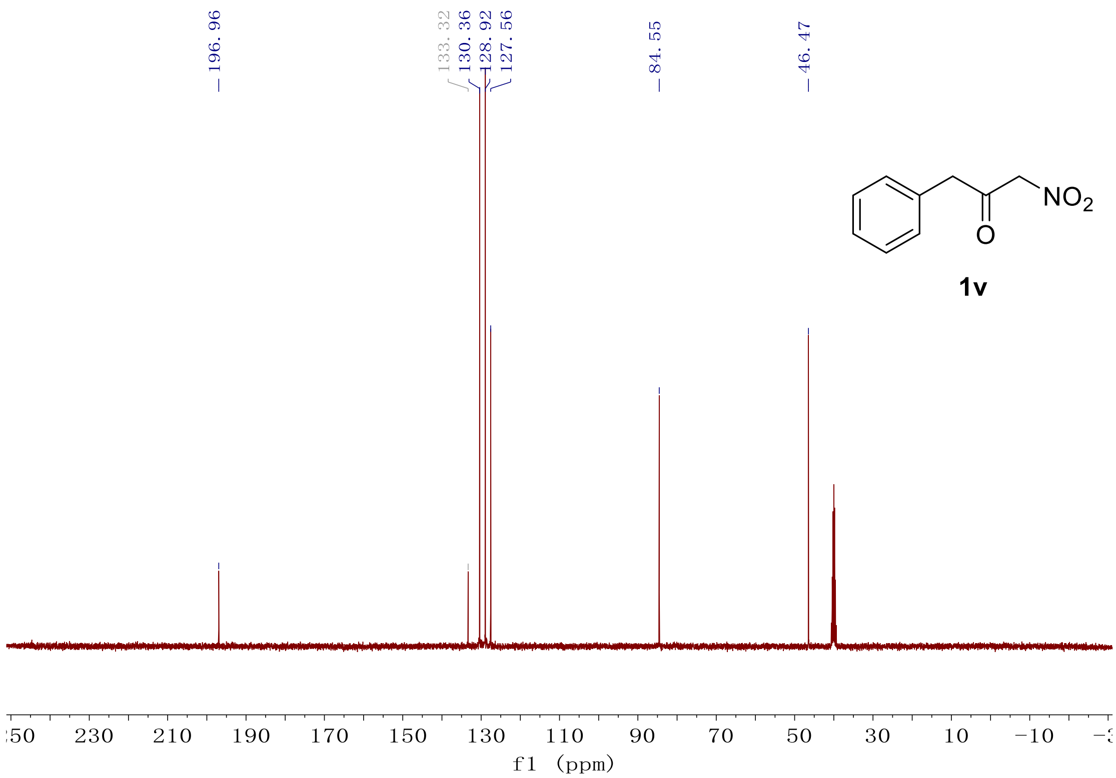
188.72
136.14
132.40
131.65
131.29
130.21
129.99
129.27
128.34
127.89
123.62
83.29
O
NO2
1u
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)



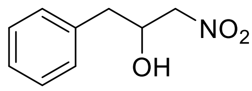
OH
NO2
2u
1.13
3.06
1.12
1.93
1.00
1.05
1.12
1.06
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



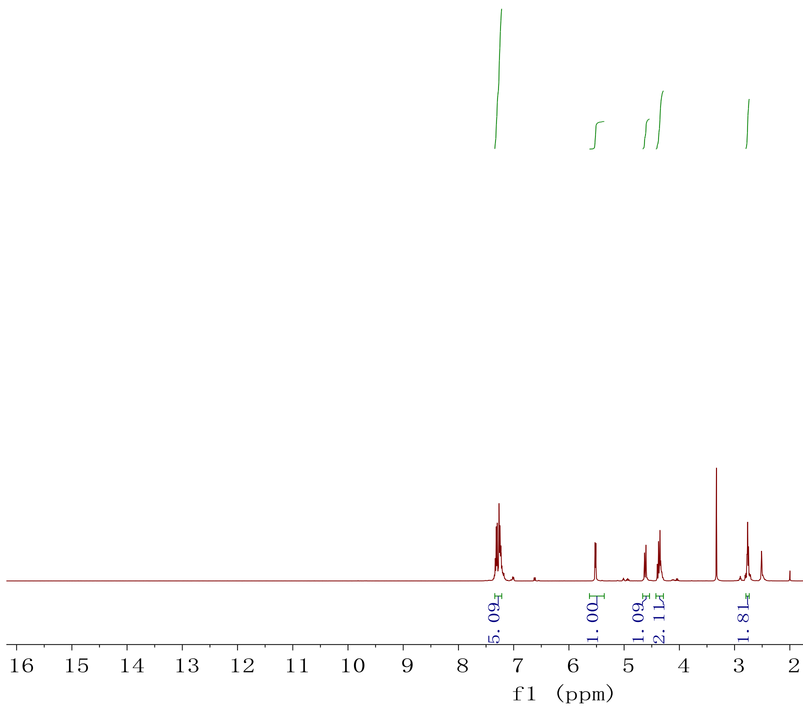
NO2
O
1v
4.60
2.00
2.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

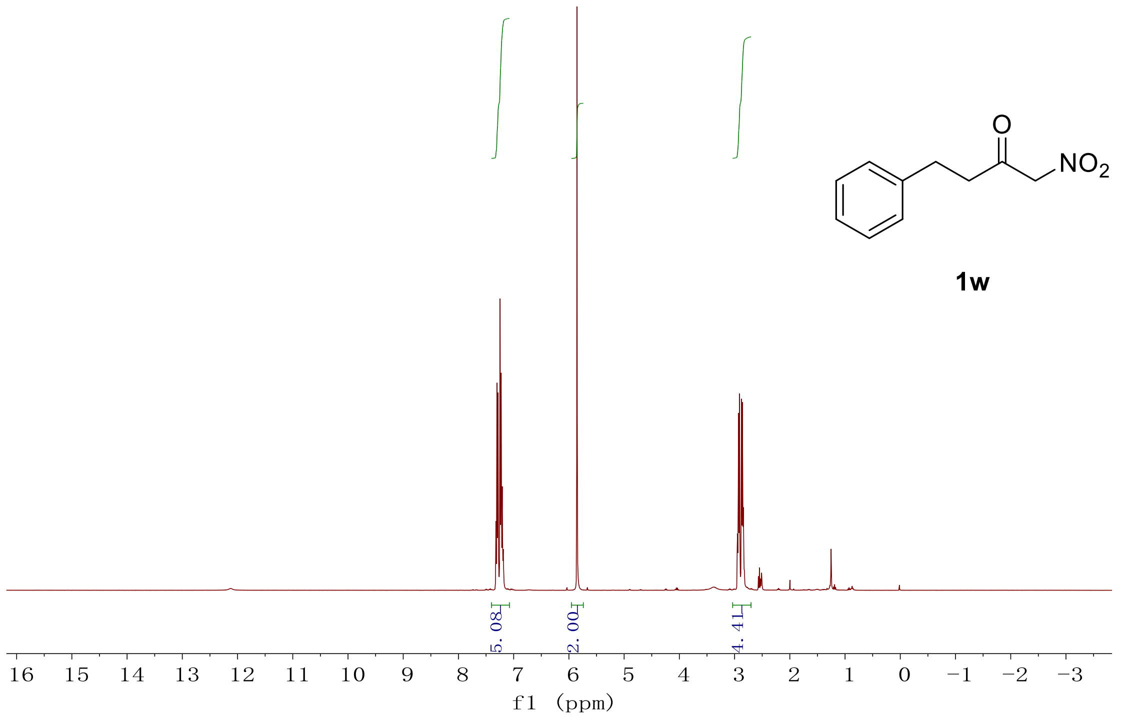


196.96
133.32
130.36
128.92
127.56
84.55
46.47
NO2
O
1v
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

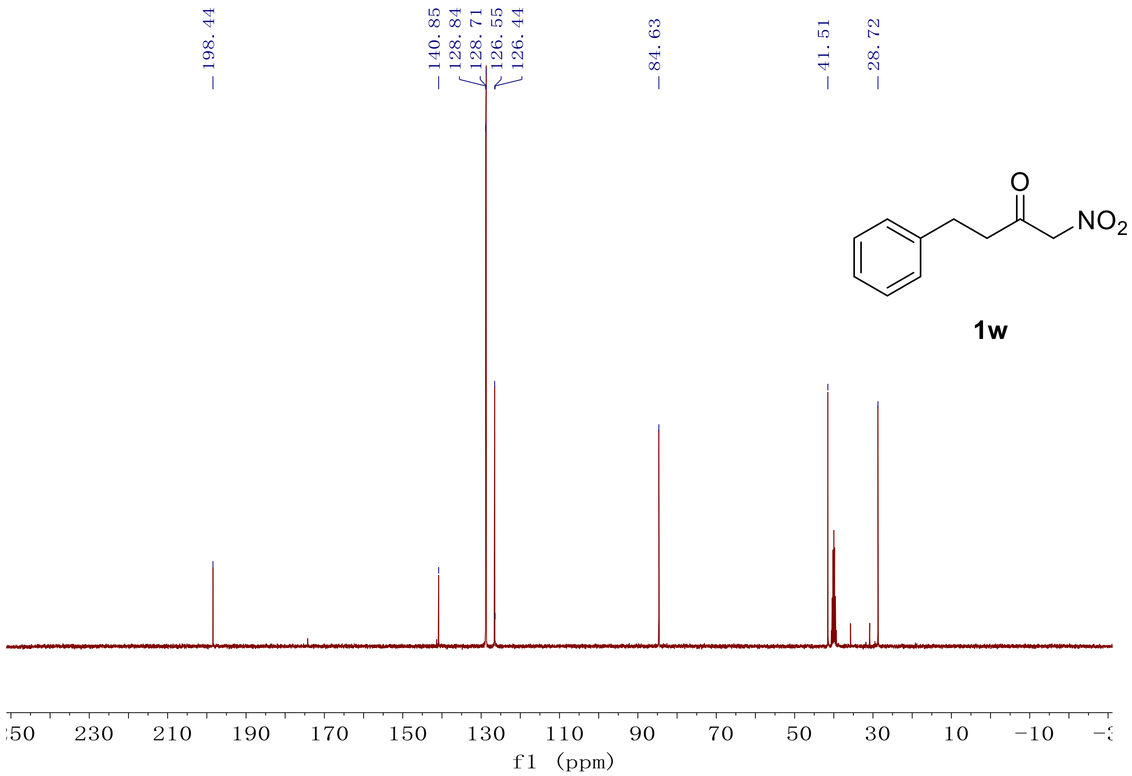

NO2
OH

2v

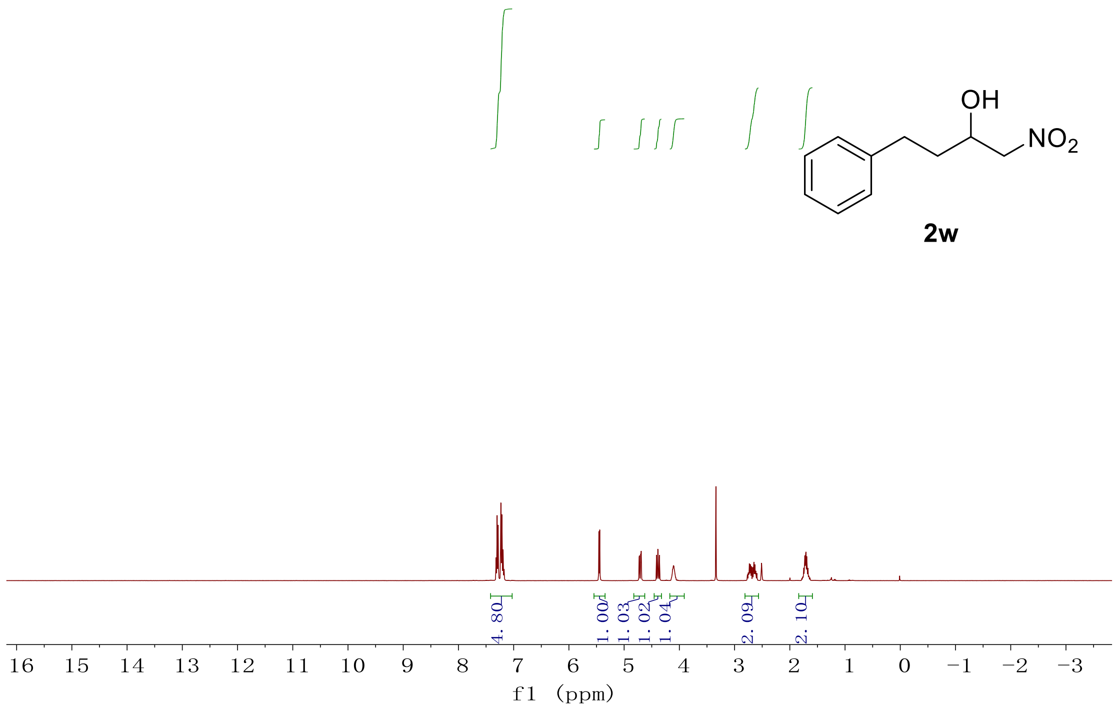

5.09
1.00
1.09
2.11
1.81
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)



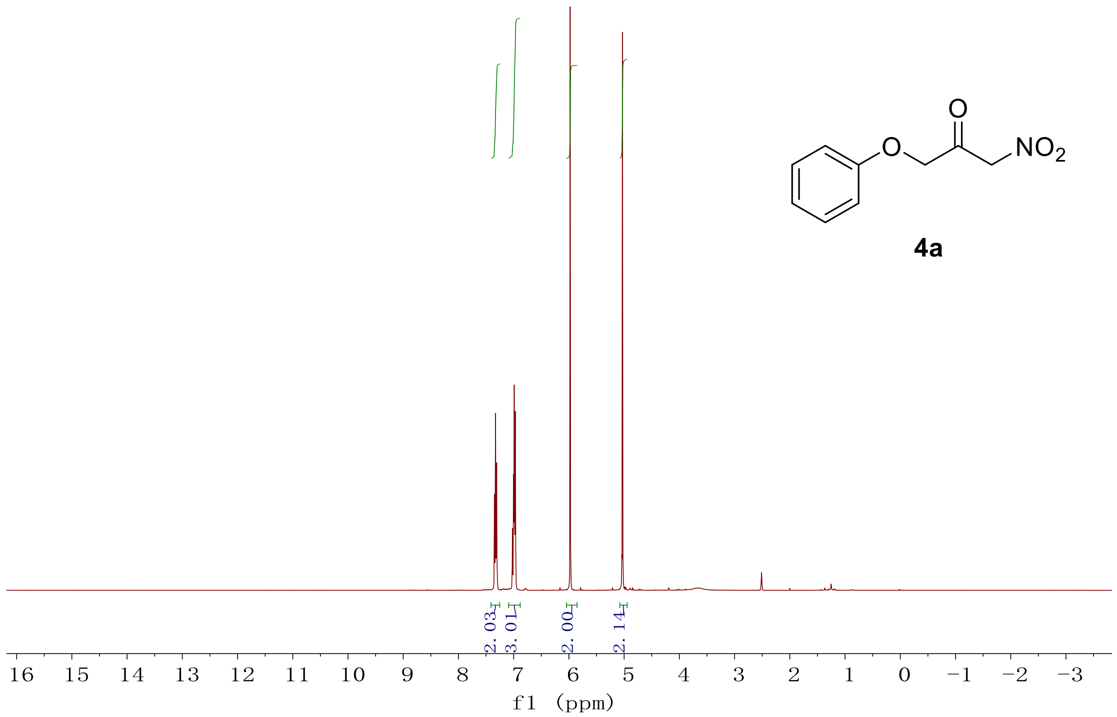
NO2
O
1w
5.08
2.00
4.41
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)



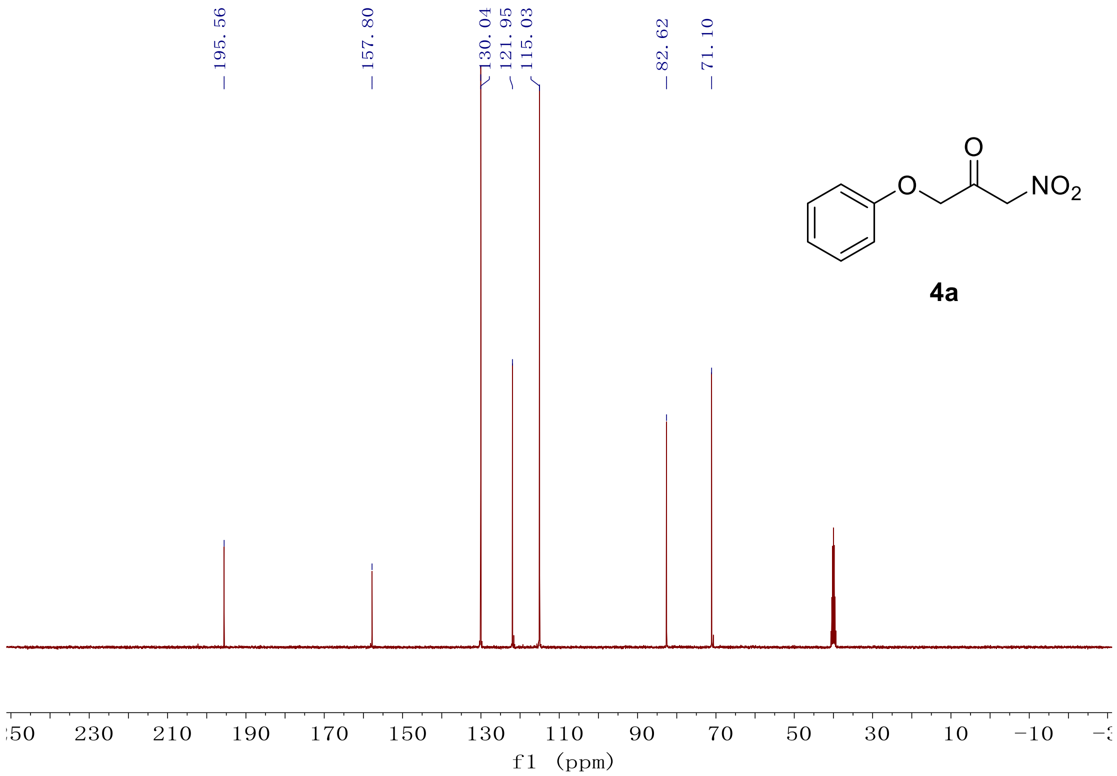
198.44
140.85
128.84
128.71
126.55
126.44
84.63
41.51
28.72
NO2
O
1w
230
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)



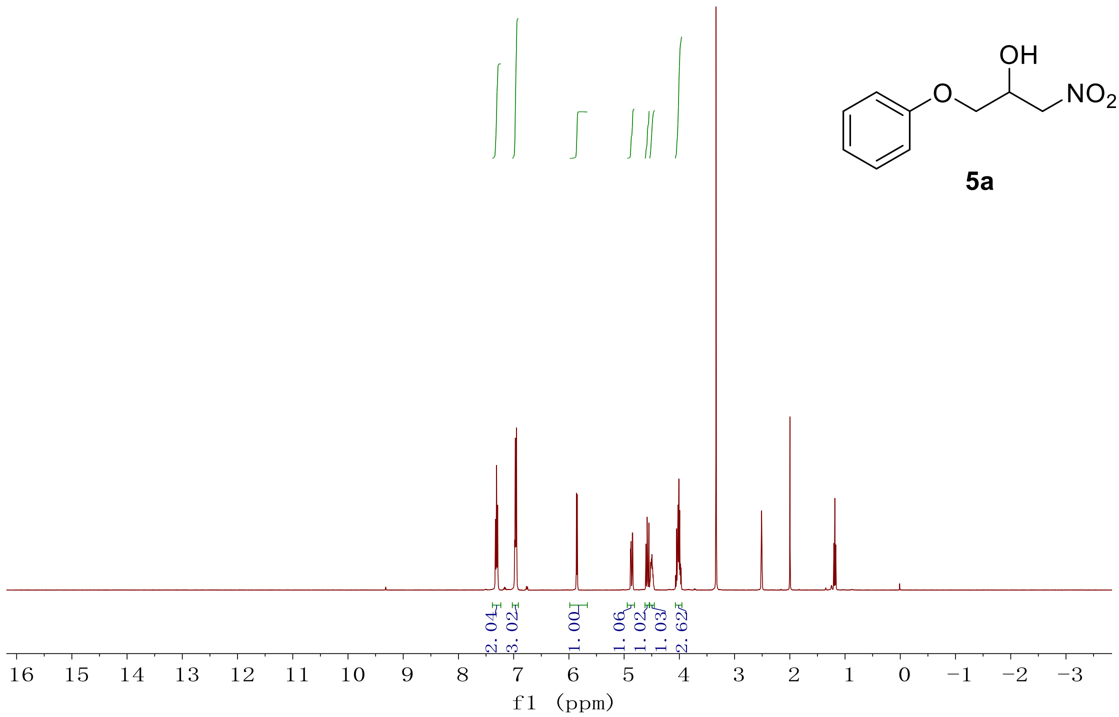
OH
NO2
2w
4.80
1.00
1.03
1.02
1.04
2.09
2.10
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

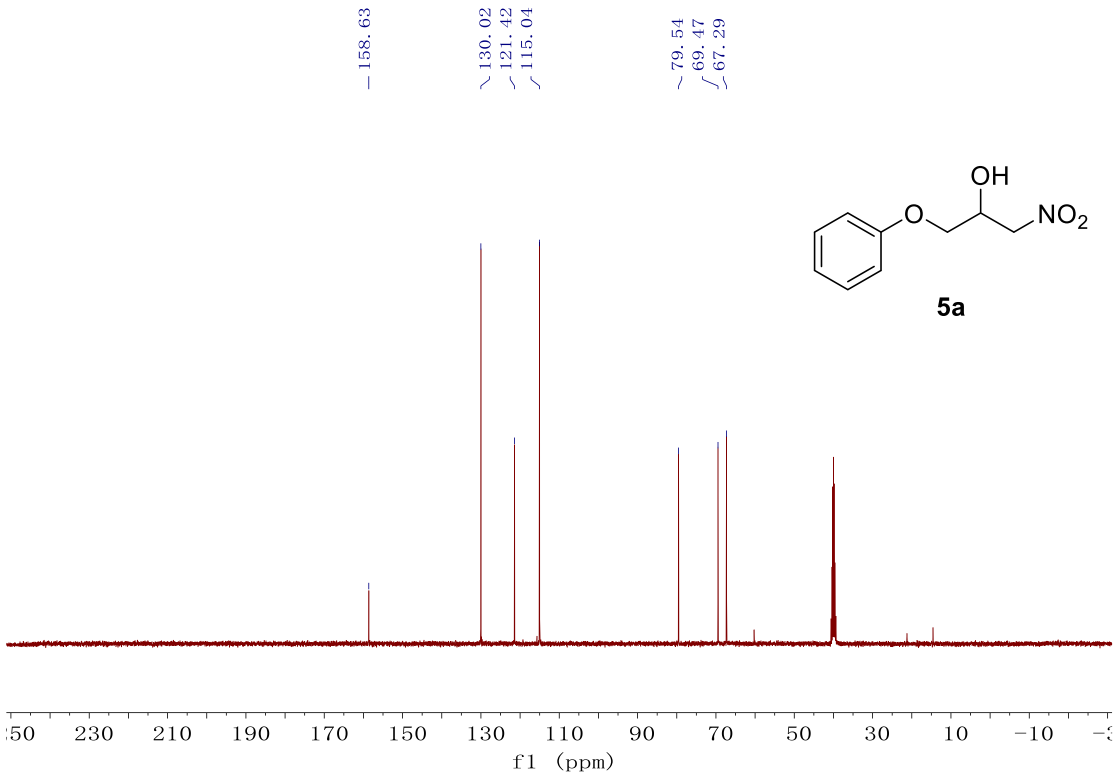


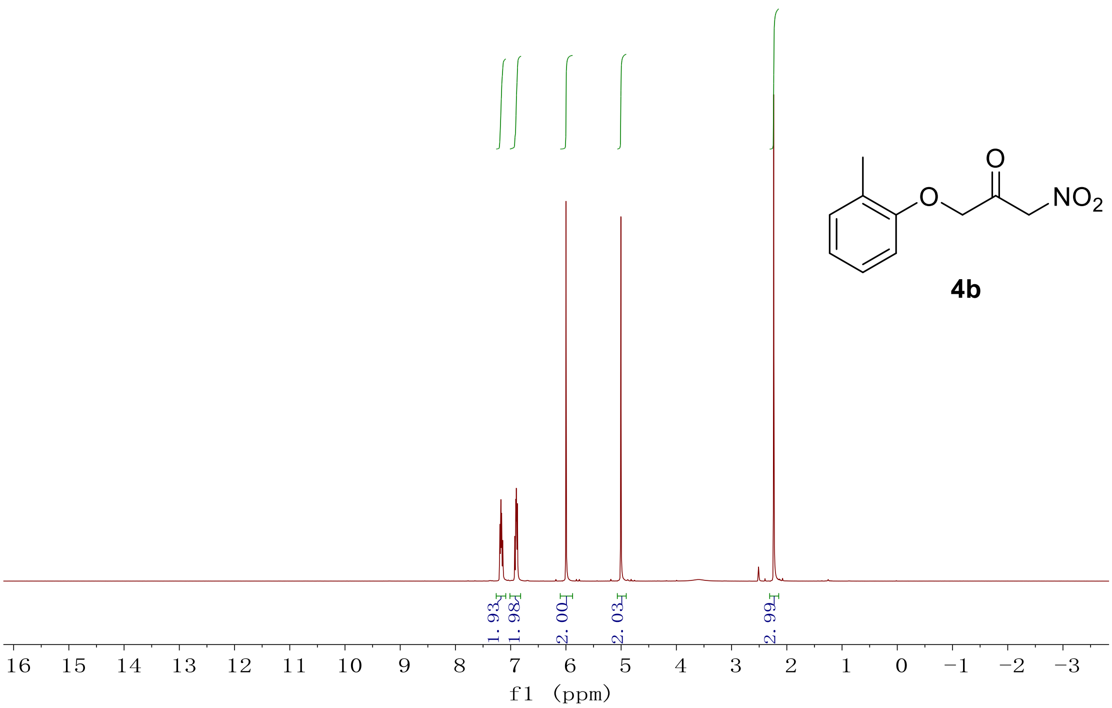
O
O
NO2
4a
2.03
3.01
2.00
2.14
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



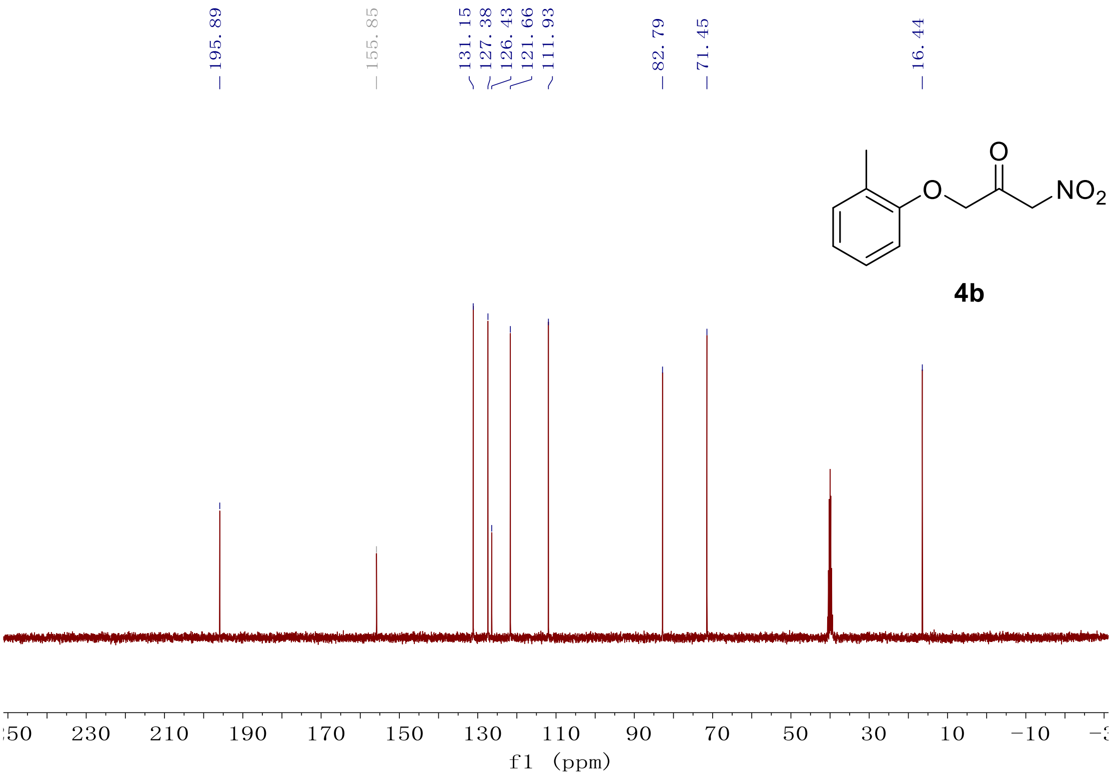
195.56
157.80
130.04
121.95
115.03
82.62
71.10
O
O
NO2
4a
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OH
O
NO2
5a
2.04
3.02
1.00
1.06
1.02
1.03
2.62
f1 (ppm)

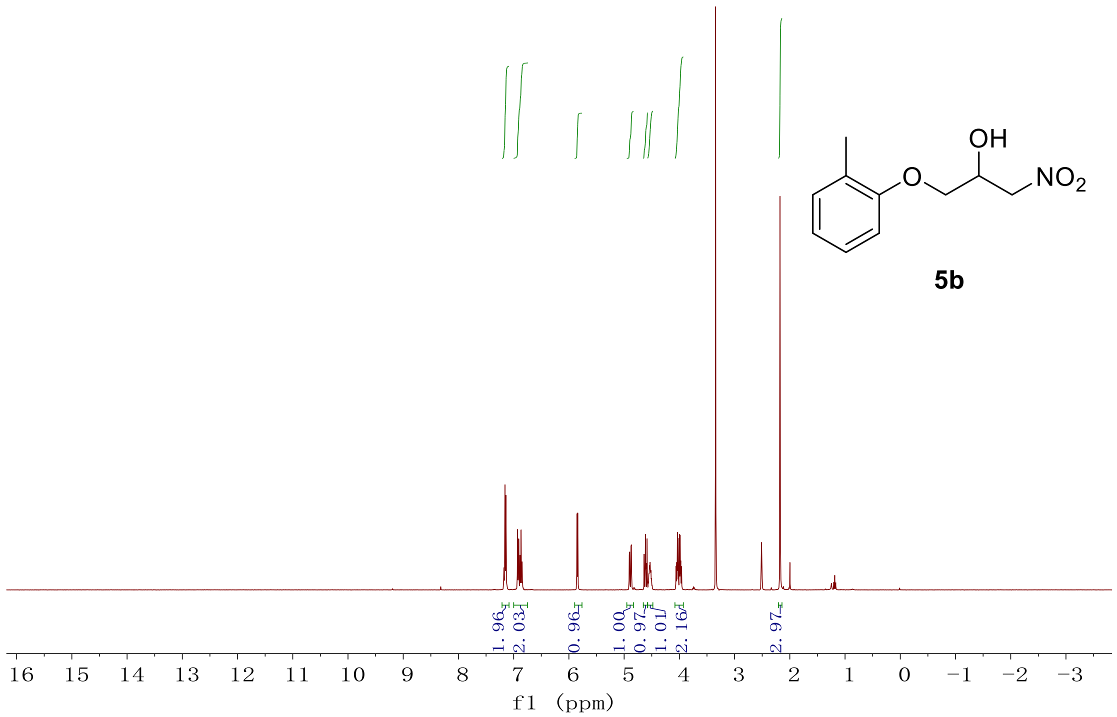

158.63
130.02
121.42
115.04
79.54
69.47
67.29
OH
O
NO2
5a
f1 (ppm)

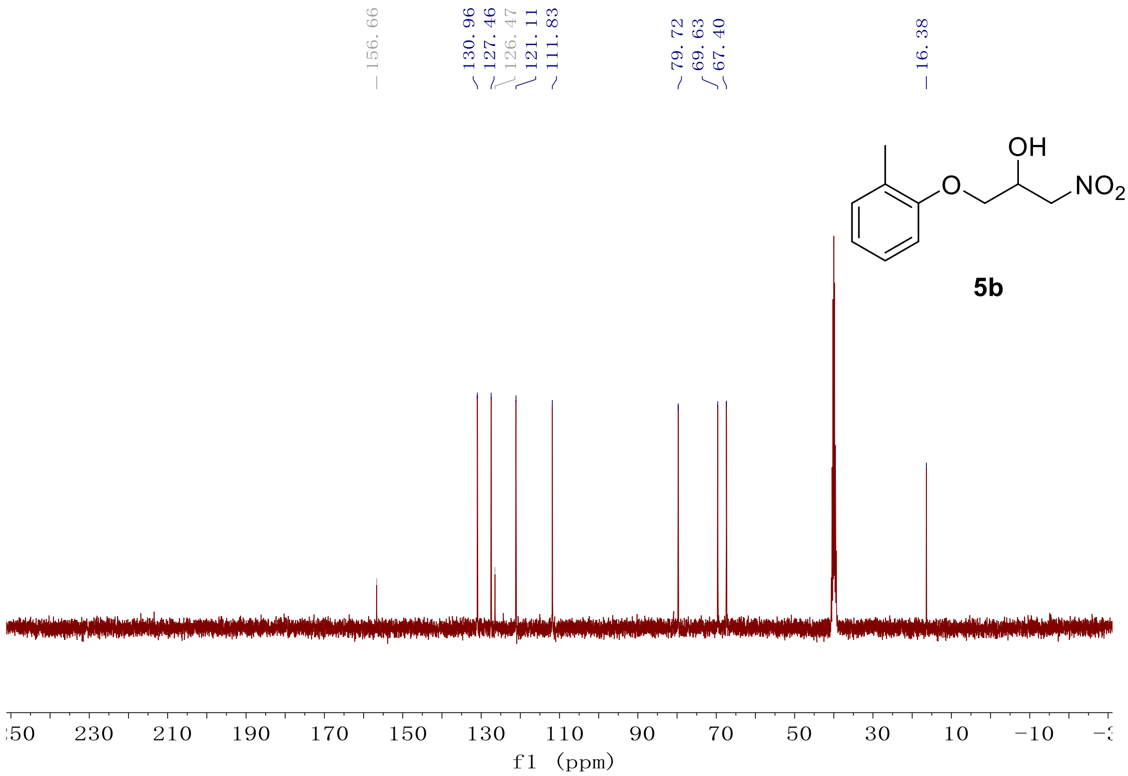

1.93
1.98
2.00
2.03
2.99
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)
O
O
NO2

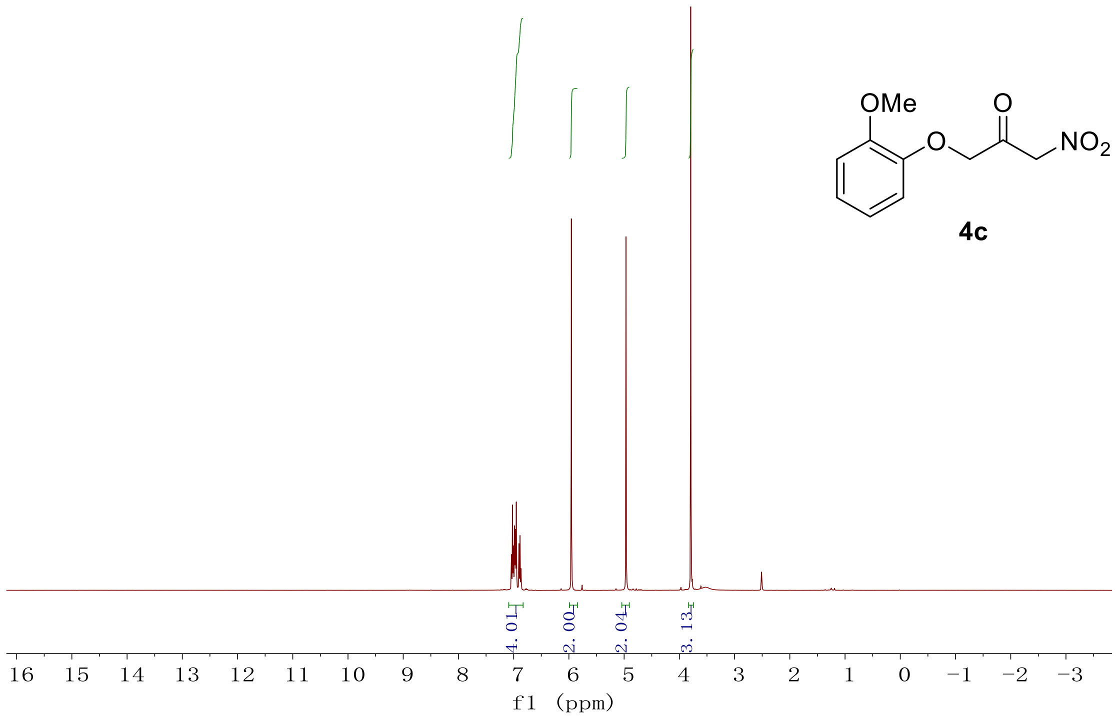
4b

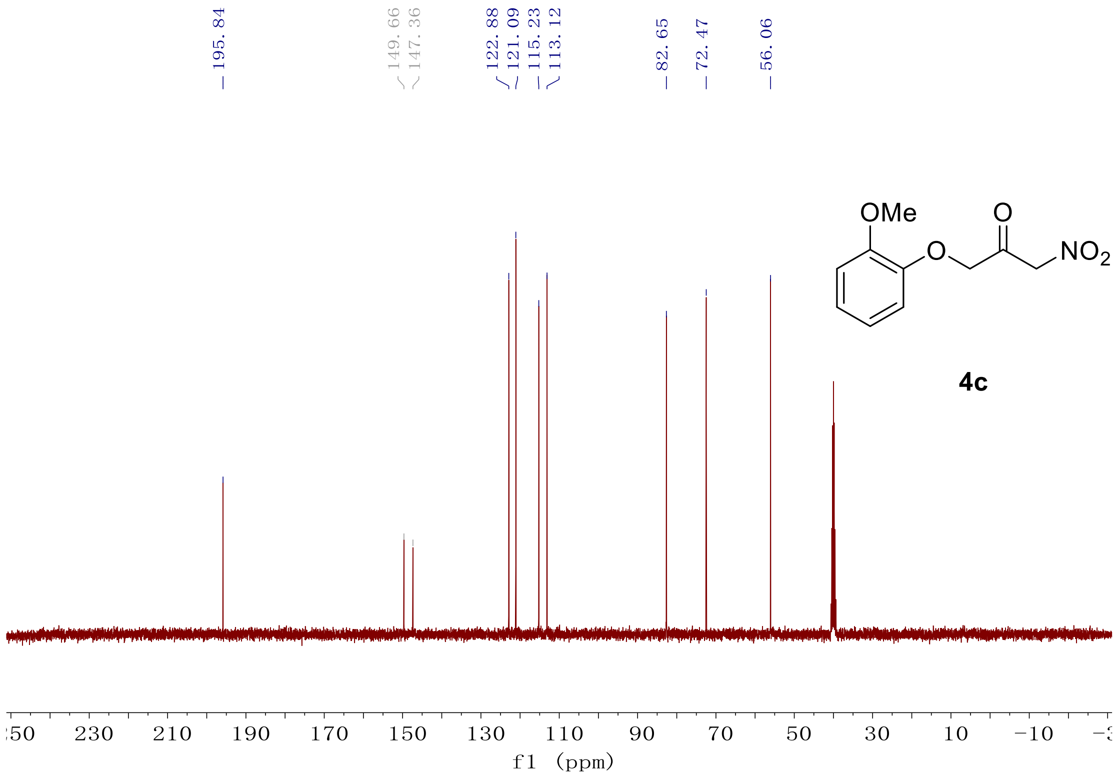

195.89
155.85
131.15
127.38
126.43
121.66
111.93
82.79
71.45
16.44
230
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)
O
O
NO2

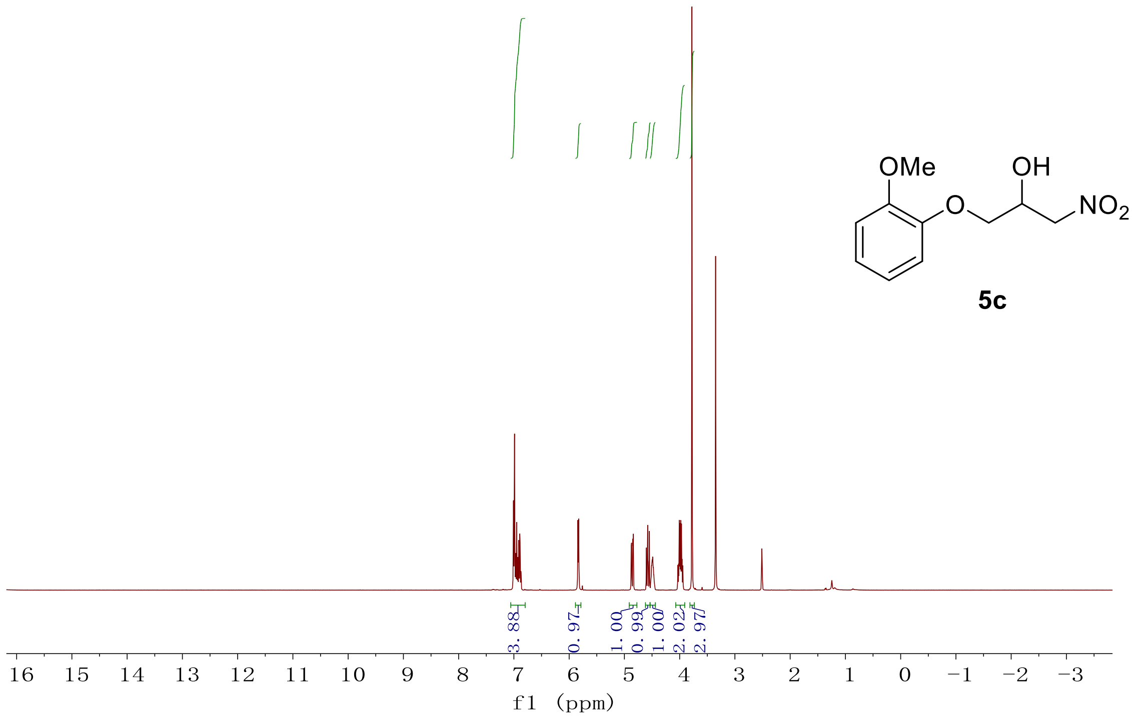
4b

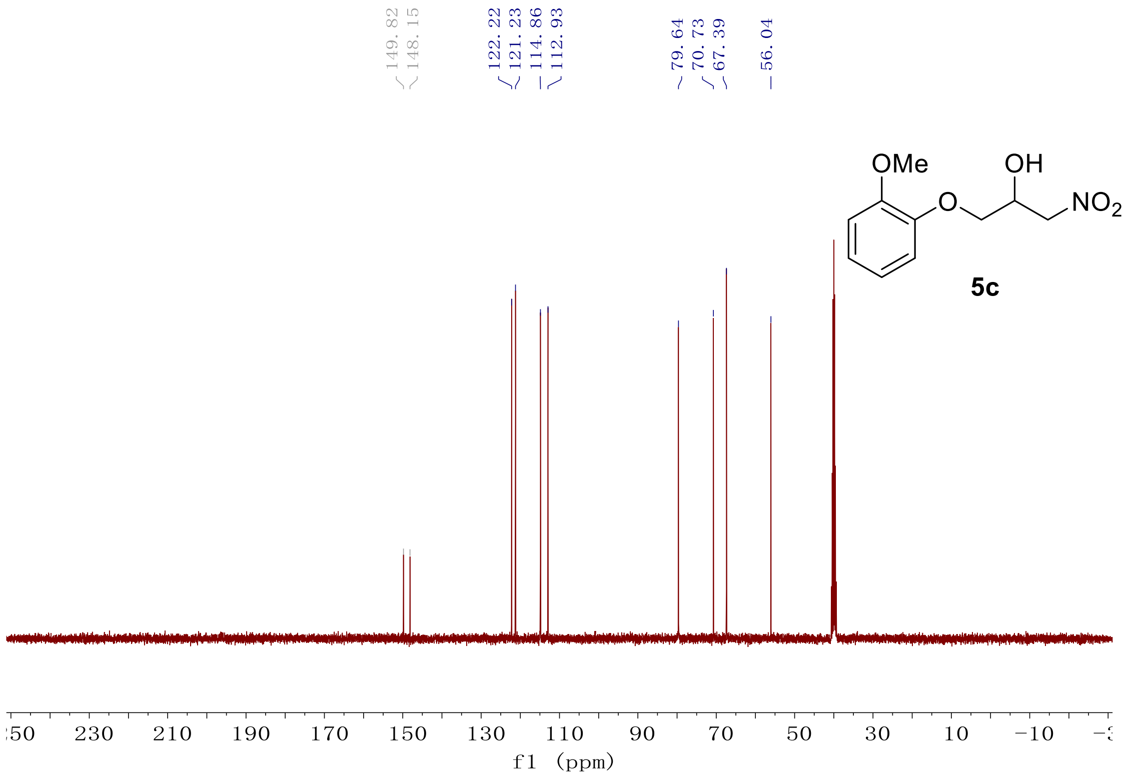

OH
O
NO2
5b
1.96
2.03
0.96
1.00
0.97
1.01
2.16
2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

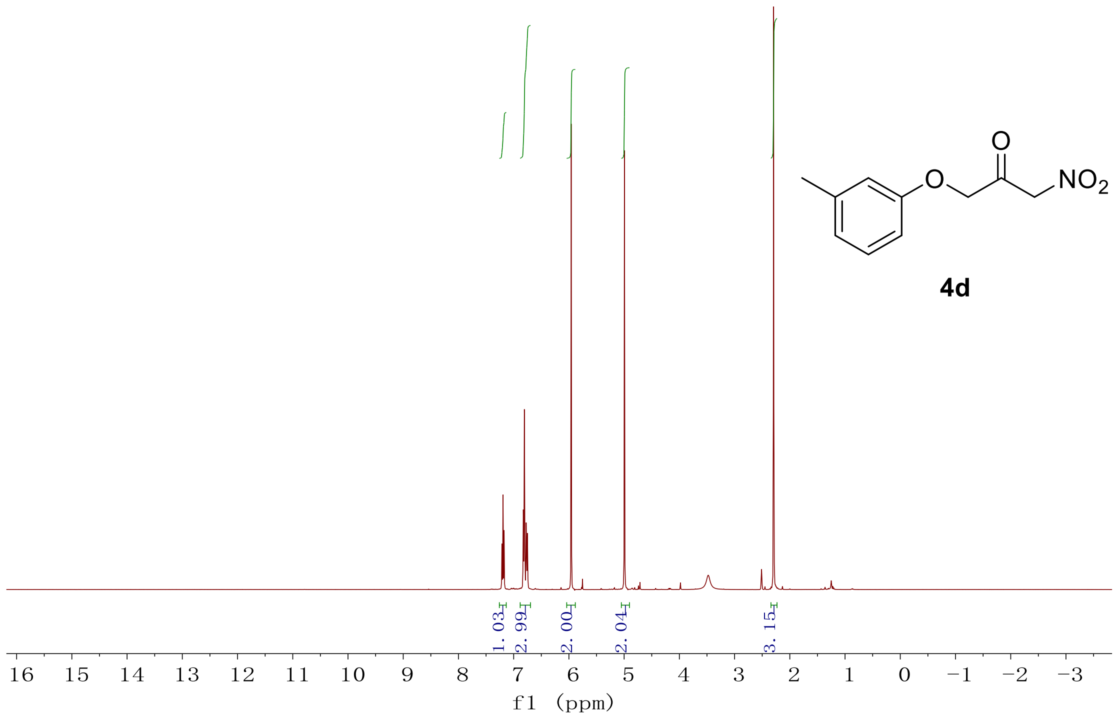

156.66
130.96
127.46
126.47
121.11
111.83
79.72
69.63
67.40
16.38
OH
O
NO2
5b
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OMe
O
NO2
4c
4.01
2.00
2.04
3.13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

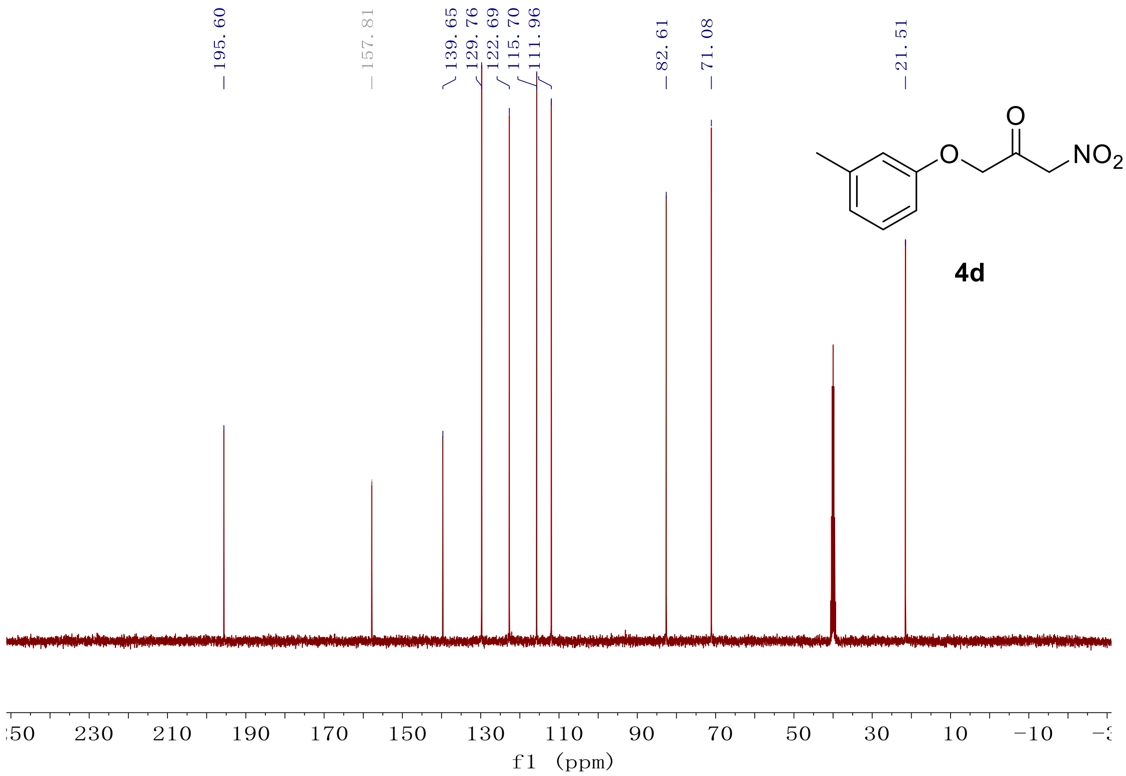

195.84
149.66
147.36
122.88
121.09
115.23
113.12
82.65
72.47
56.06
OMe
O
NO2
4c
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


OMe
OH
O
NO2
5c
3.88
0.97
1.00
0.99
1.00
2.02
2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

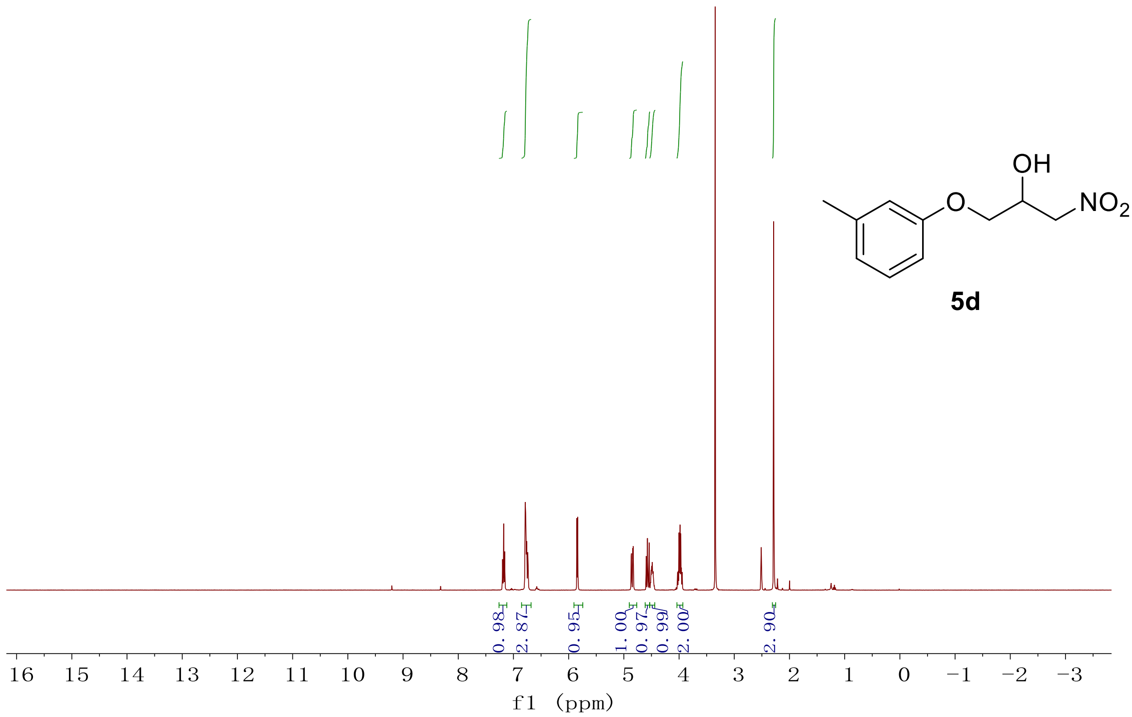

149.82
148.15
122.22
121.23
114.86
112.93
79.64
70.73
67.39
56.04
OMe
OH
O
NO2
5c
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

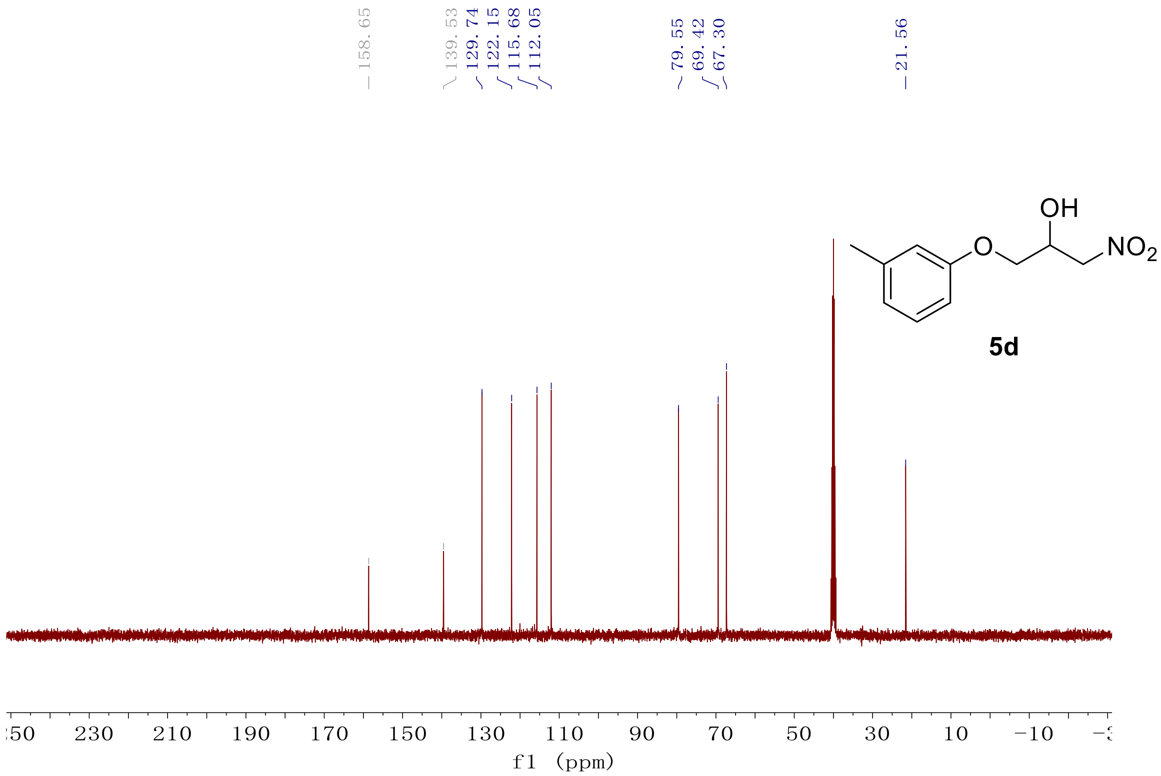

O
O
NO2
1.03
2.99
2.00
2.04
3.15
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

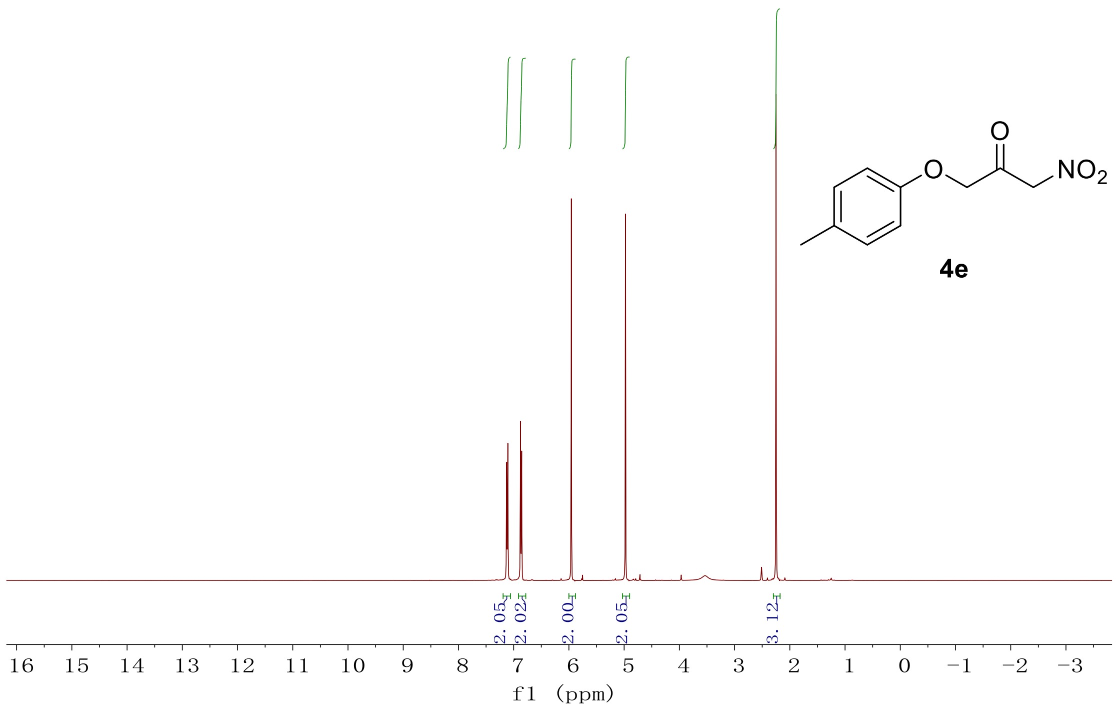
4d

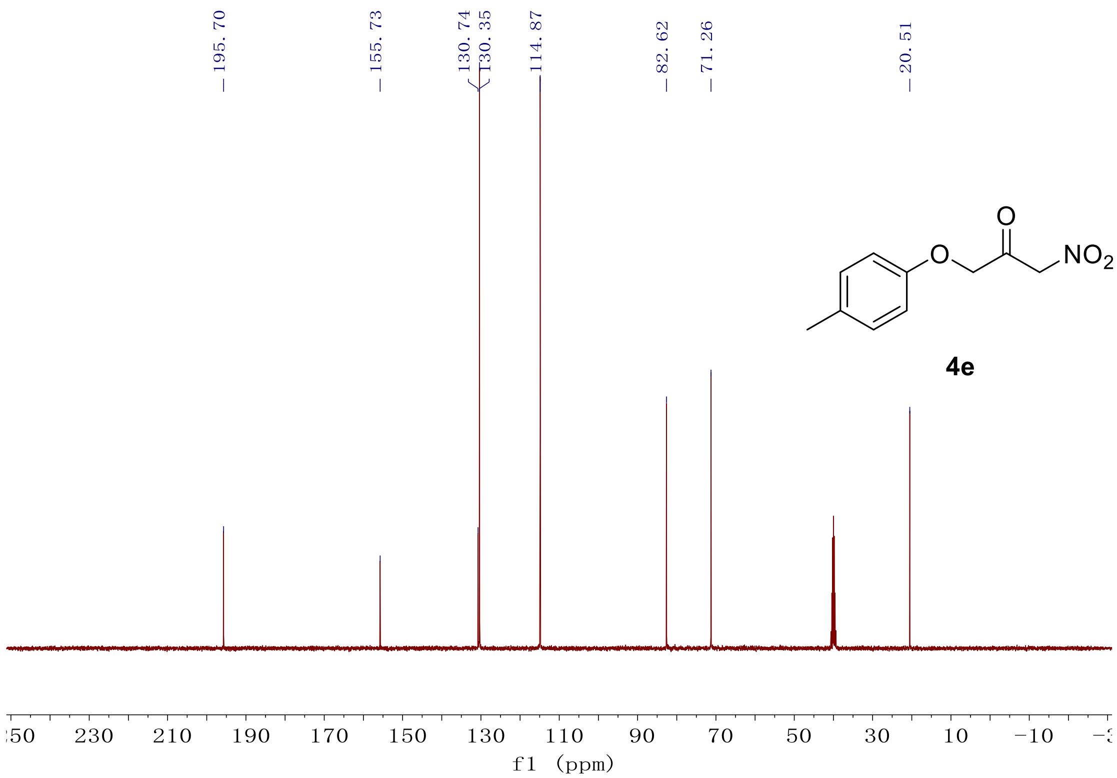

195.60
157.81
139.65
129.76
122.69
115.70
111.96
82.61
71.08
21.51
O
O
NO2
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

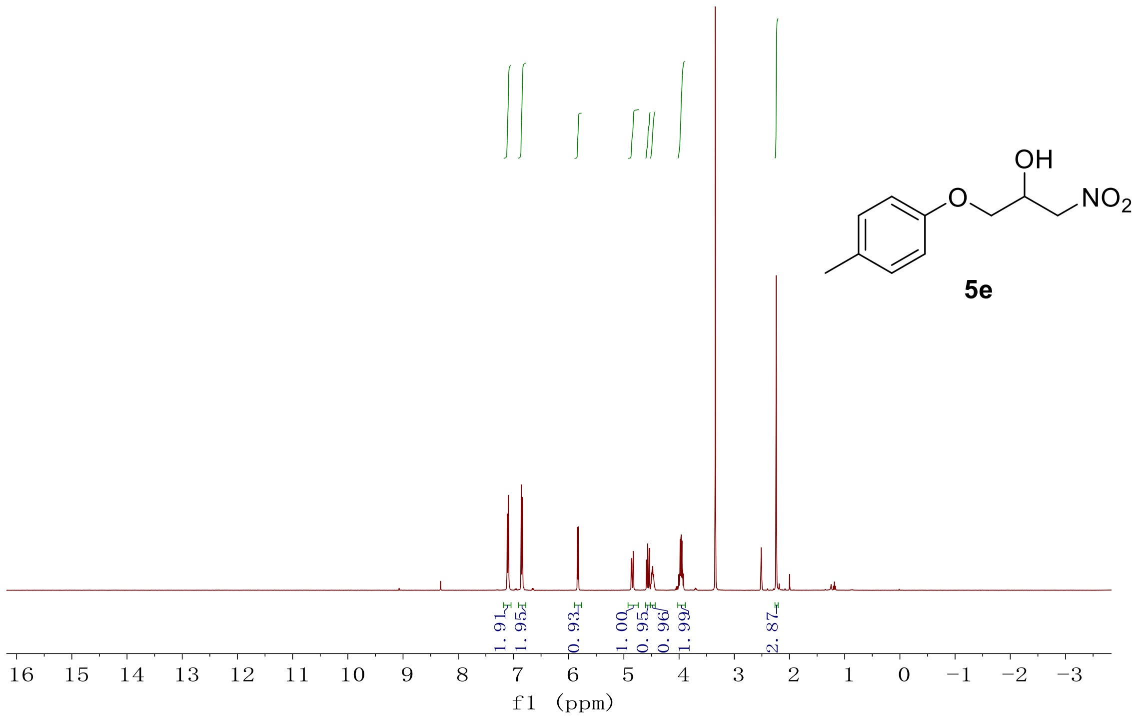
4d


OH
O
NO2
5d
0.98
2.87
0.95
1.00
0.97
0.99
2.00
2.90
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

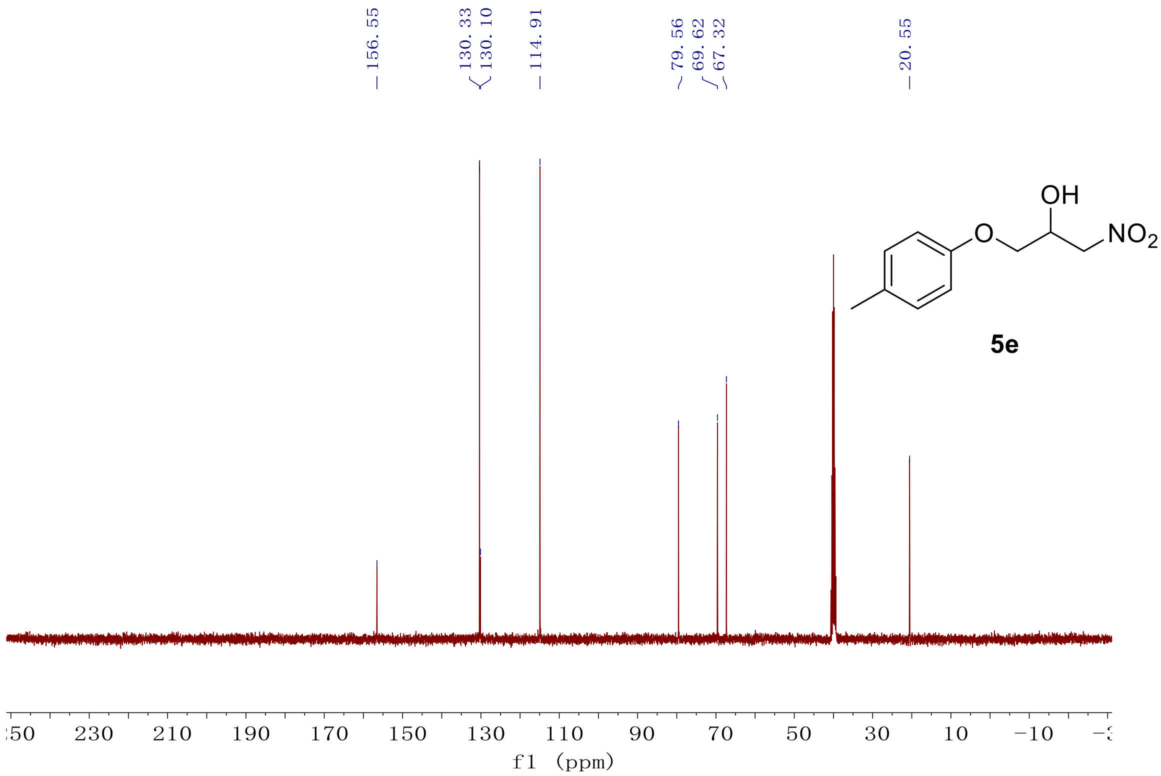

158.65
139.53
129.74
122.15
115.68
112.05
79.55
69.42
67.30
21.56
OH
O
NO2
5d
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


4e
2.05
2.02
2.00
2.05
3.12
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

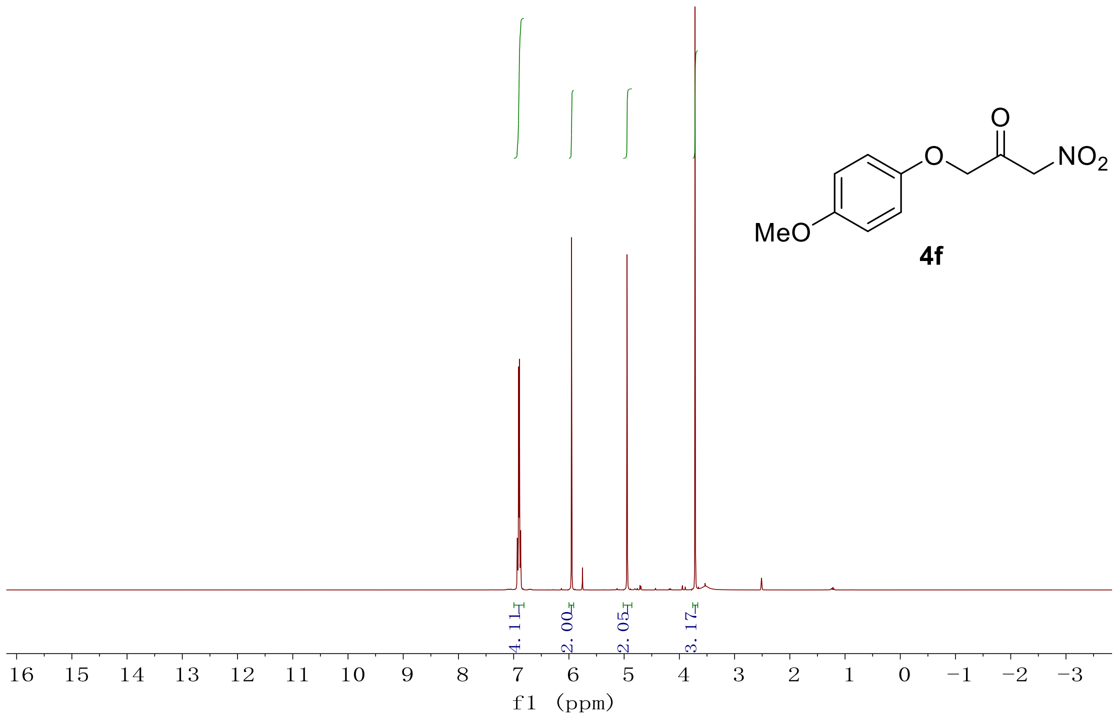

195.70
155.73
130.74
130.35
114.87
82.62
71.26
20.51
4e
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

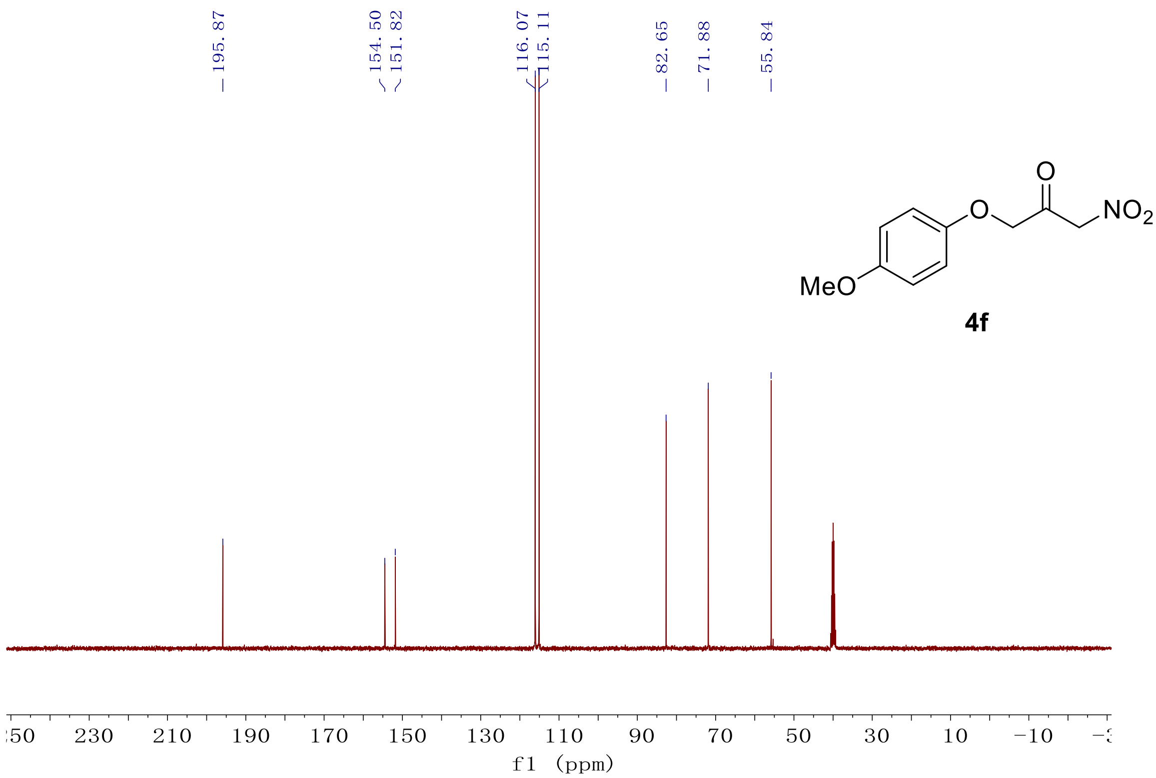


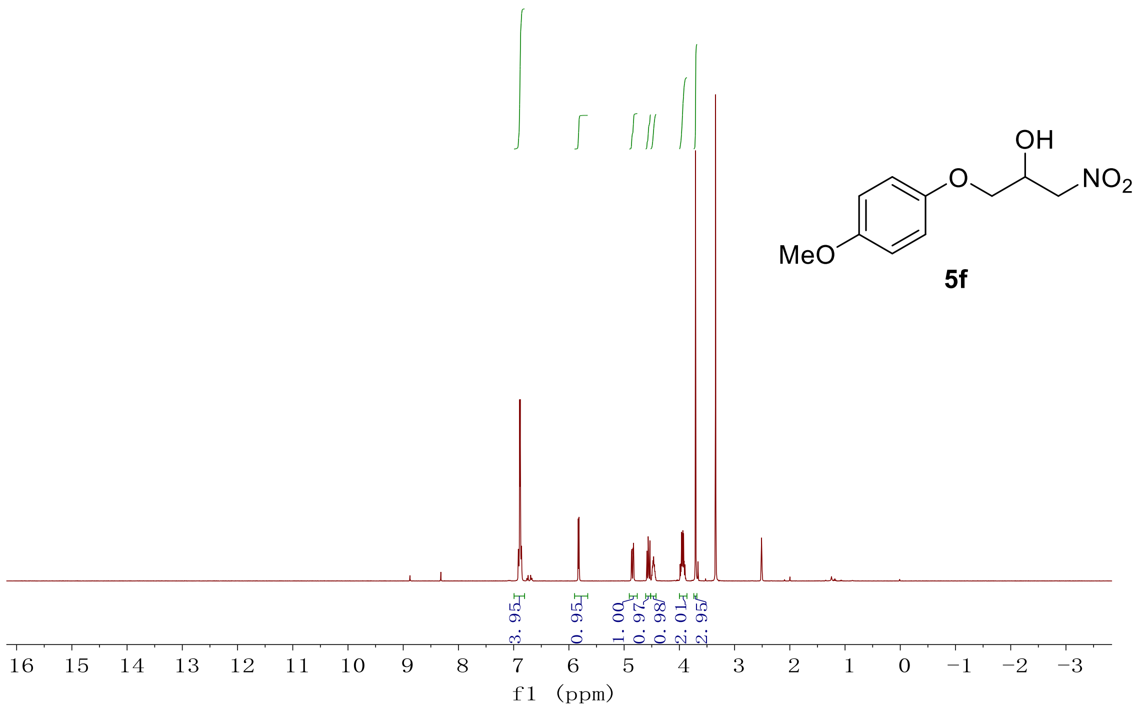
OH
O
NO2
5e
1.91
1.95
0.93
1.00
0.95
0.96
1.99
2.87
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



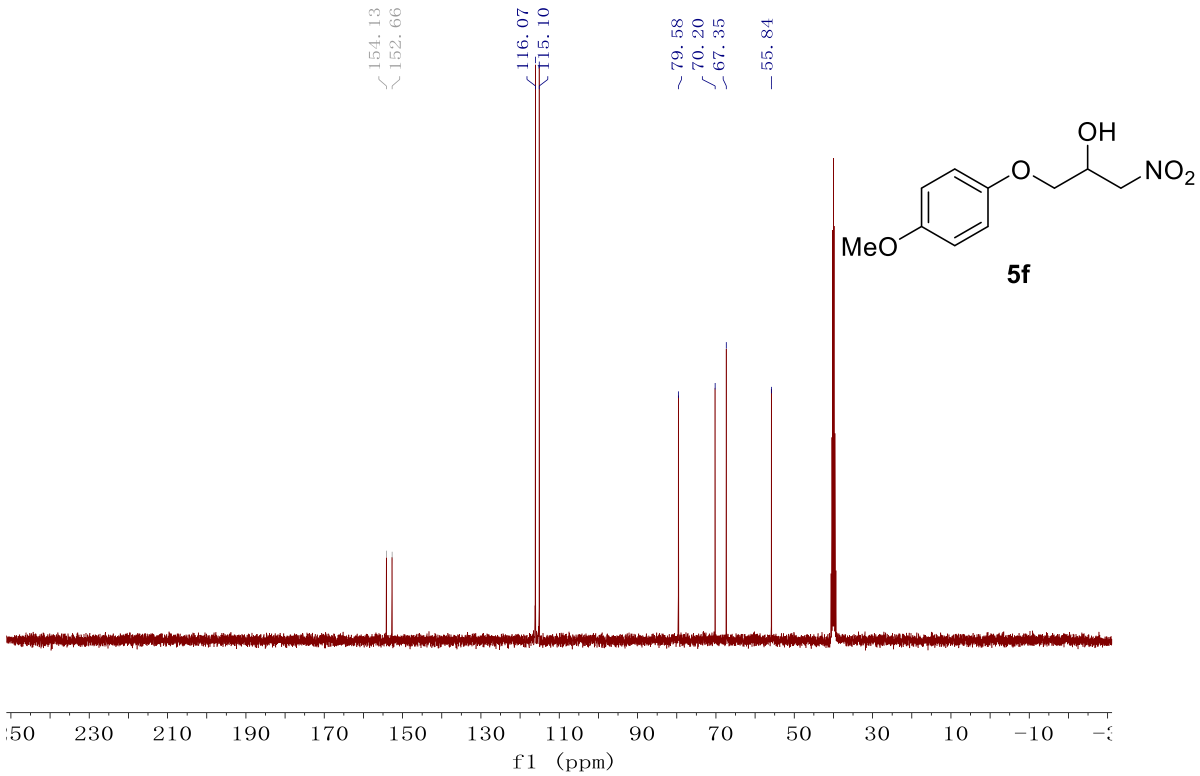
156.55
130.33
130.10
114.91
79.56
69.62
67.32
20.55
OH
O
NO2
5e
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


4.11
2.00
2.05
3.17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)
O
NO2
O
MeO
4f

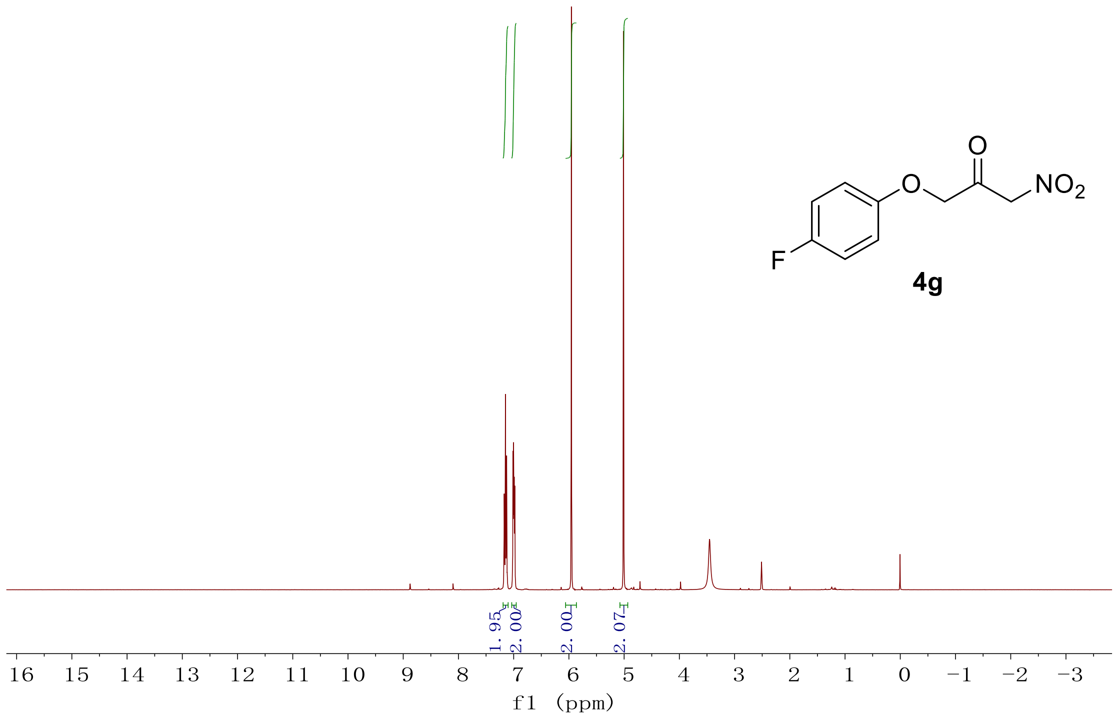

195.87
154.50
151.82
116.07
115.11
82.65
71.88
55.84
O
NO2
O
MeO
4f
230
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)

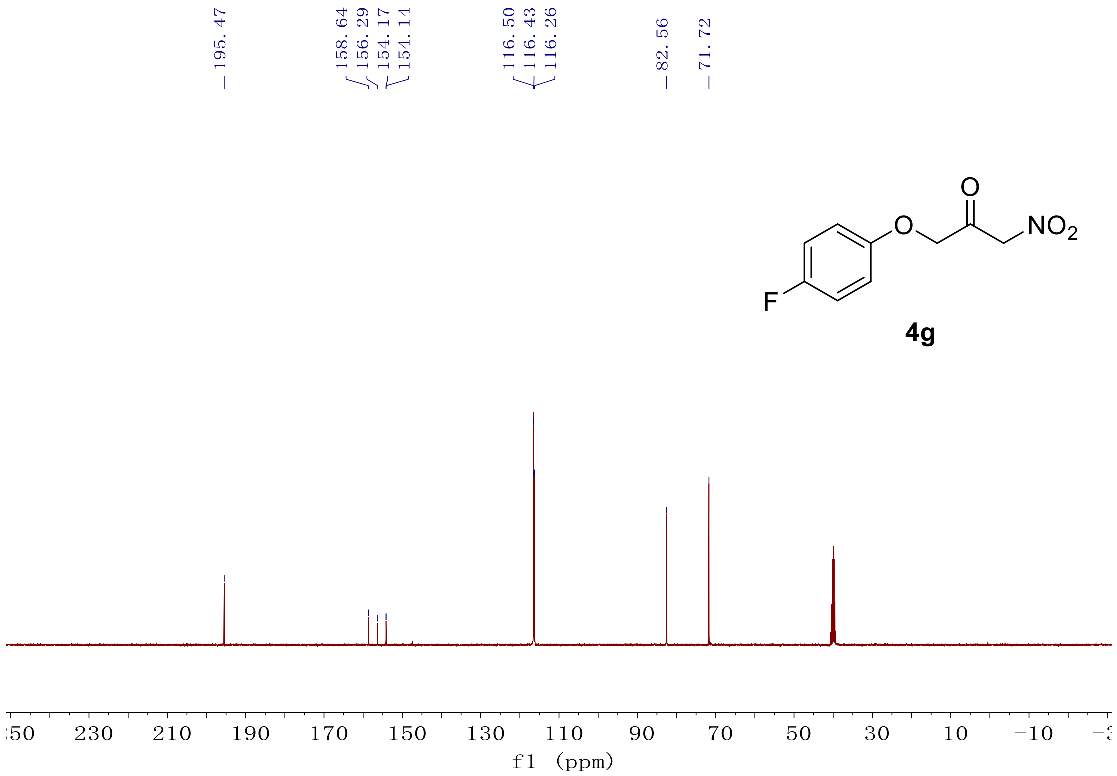


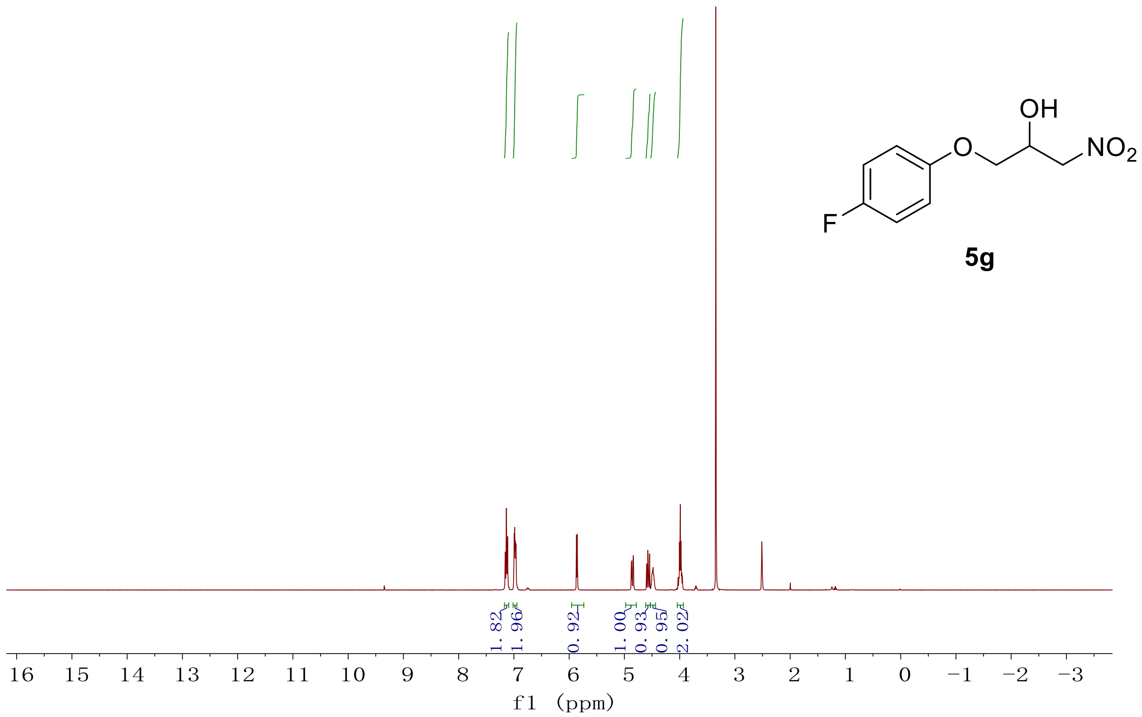
OH
O
NO2
MeO
5f
3.95
0.95
1.00
0.97
0.98
2.01
2.95
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



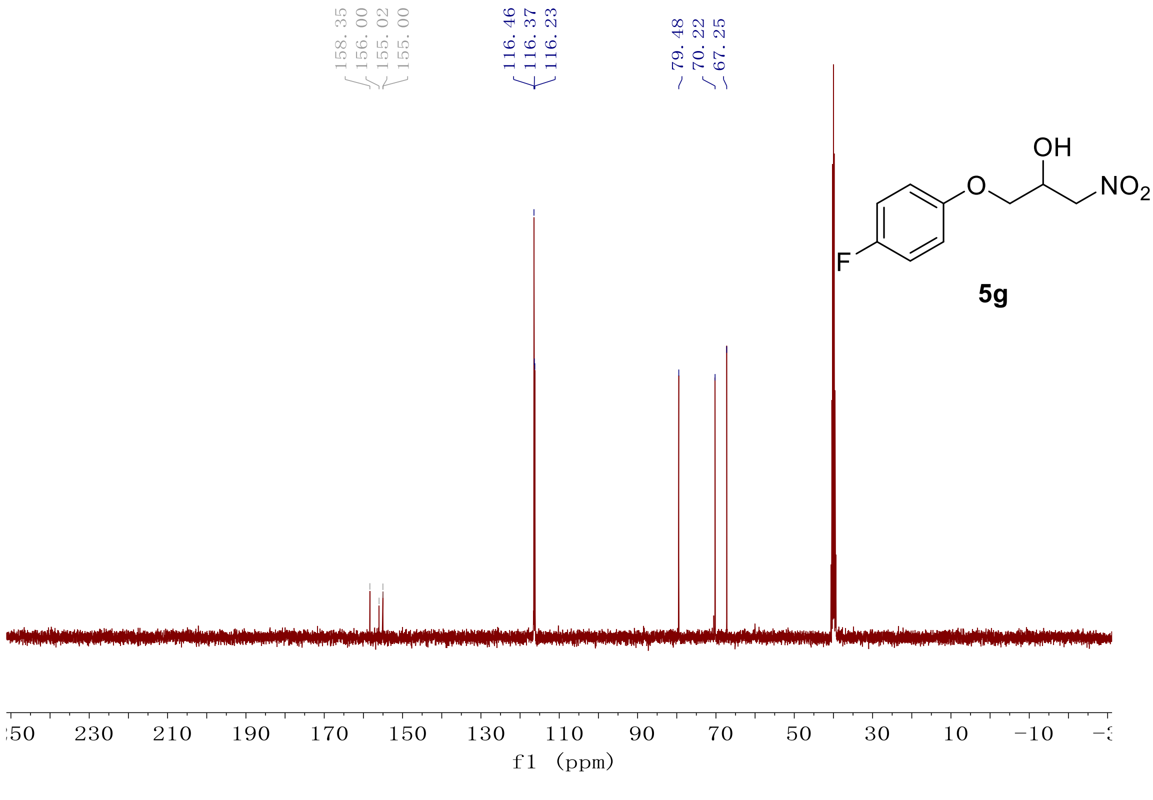
154.13
152.66
116.07
115.10
79.58
70.20
67.35
55.84
OH
O
NO2
MeO
5f
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


NO2
O
O
F
4g
1.95
2.00
2.00
2.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

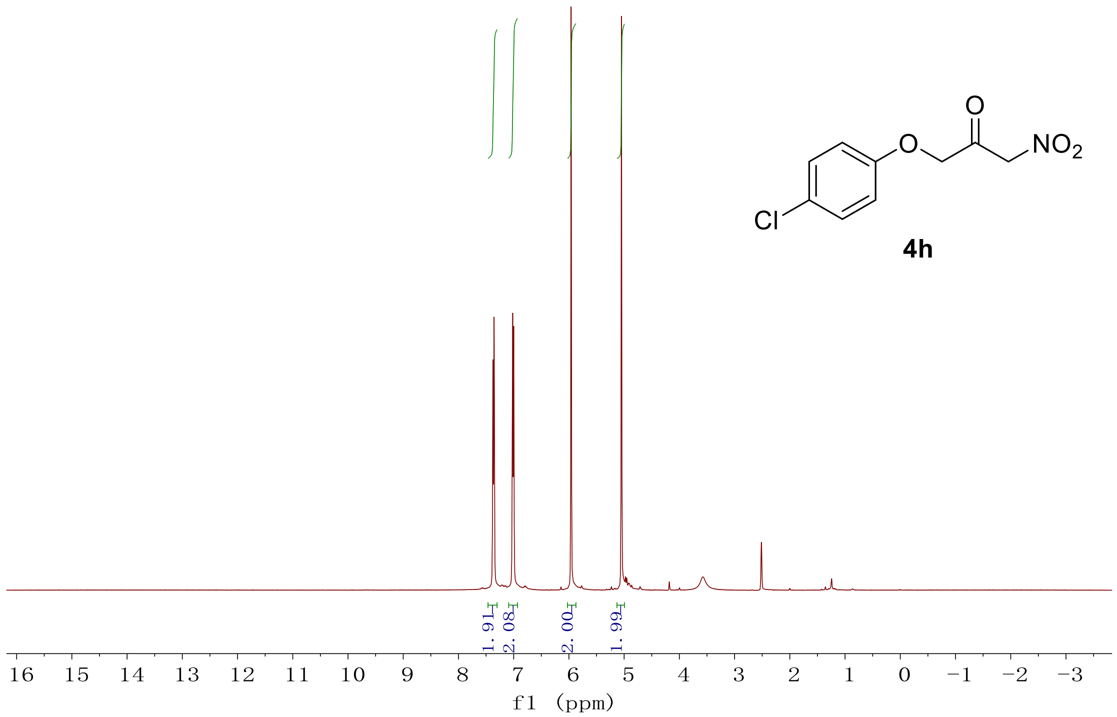

195.47
158.64
156.29
154.17
154.14
116.50
116.43
116.26
82.56
71.72
NO2
O
O
F
4g
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

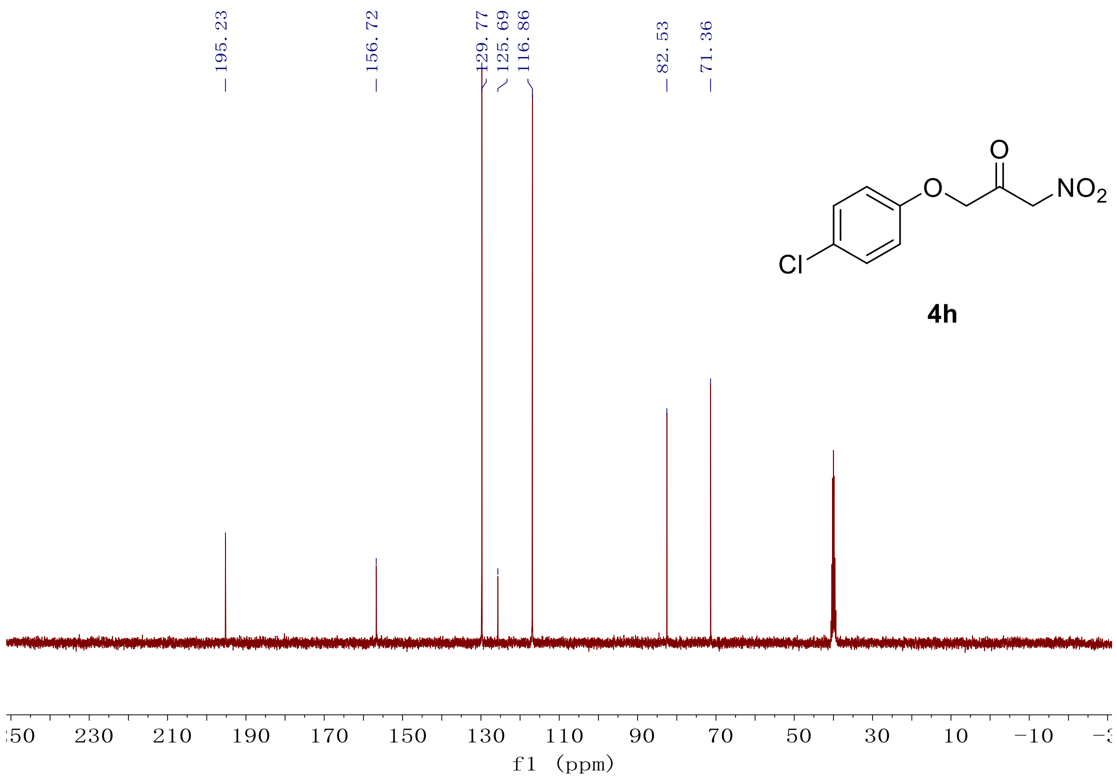


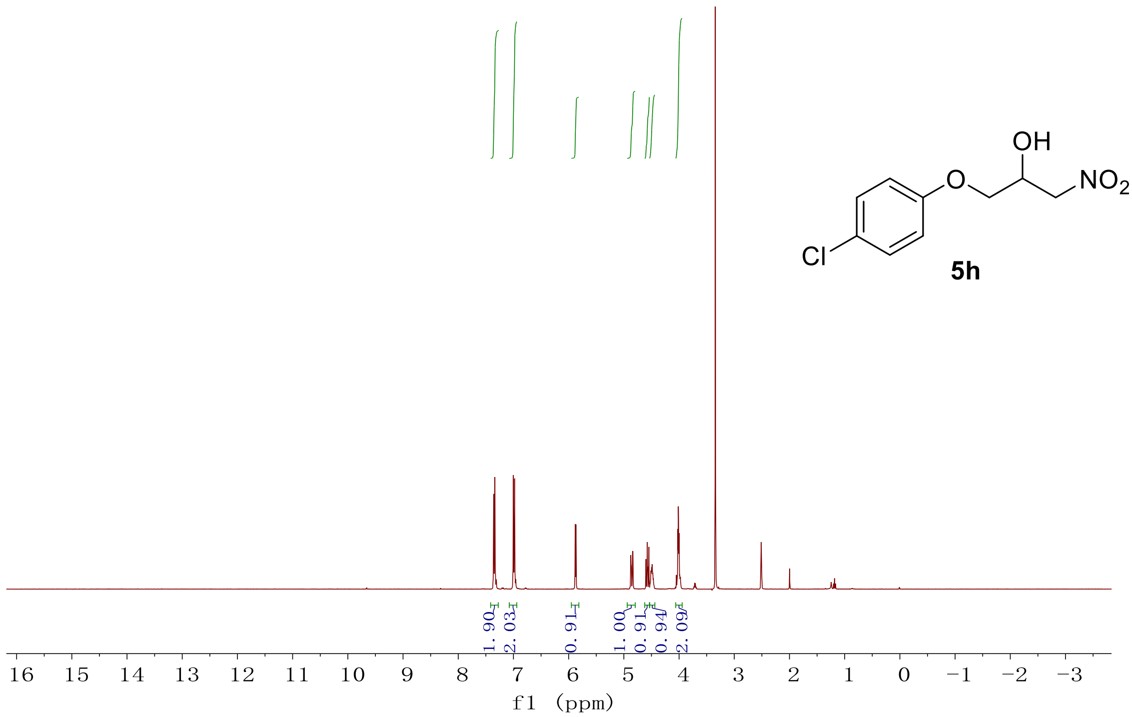
OH
O
NO2
F
5g
1.82
1.96
0.92
1.00
0.93
0.95
2.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

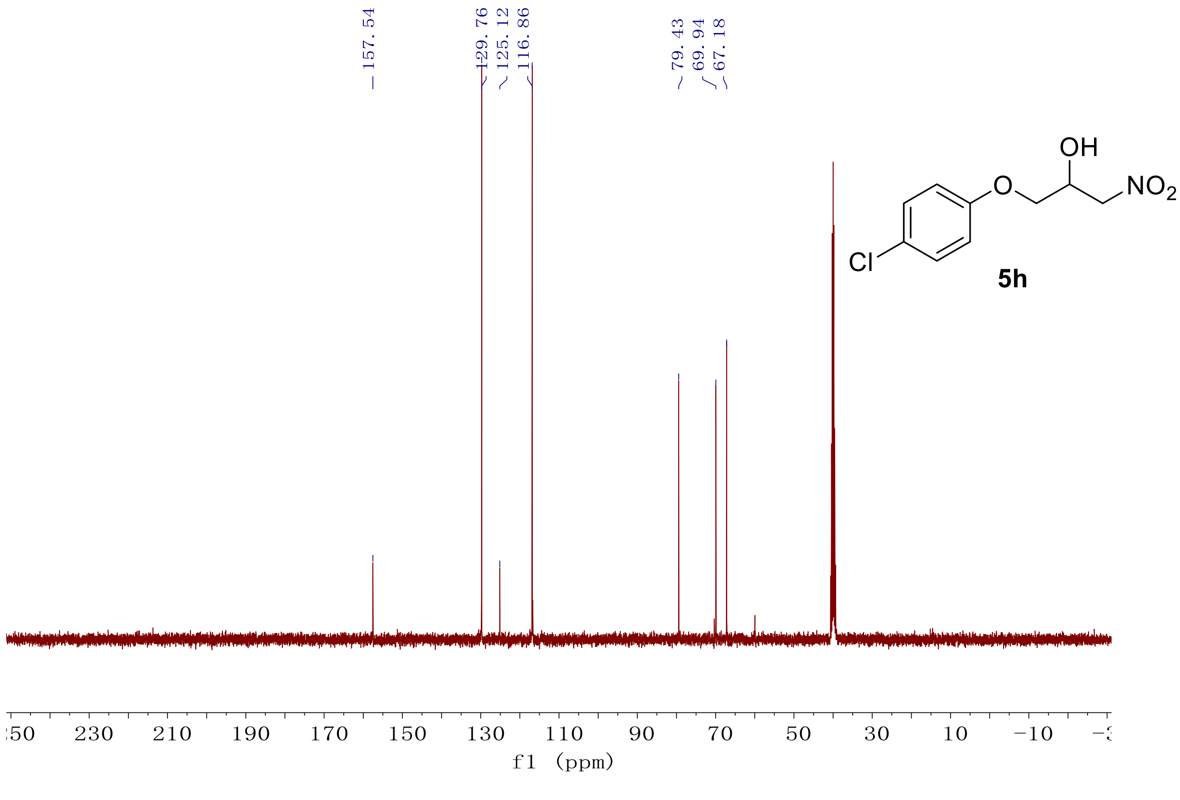


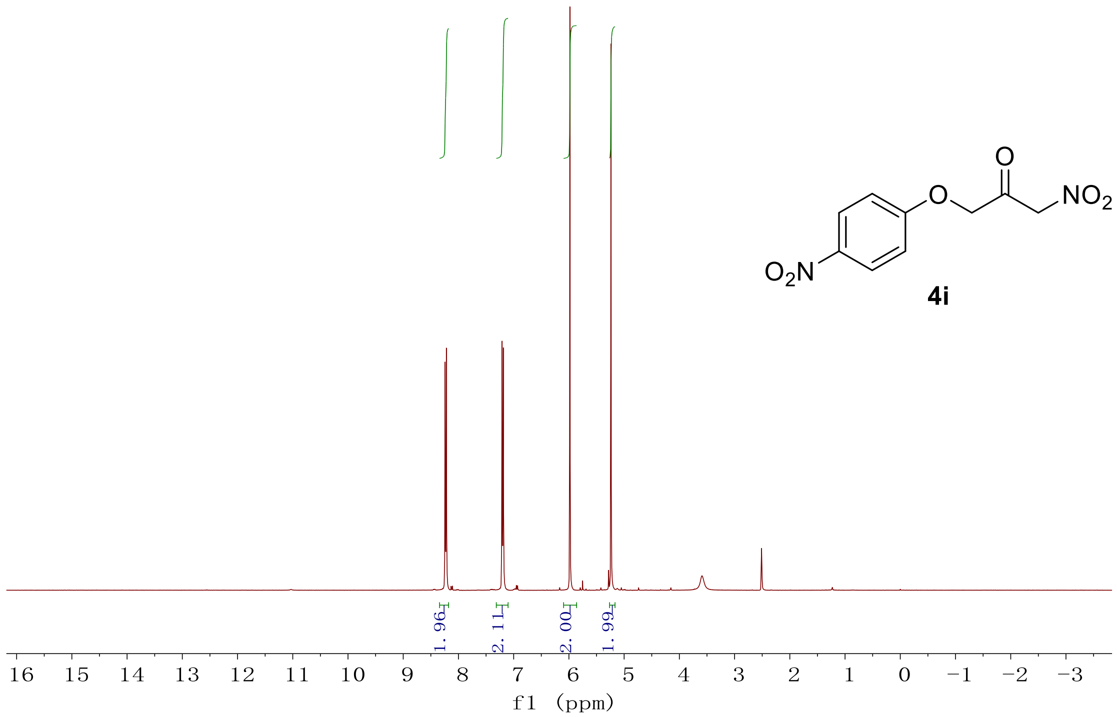
158.35
156.00
155.02
155.00
116.46
116.37
116.23
79.48
70.22
67.25
OH
O
NO2
F
5g
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

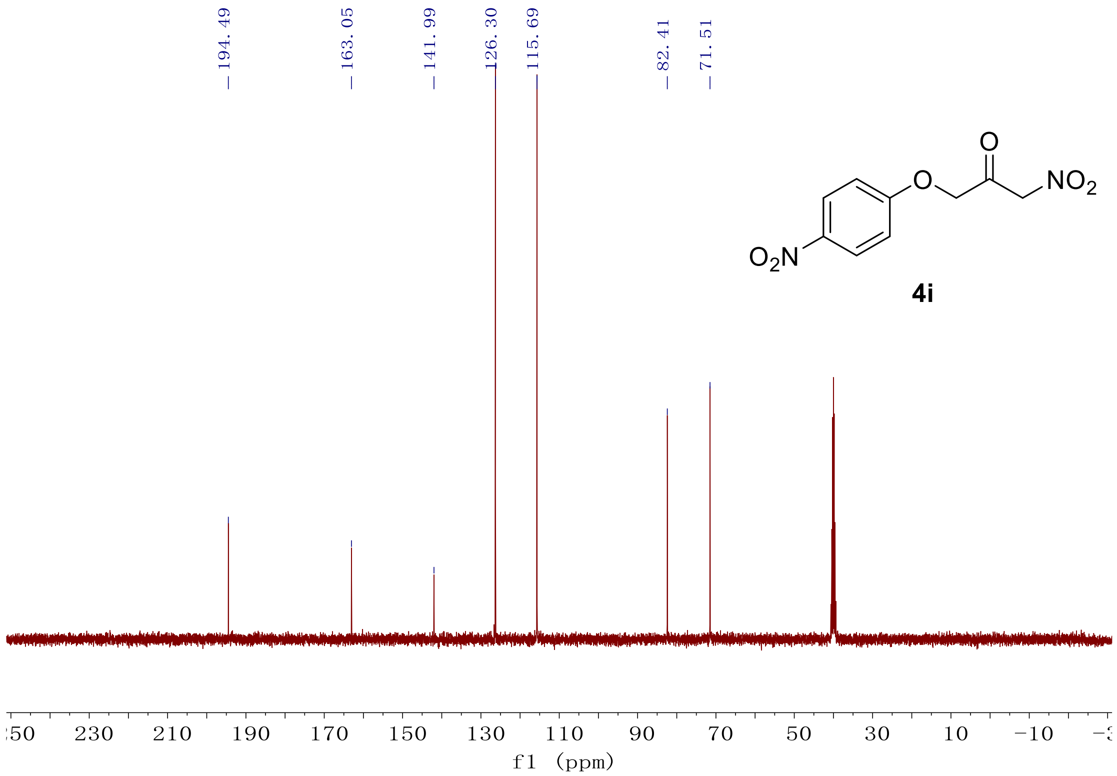

O
NO2
O
Cl
4h
1.91
2.08
2.00
1.99
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)

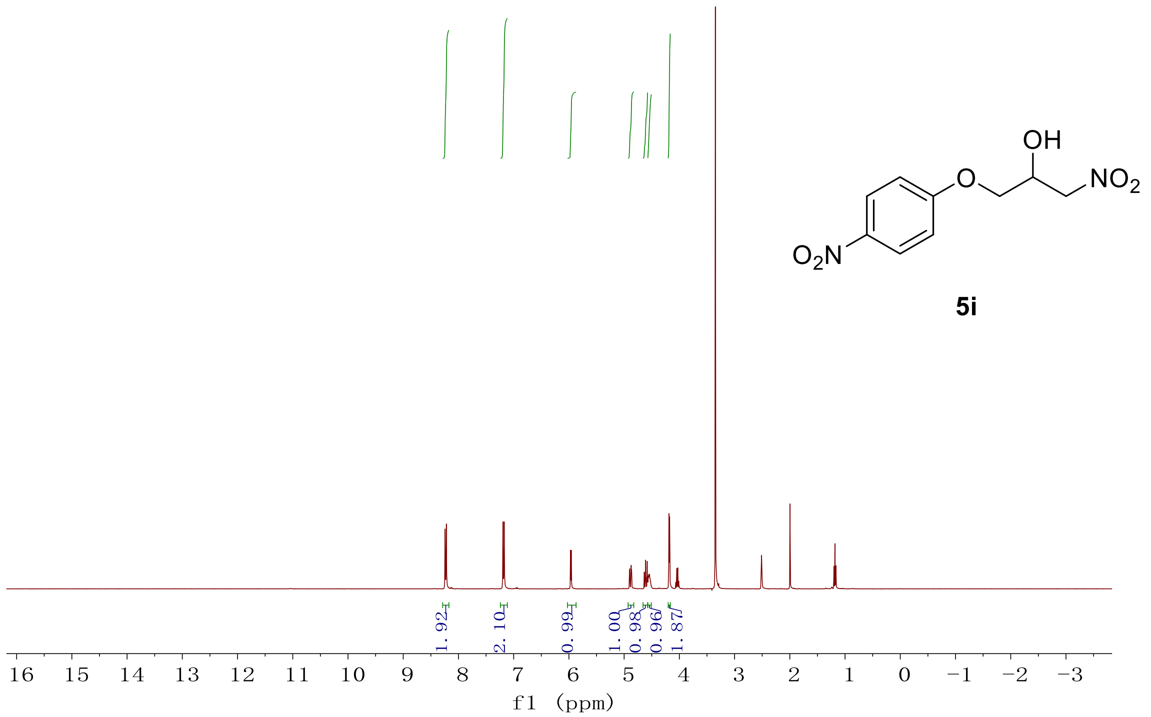

195.23
156.72
129.77
125.69
116.86
82.53
71.36
O
NO2
O
Cl
4h
230
210
190
170
150
130
110
90
70
50
30
10
−10
f1 (ppm)

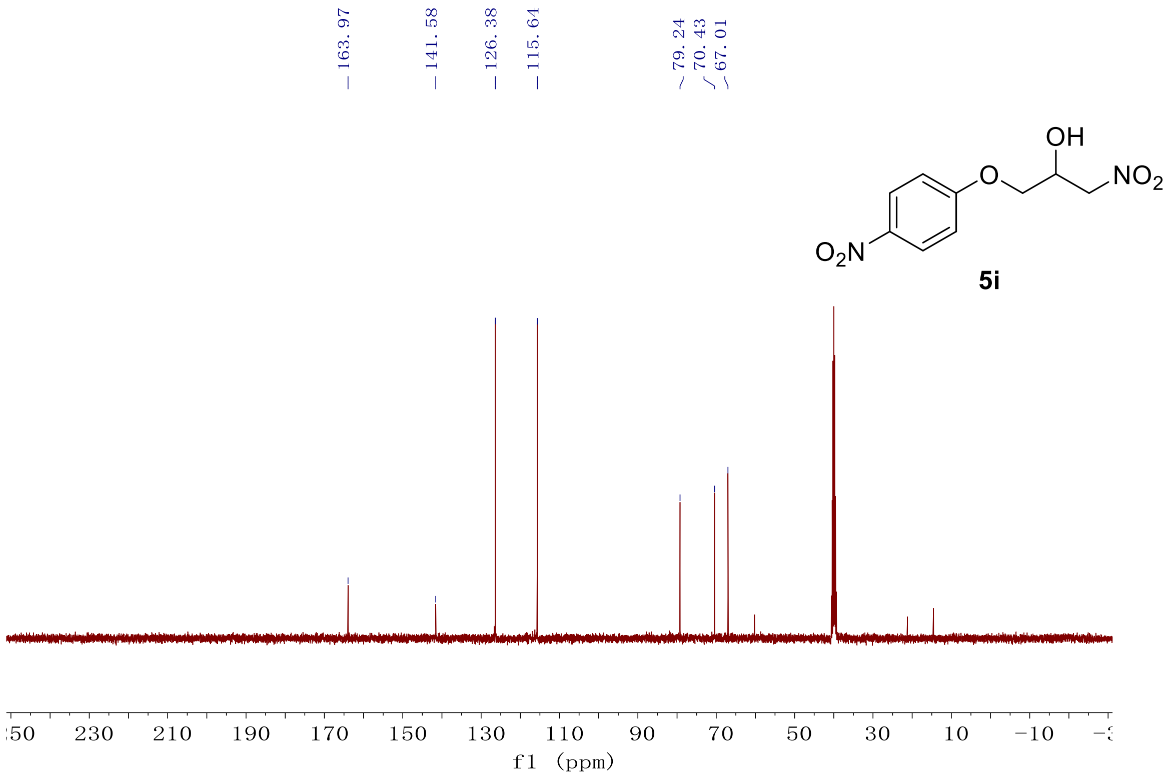

OH
O
NO2
Cl
5h
1.90
2.03
0.91
1.00
0.91
0.94
2.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

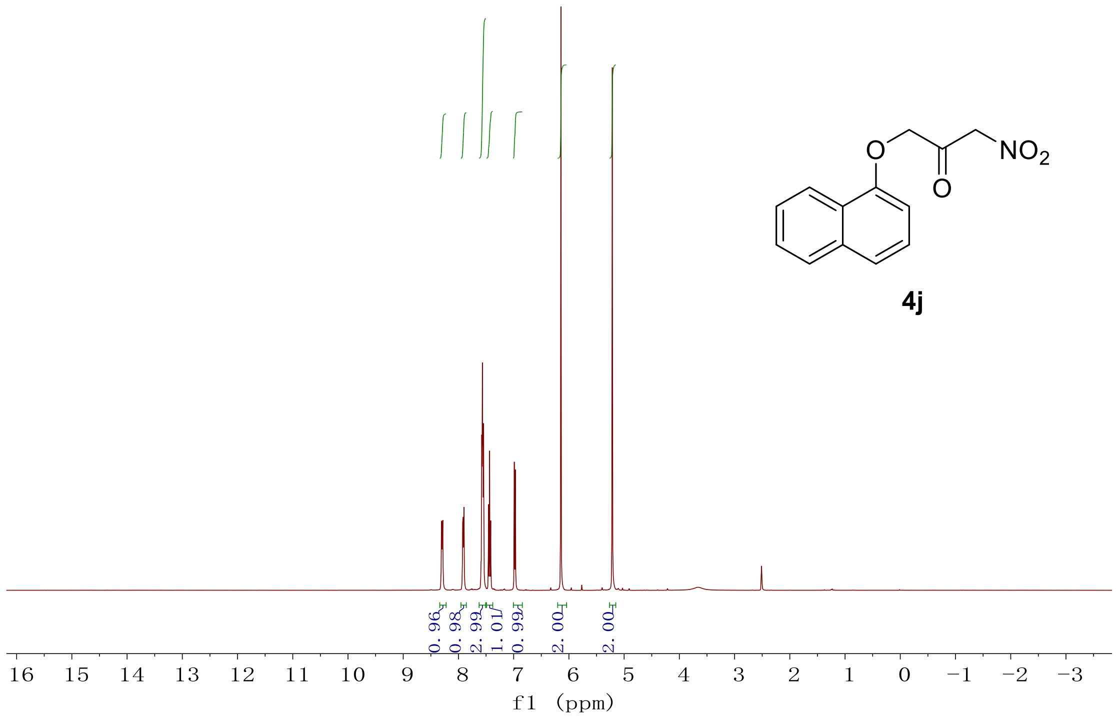

157.54
129.76
125.12
116.86
79.43
69.94
67.18
OH
O
NO2
Cl
5h
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

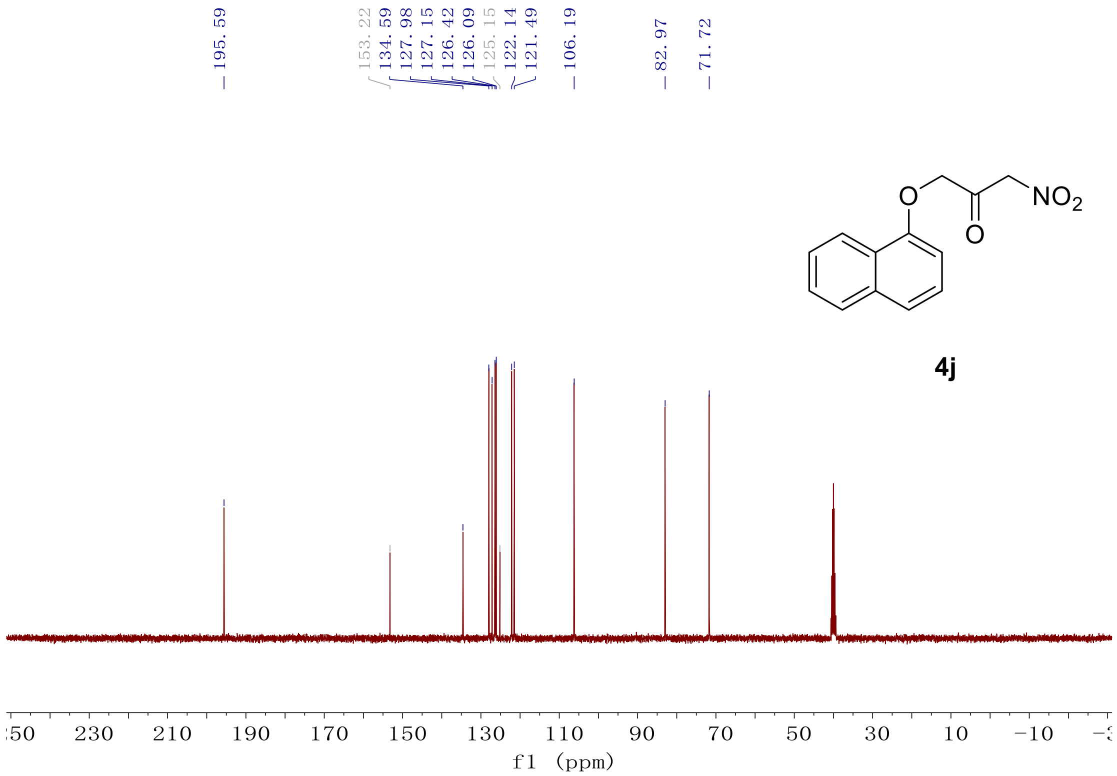

O
NO2
O
O2N
4i
1.96
2.11
2.00
1.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

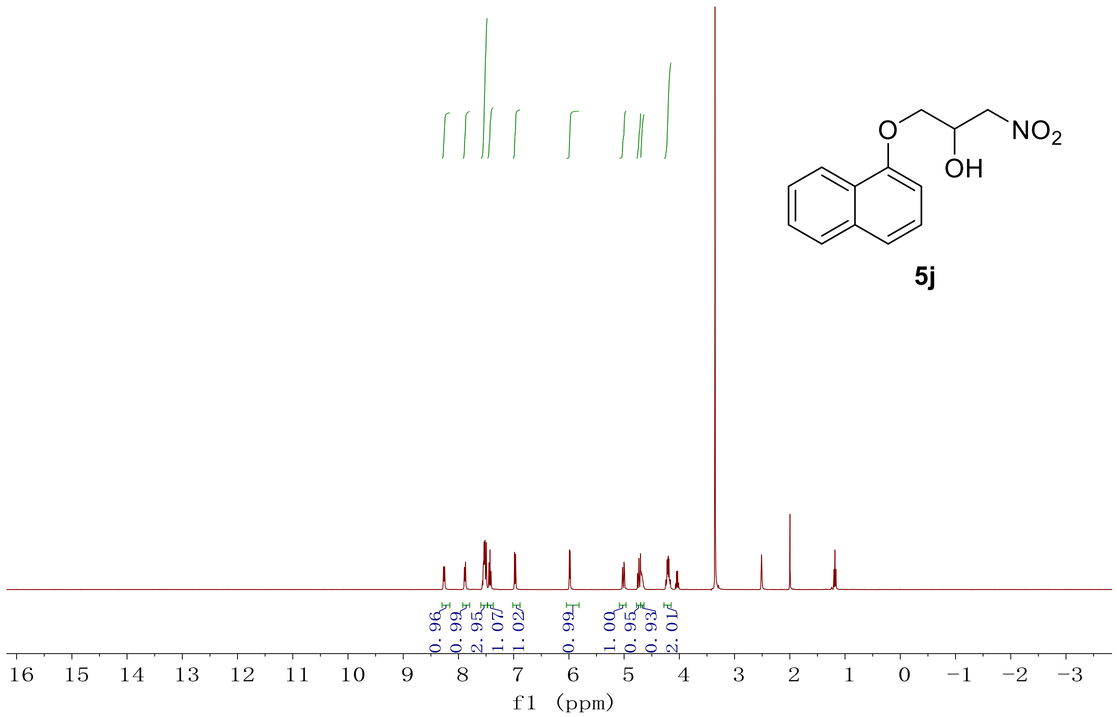

194.49
163.05
141.99
126.30
115.69
82.41
71.51
O
NO2
O
O2N
4i
250 230 210 190 170 150 130 110 90 70 50 30 10 −10 −30
f1 (ppm)


OH
O
NO2
O2N
5i
1.92
2.10
0.99
1.00
0.98
0.96
1.87
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

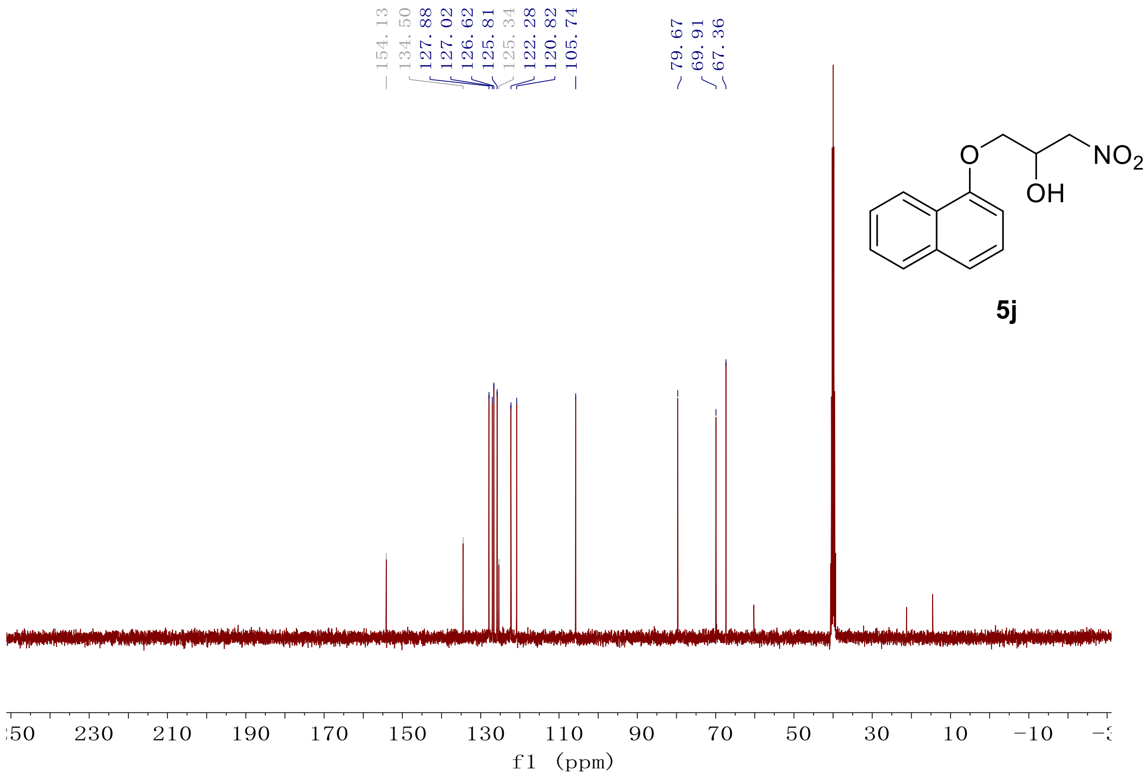

163.97
141.58
126.38
115.64
79.24
70.43
67.01
OH
O
NO2
O2N
5i
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)


NO2
O
O
4j
0.96
0.98
2.99
1.01
0.99
2.00
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


195.59
153.22
134.59
127.98
127.15
126.42
126.09
125.15
122.14
121.49
106.19
82.97
71.72
NO2
O
O
4j
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

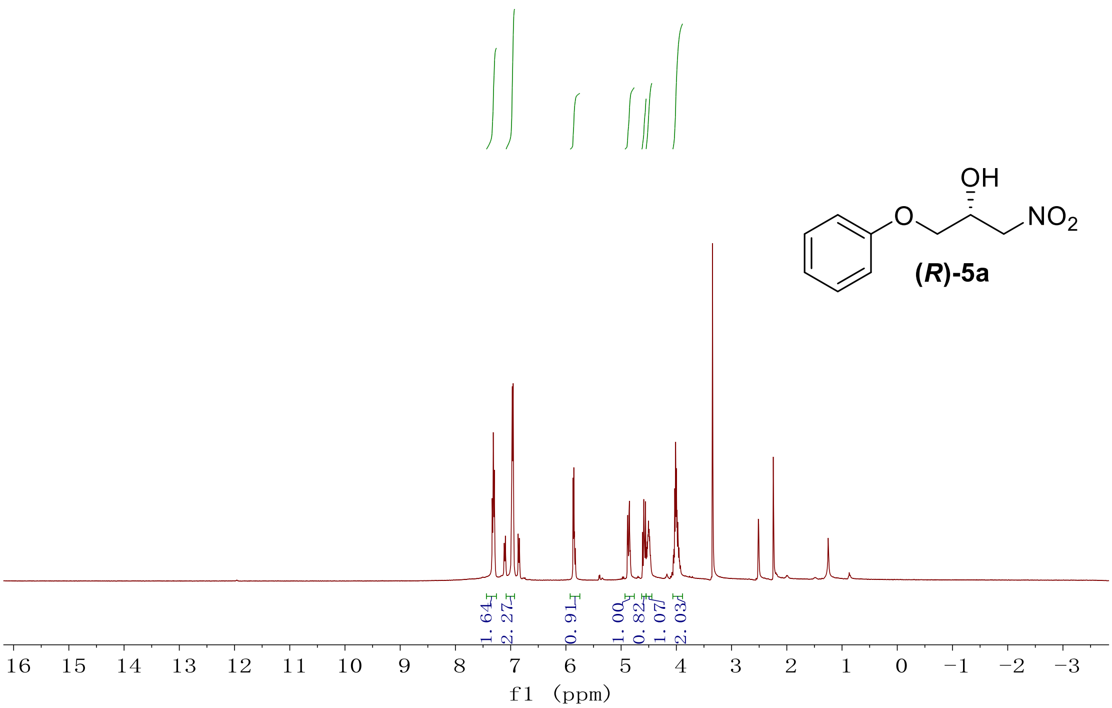


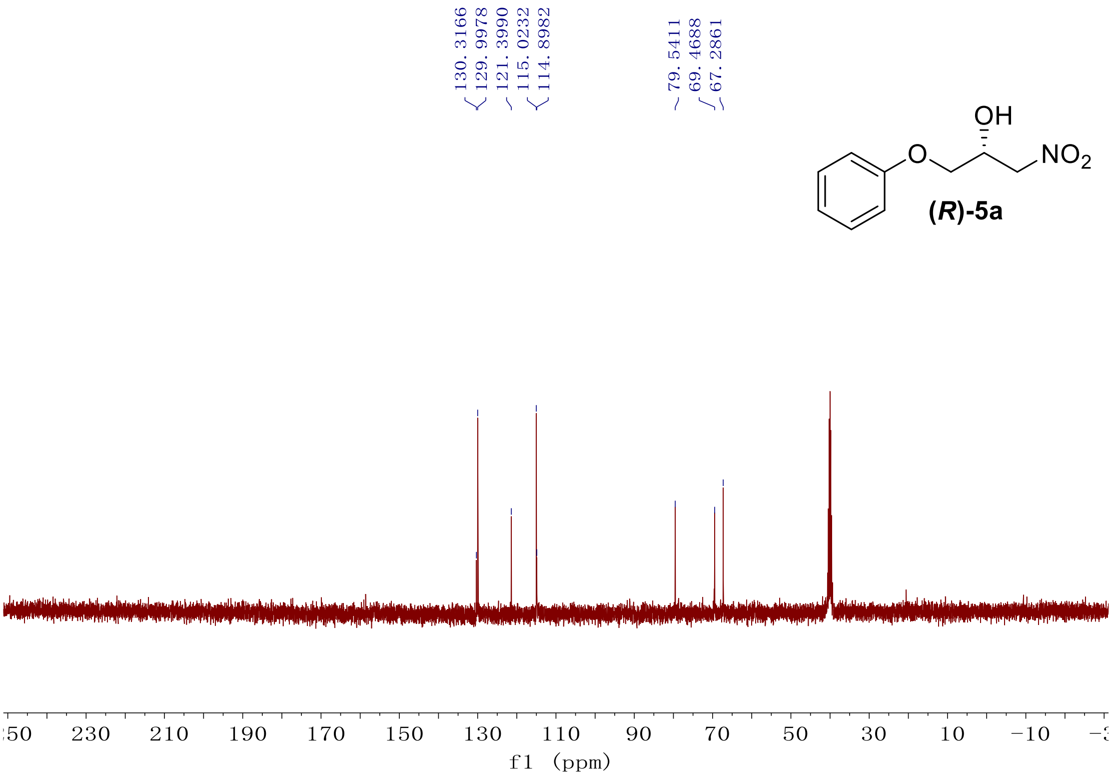
0.96
0.99
2.95
1.07
1.02
0.99
1.00
0.95
0.93
2.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
NO2
OH
O
5j

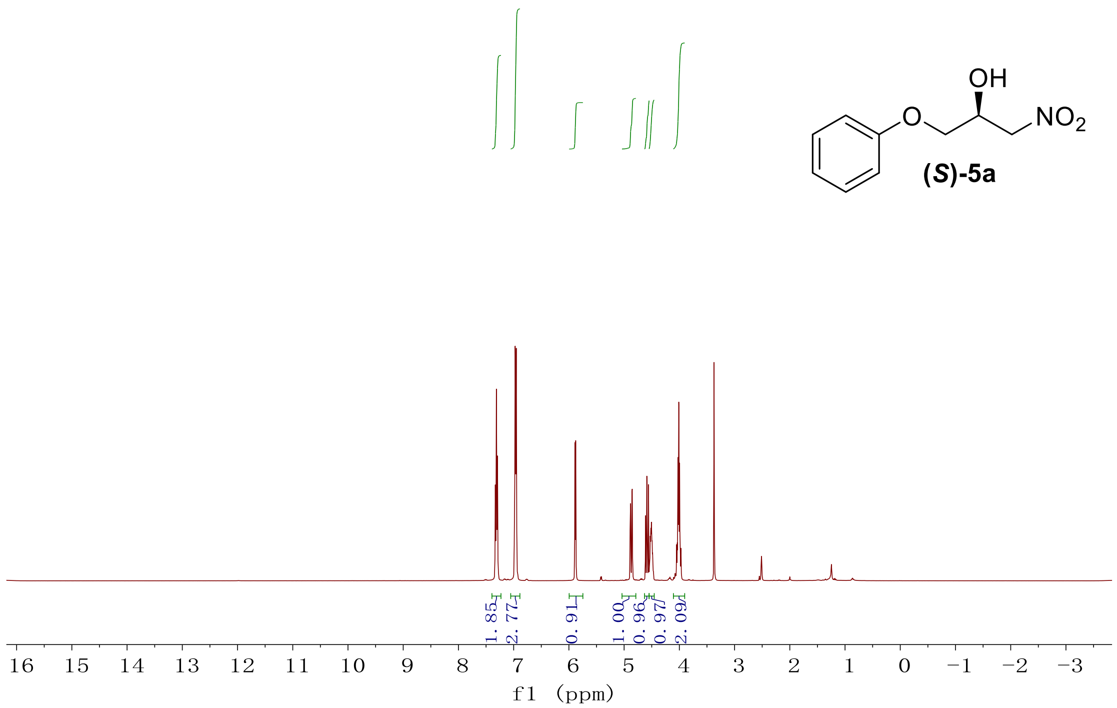


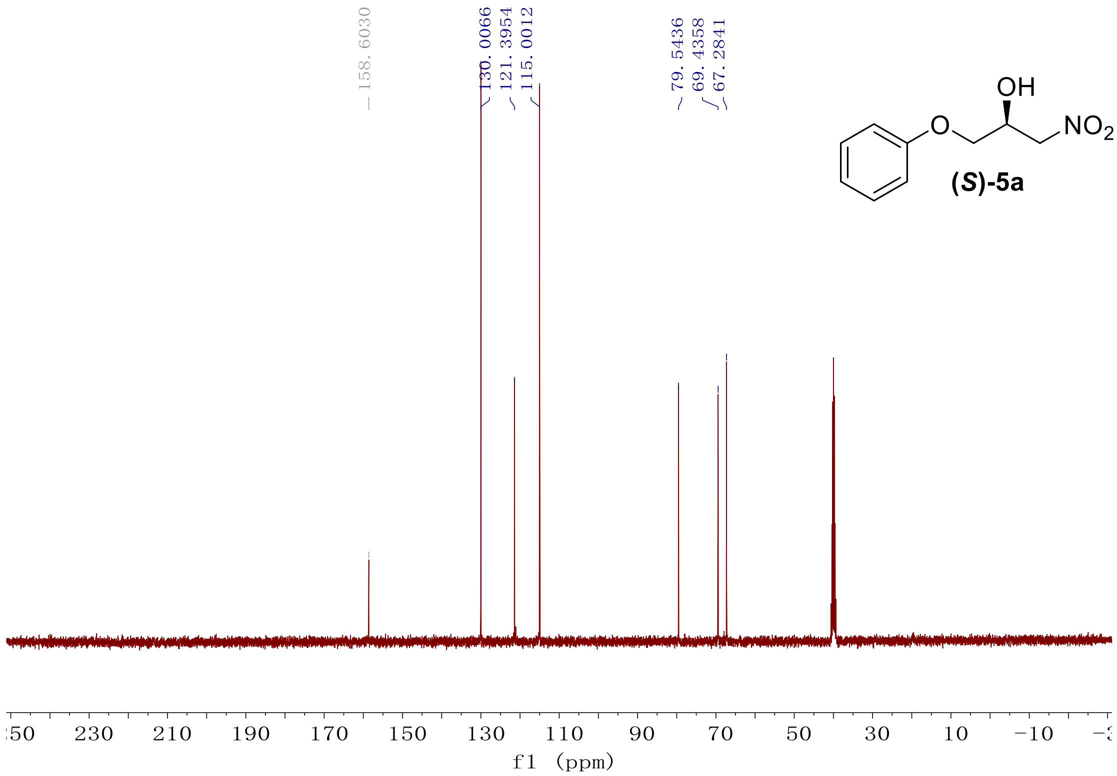
154.13
134.50
127.88
127.02
126.62
125.81
125.34
122.28
120.82
105.74
79.67
69.91
67.36
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)
NO2
OH
O
5j

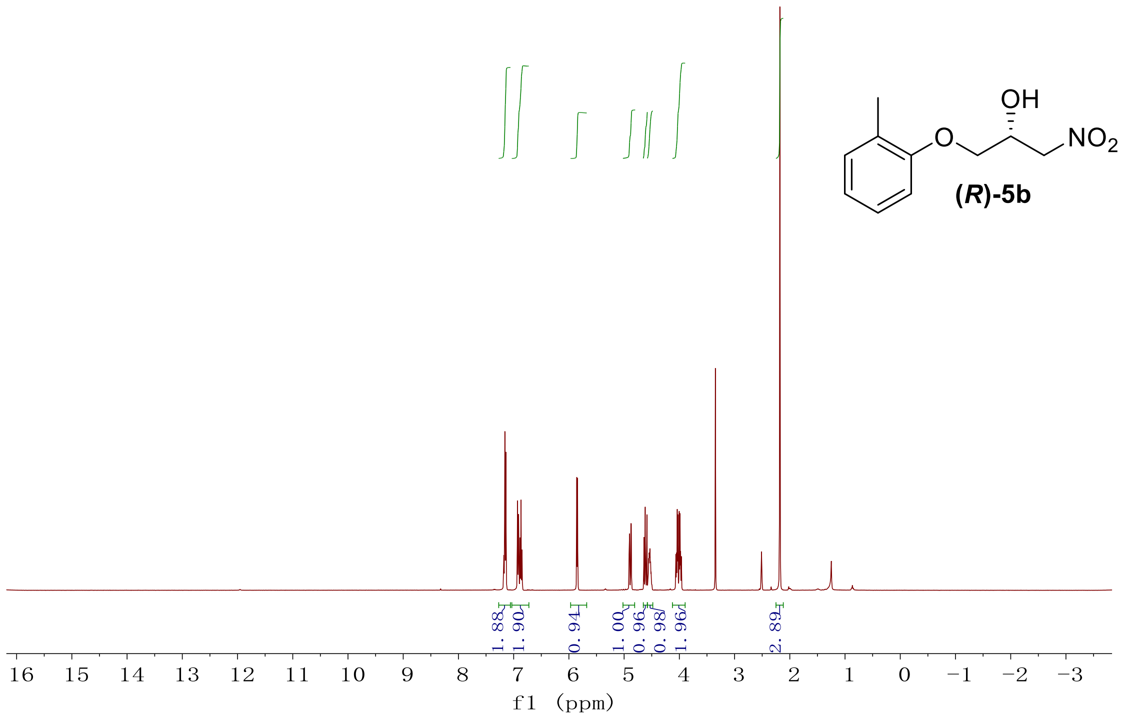
NMR of the products from CFE catalyzed preparative scale reactions



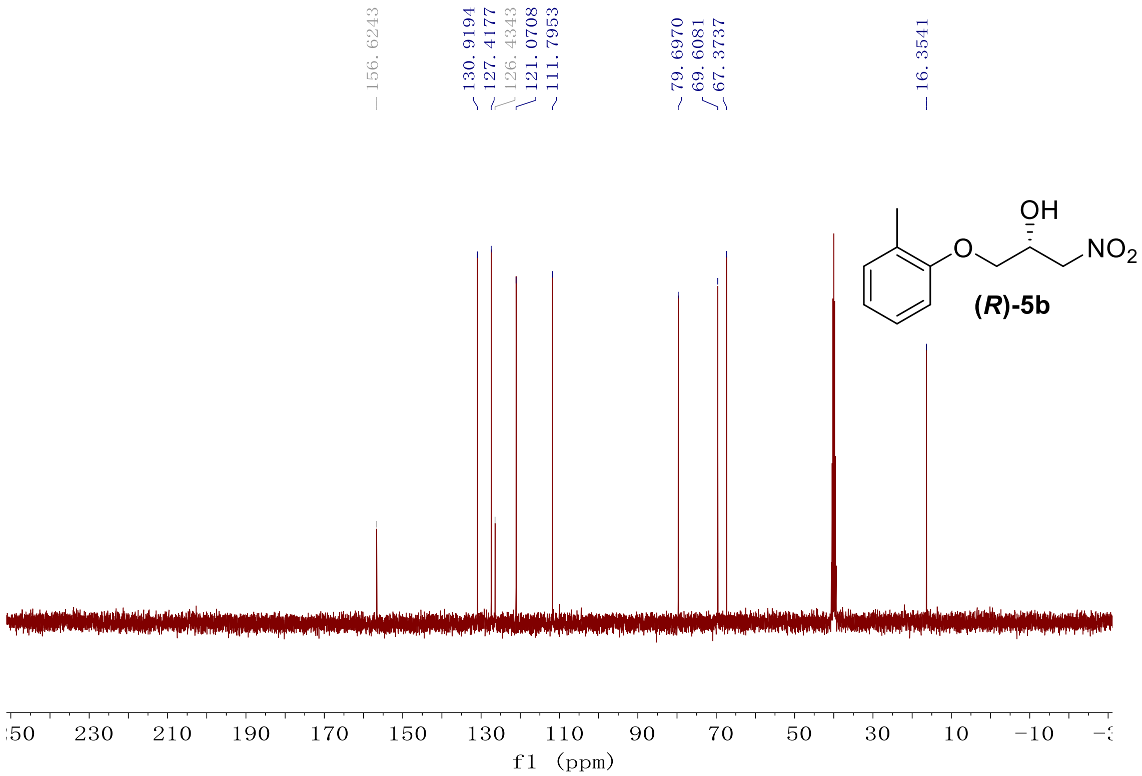



OH
O
NO2
(S)-5a
1.85
2.77
0.91
1.00
0.96
0.97
2.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

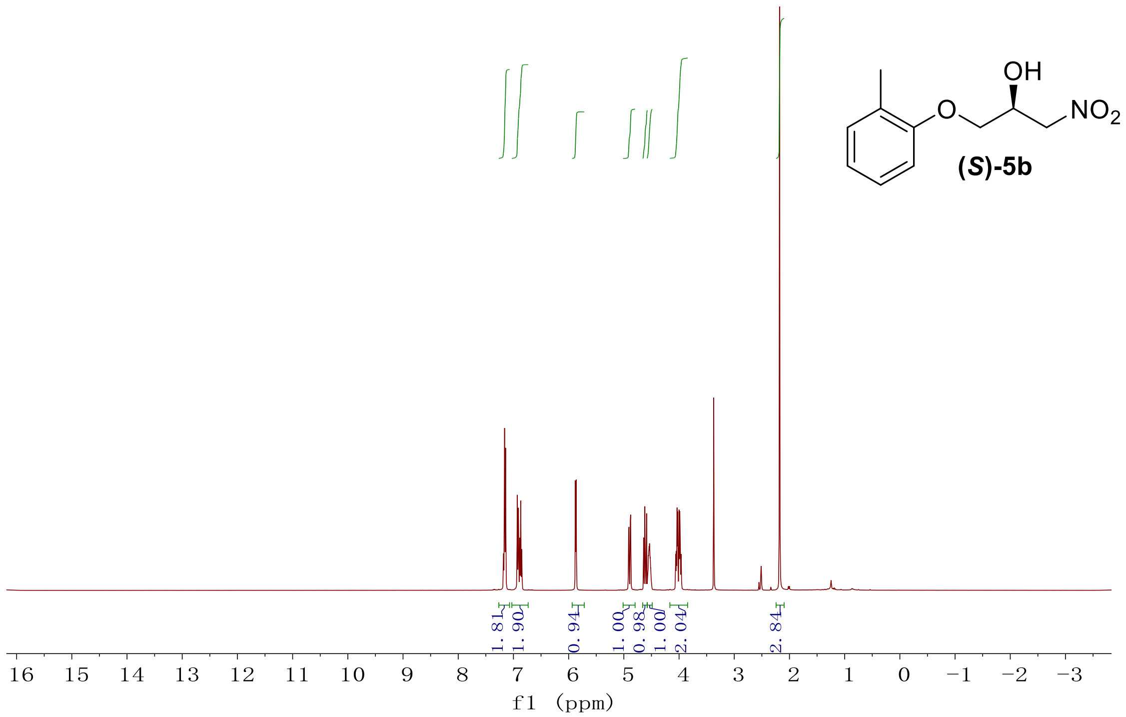

158.6030
130.0066
121.3954
115.0012
79.5436
69.4358
67.2841
OH
O
NO2
(S)-5a
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)



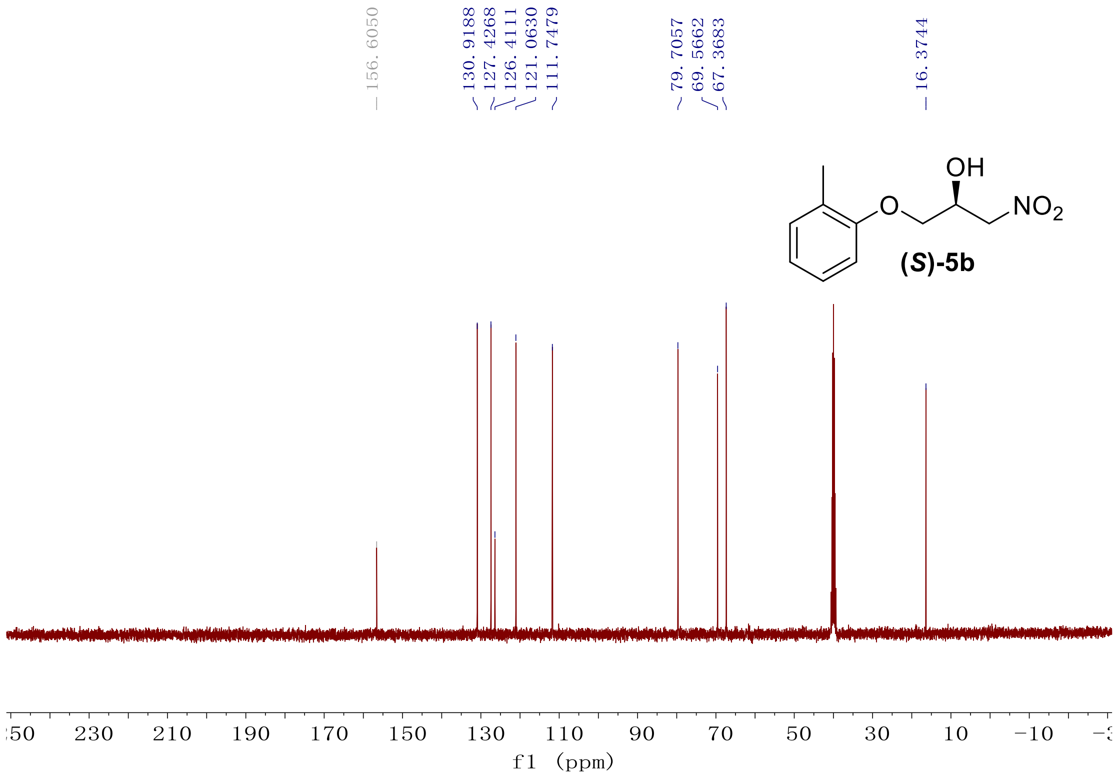
OH
O
NO2
(R)-5b
1.88
1.90
0.94
1.00
0.96
0.98
1.96
2.89
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)



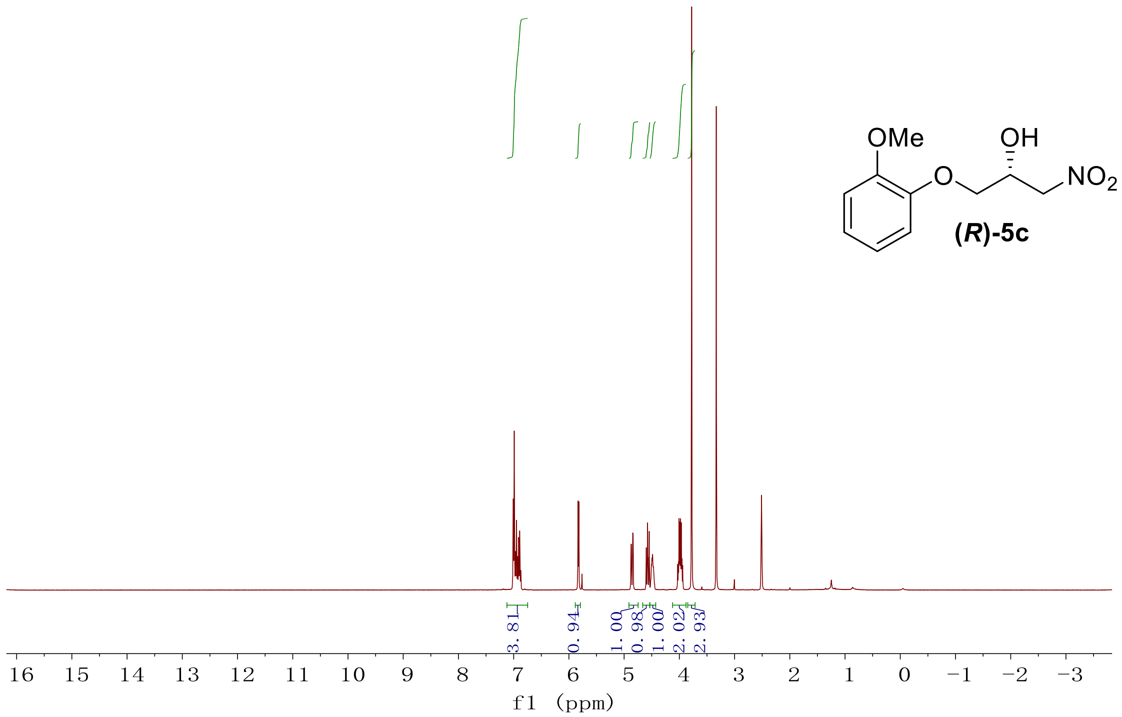
156.6243
130.9194
127.4177
126.4343
121.0708
111.7953
79.6970
69.6081
67.3737
16.3541
OH
O
NO2
(R)-5b
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

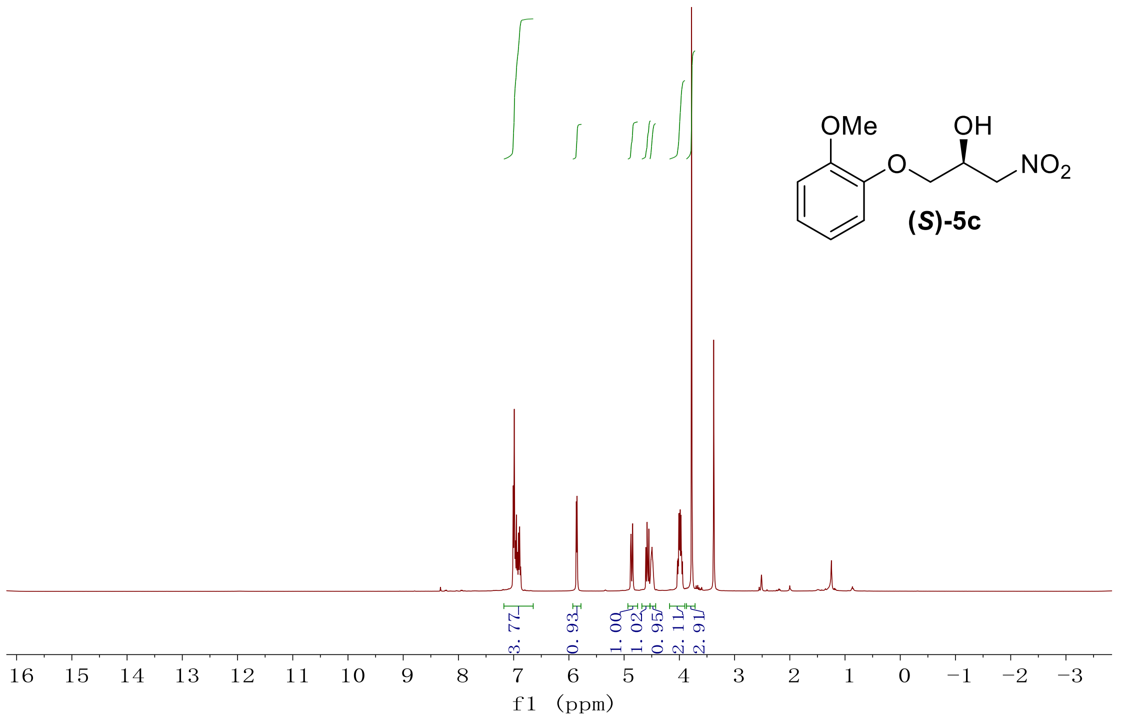


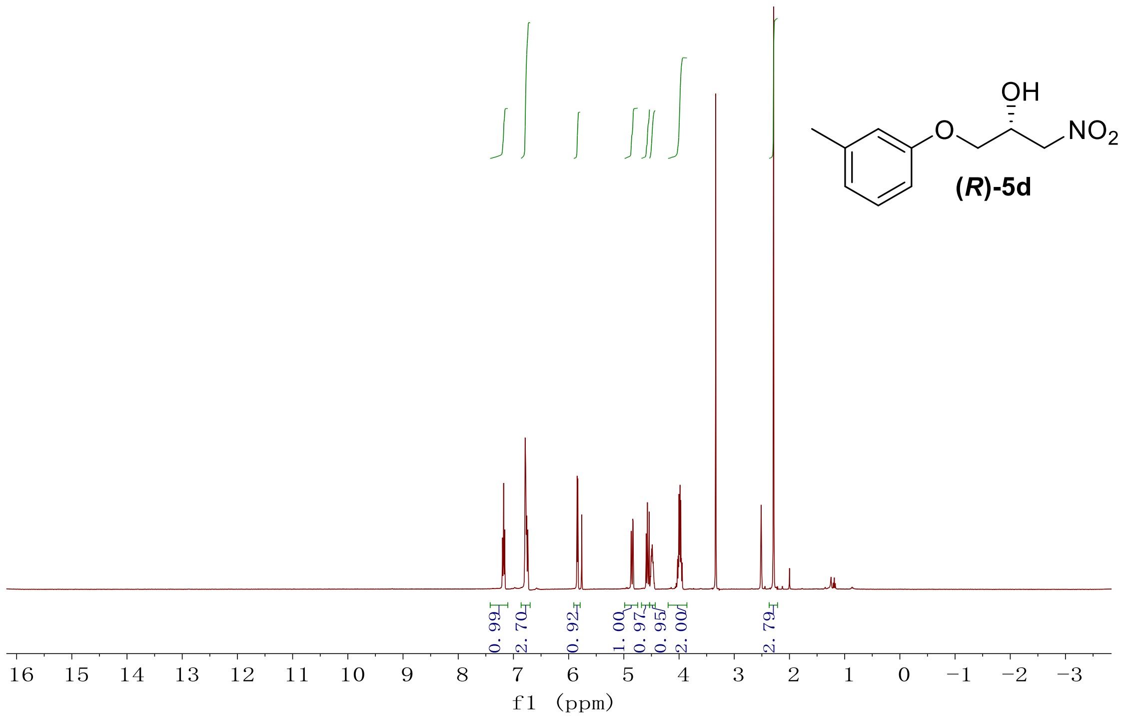
OH
O
NO2
(S)-5b
1.81
1.90
0.94
1.00
0.98
1.00
2.04
2.84
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

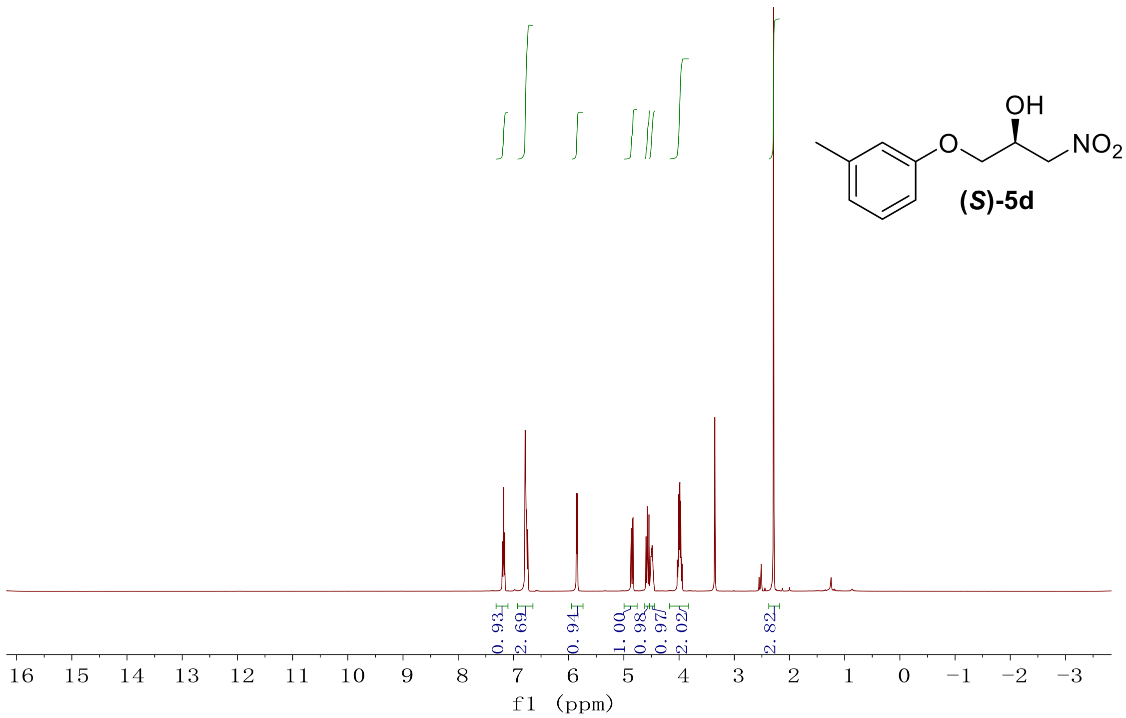


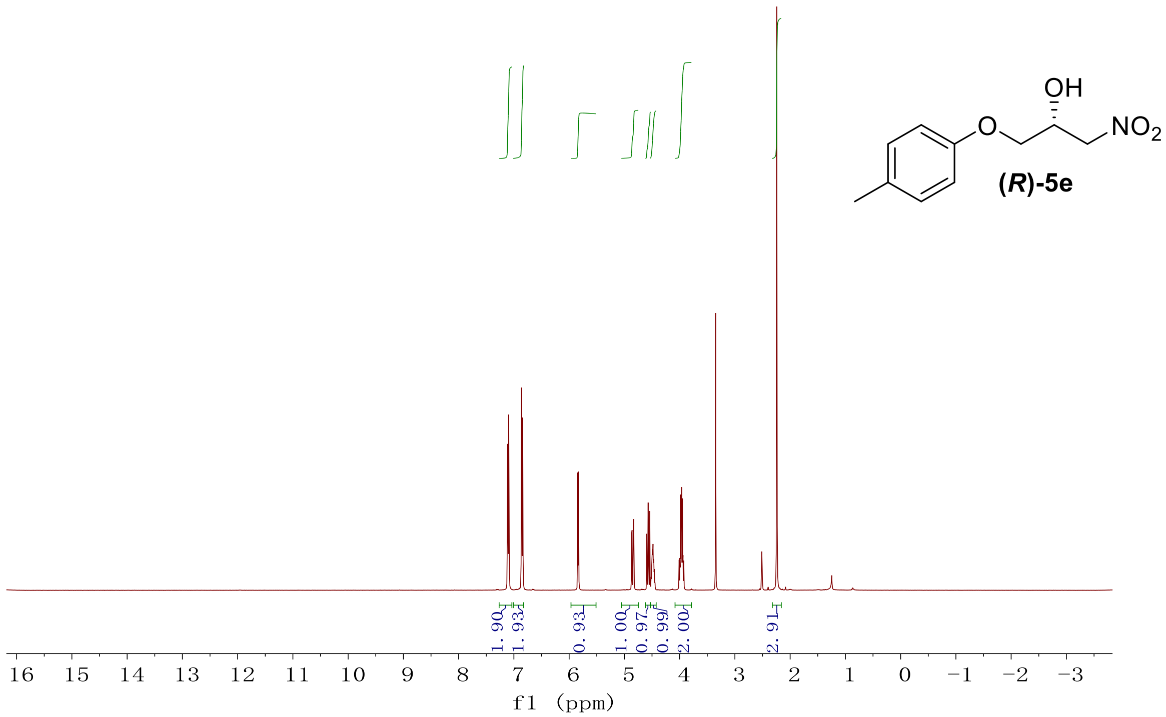
156.6050
130.9188
127.4268
126.4111
121.0630
111.7479
79.7057
69.5662
67.3683
16.3744
OH
O
NO2
(S)-5b
250 230 210 190 170 150 130 110 90 70 50 30 10 −10 −30
f1 (ppm)

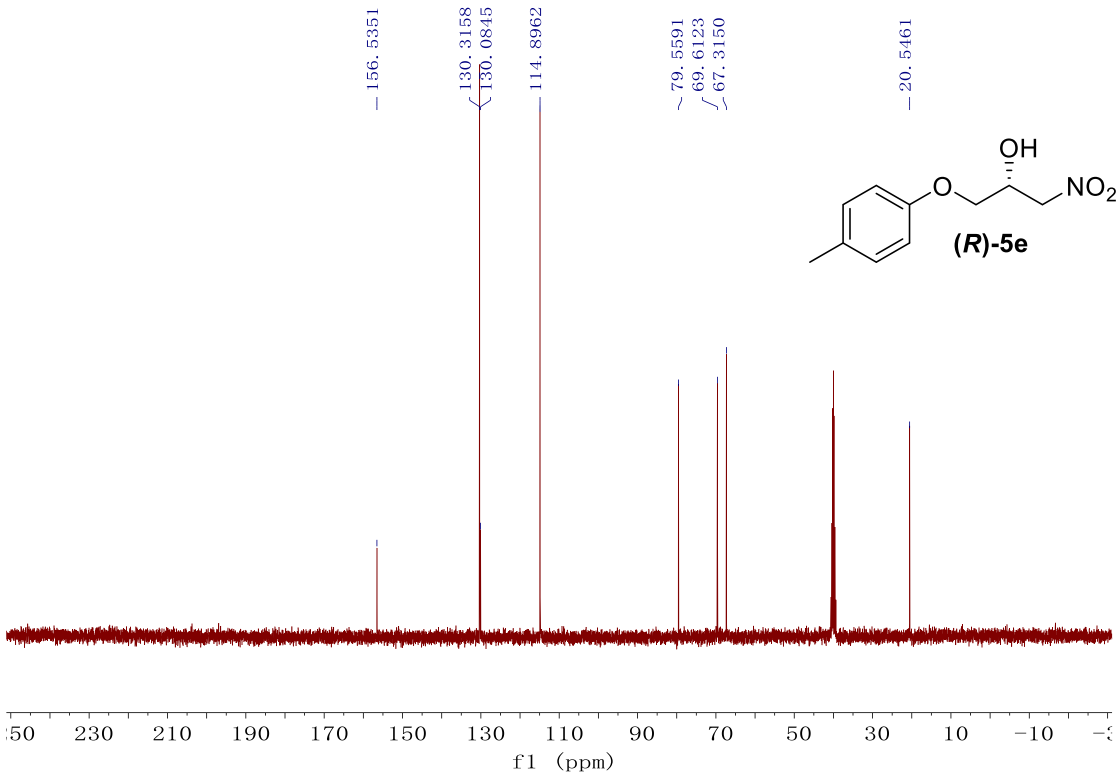

OMe
OH
O
NO2
(R)-5c
3.81
0.94
1.00
0.98
1.00
2.02
2.93
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

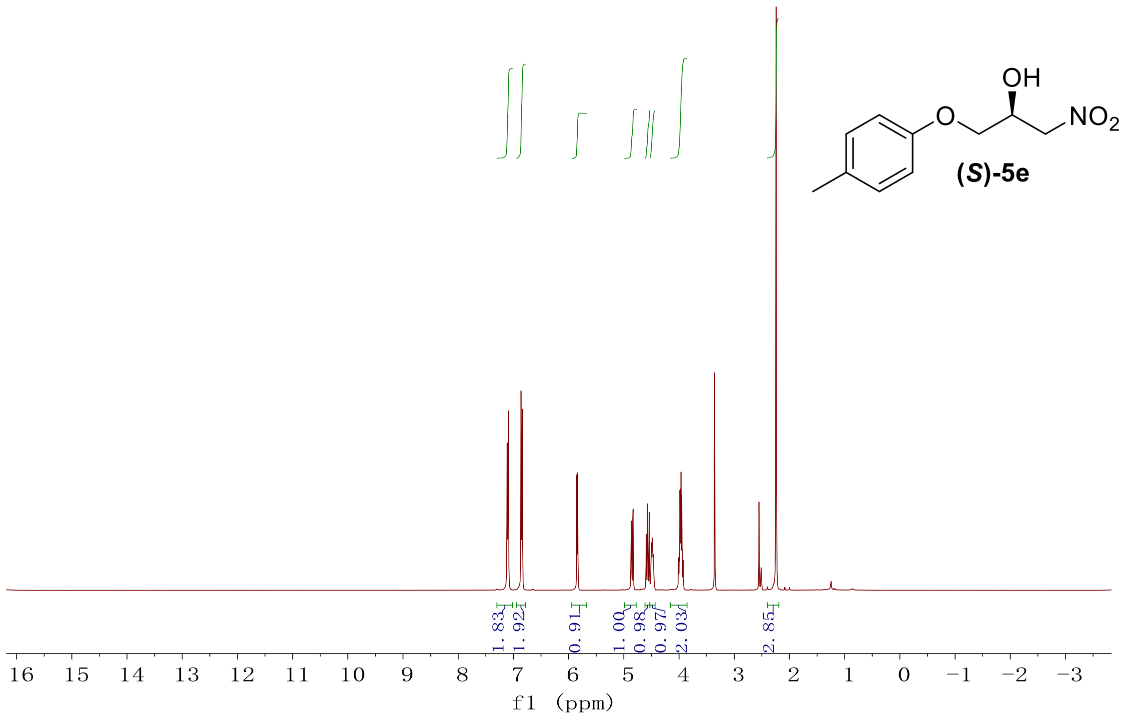

OMe
OH
O
NO2
(S)-5c
3.77
0.93
1.00
1.02
0.95
2.11
2.91
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

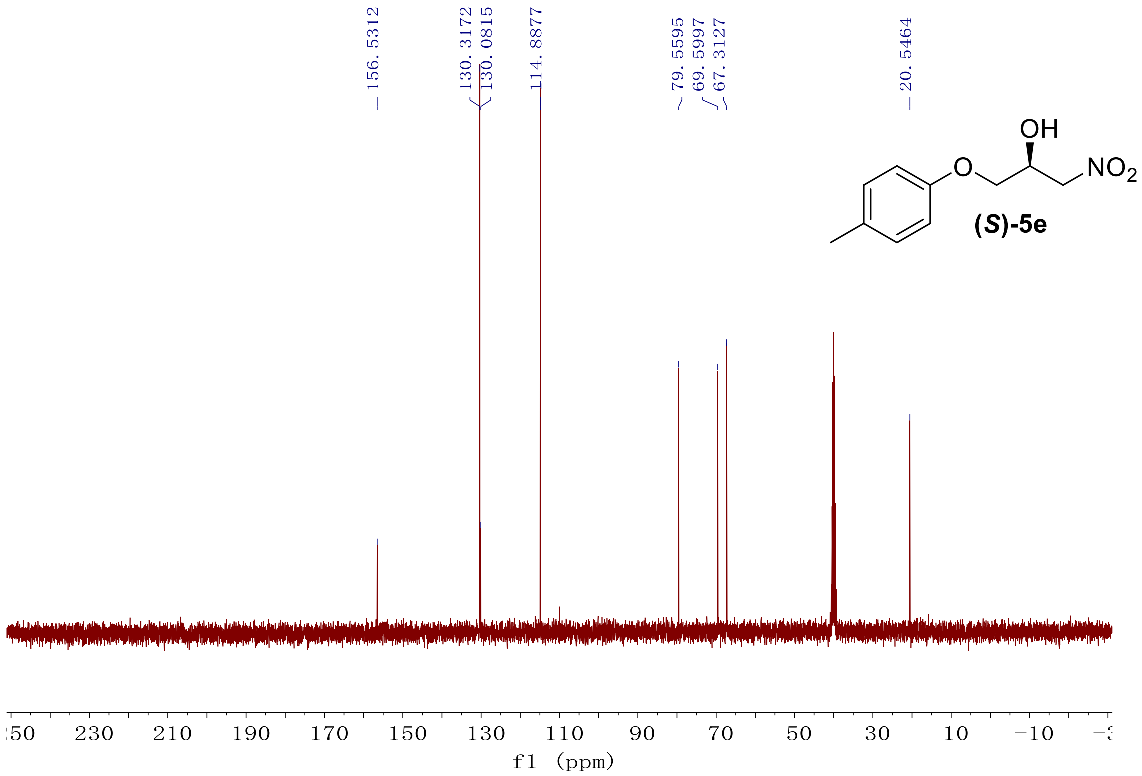

OH
O
NO2
(R)-5d
0.99
2.70
0.92
1.00
0.97
0.95
2.00
2.79
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

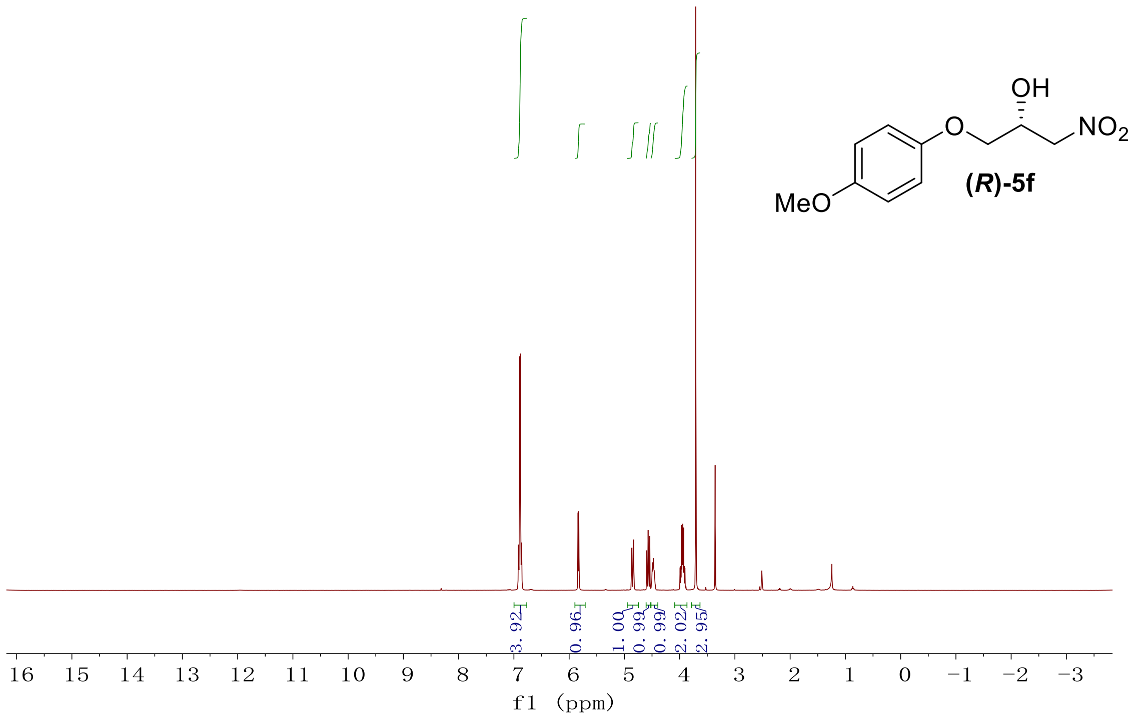

OH
O
NO2
(S)-5d
0.93
2.69
0.94
1.00
0.98
0.97
2.02
2.82
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

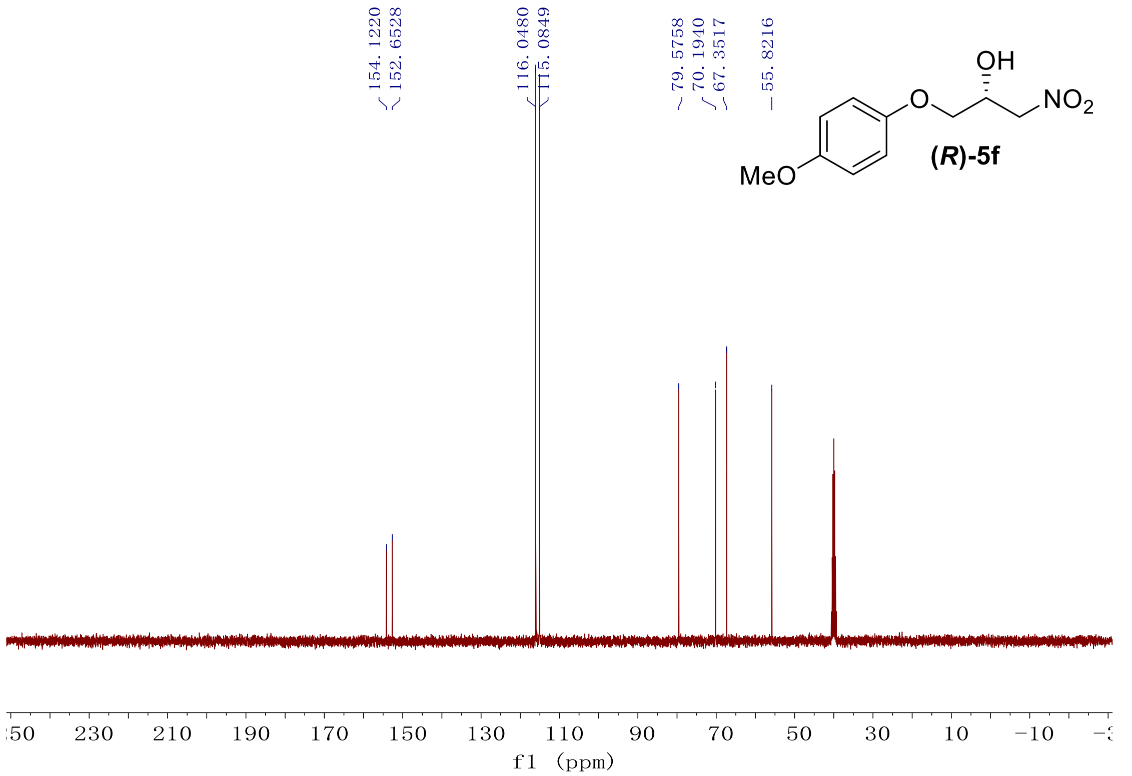

OH
O
NO2
(R)-5e
1.90
1.93
0.93
1.00
0.97
0.99
2.00
2.91
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

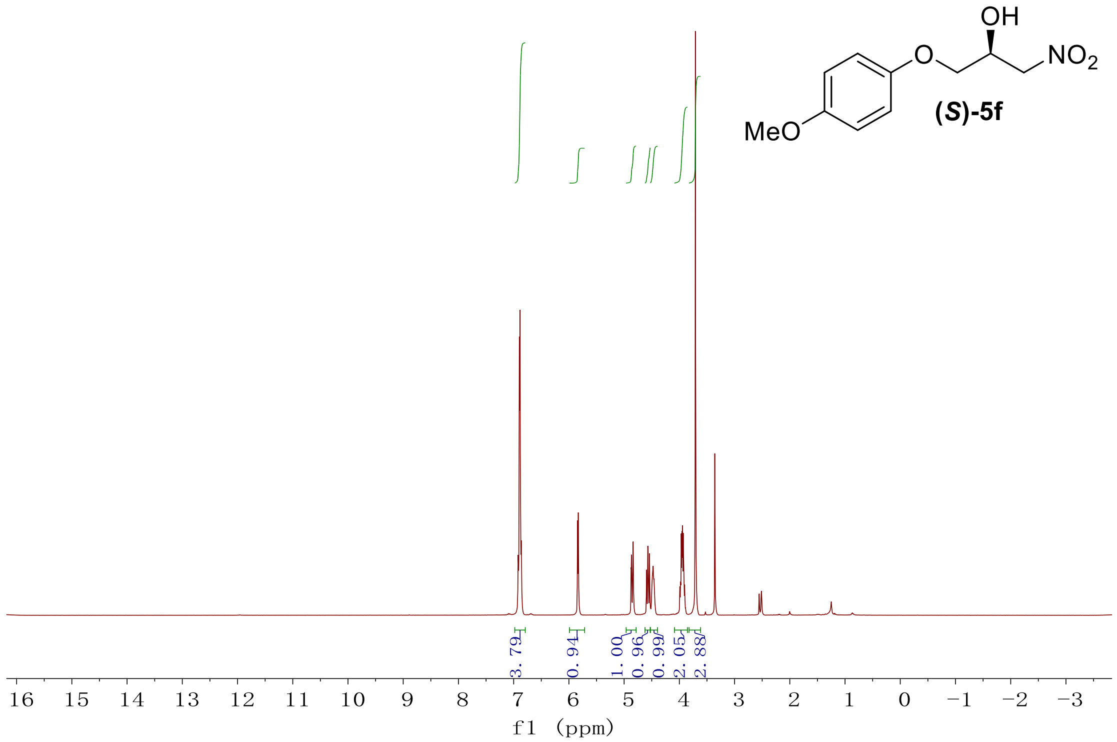

156.5351
130.3158
130.0845
114.8962
79.5591
69.6123
67.3150
20.5461
OH
O
NO2
(R)-5e
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

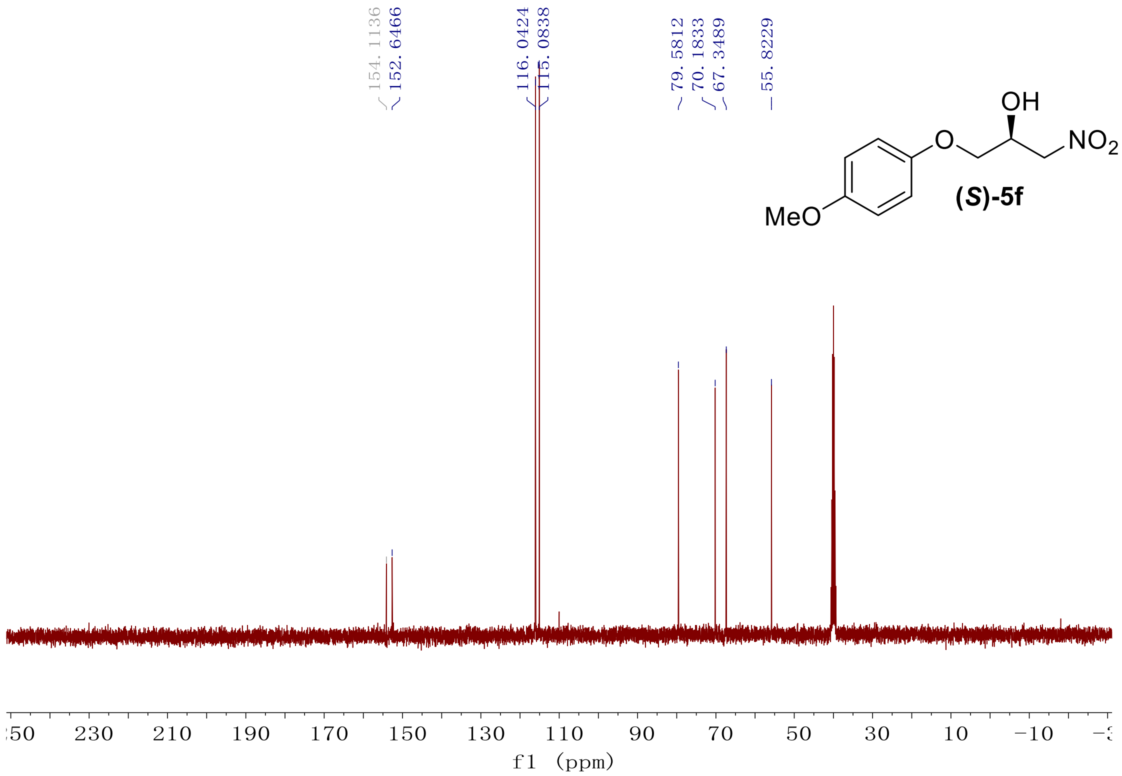

OH
O
NO_2
(S)-5e
1.83
1.92
0.91
1.00
0.98
0.97
2.03
2.85
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

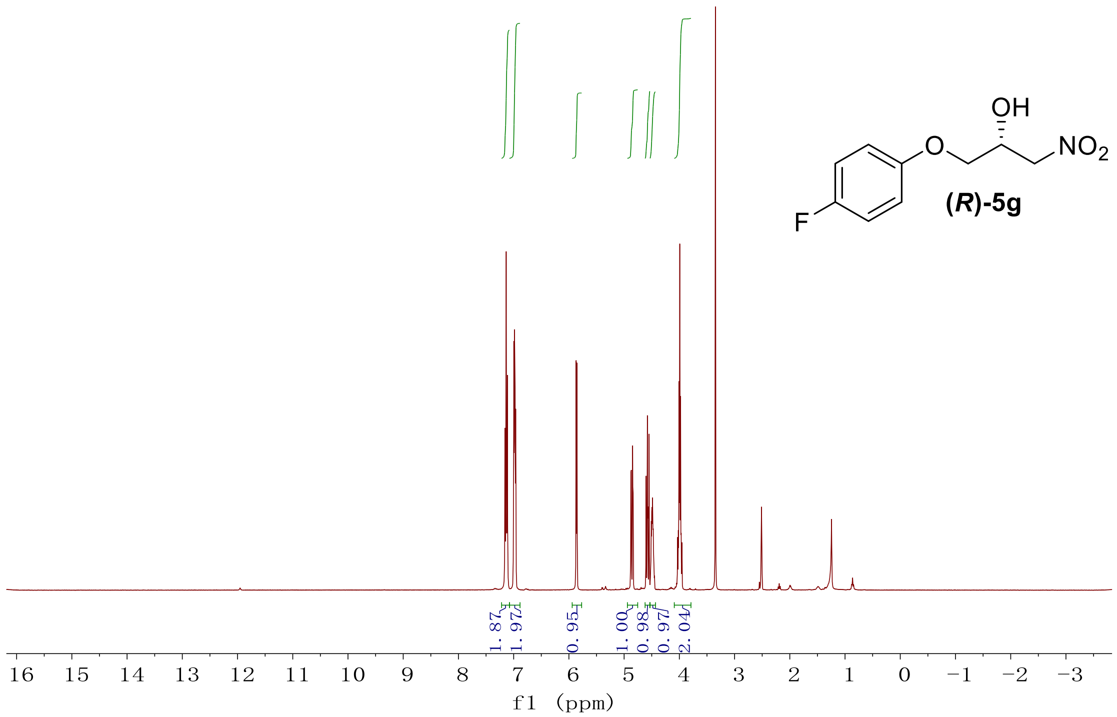

156.5312
130.3172
130.0815
114.8877
79.5595
69.5997
67.3127
20.5464
OH
O
NO_2
(S)-5e
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

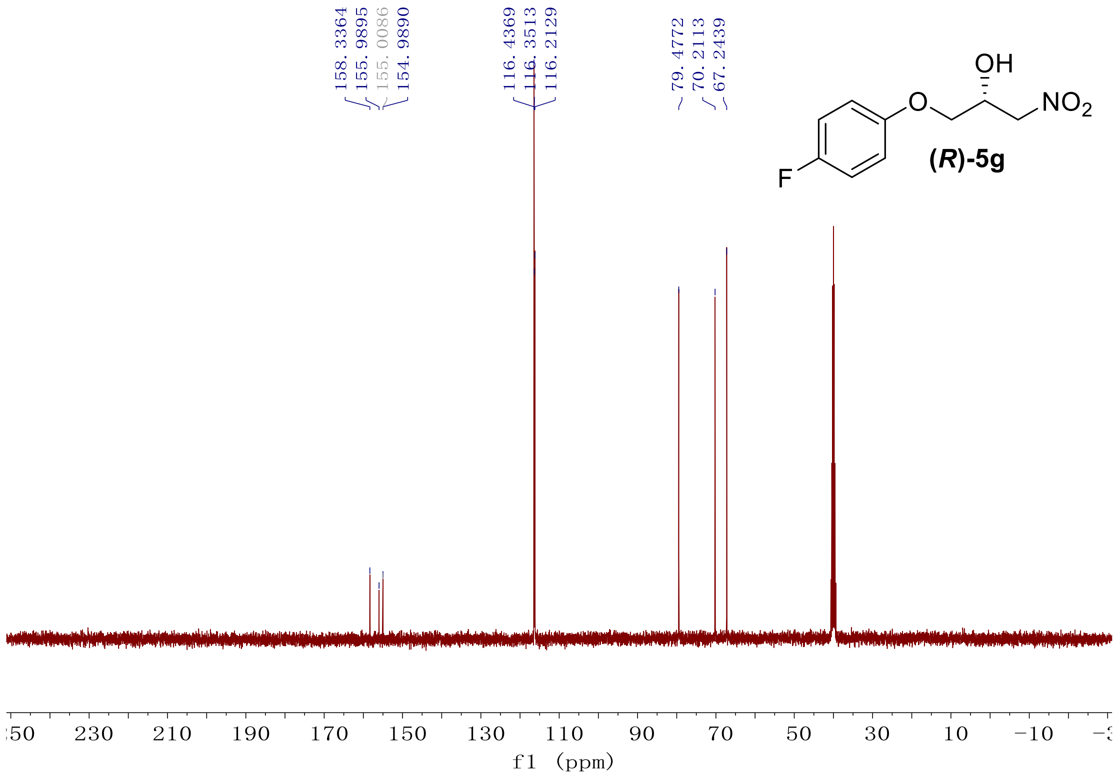

OH
O
NO2
MeO
(R)-5f
3.92
0.96
1.00
0.99
0.99
2.02
2.95
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

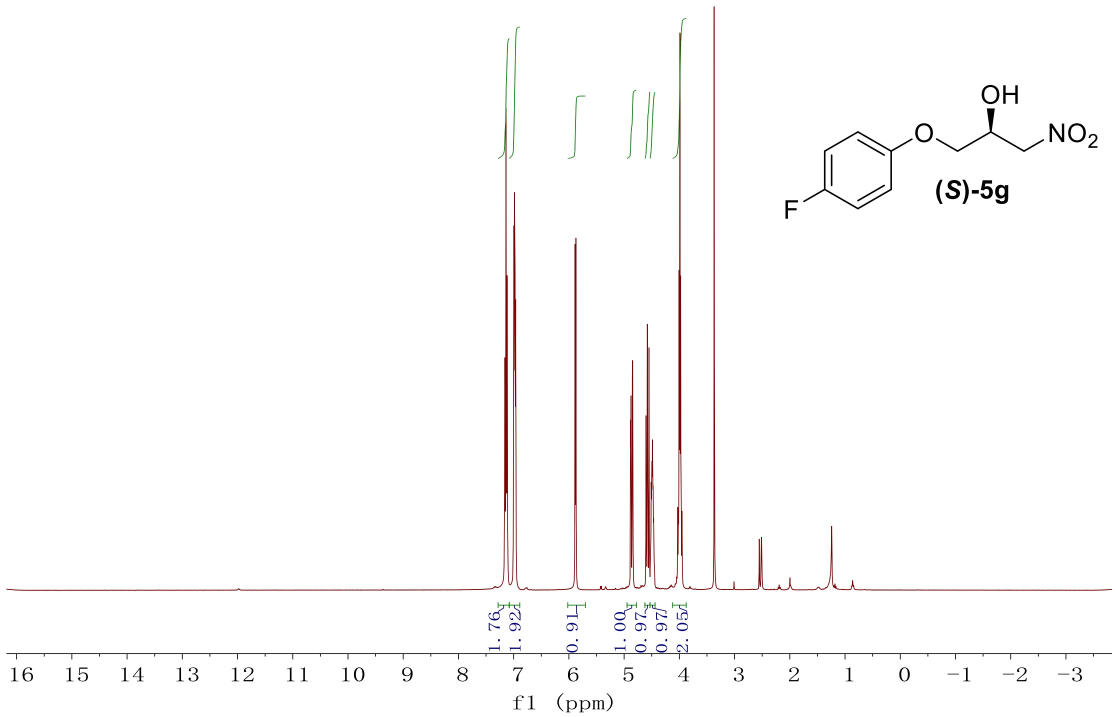

154.1220
152.6528
116.0480
115.0849
79.5758
70.1940
67.3517
55.8216
OH
O
NO2
MeO
(R)-5f
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

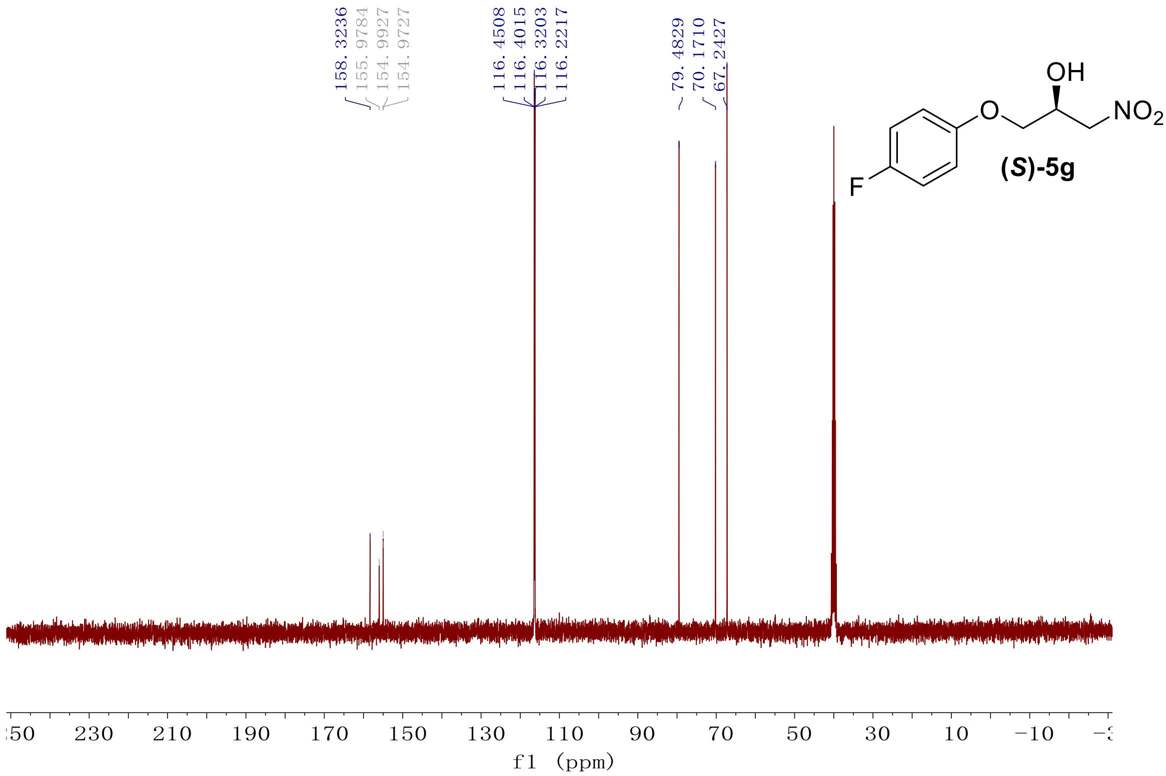

OH
O
NO2
MeO
(S)-5f
3.79
0.94
1.00
0.96
0.99
2.05
2.88
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

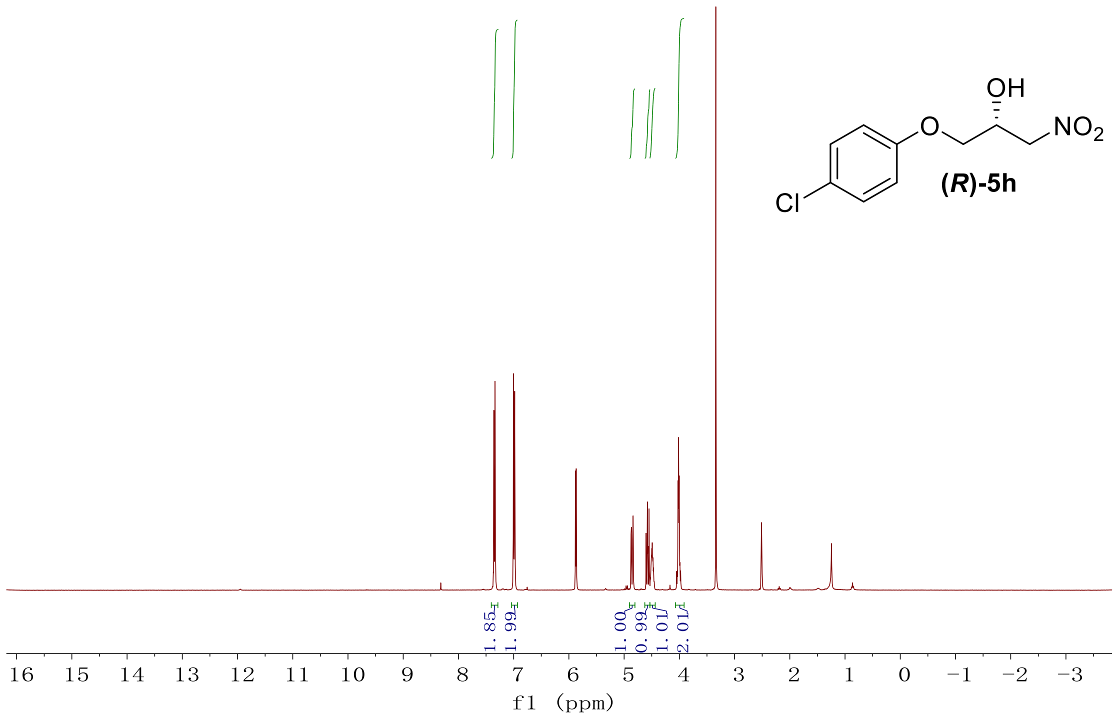

154.1136
152.6466
116.0424
115.0838
79.5812
70.1833
67.3489
55.8229
OH
O
NO2
MeO
(S)-5f
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

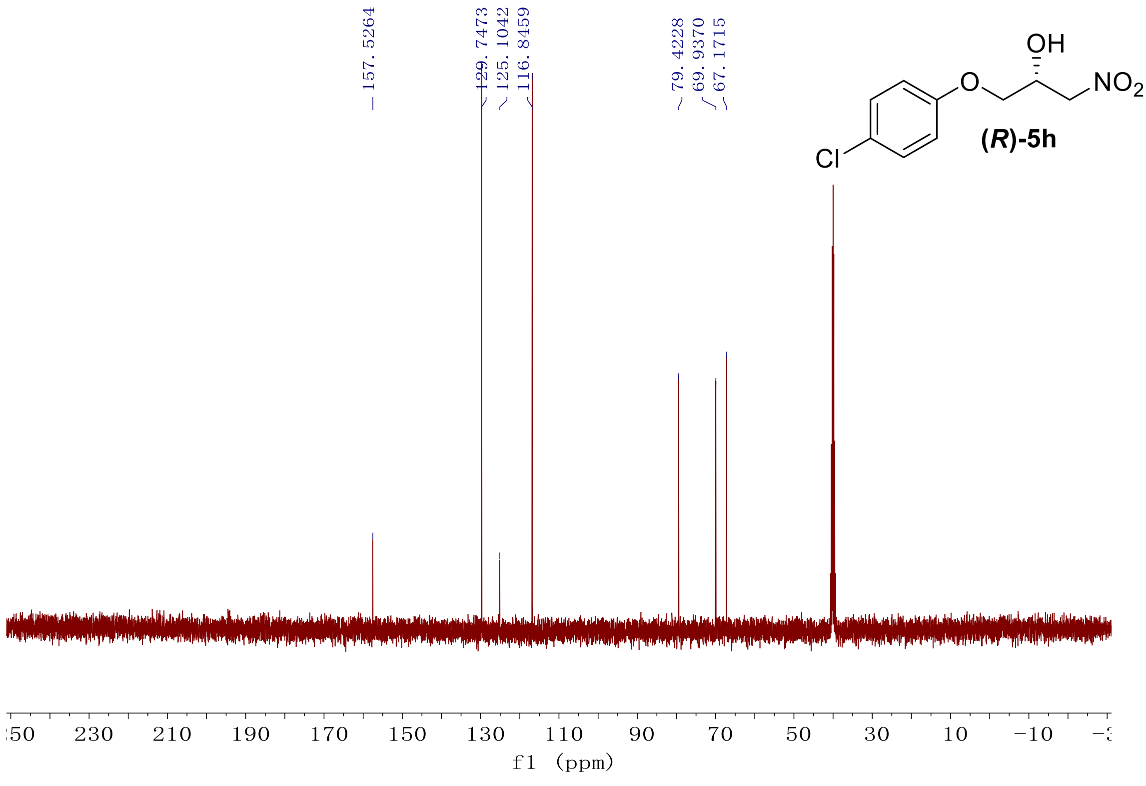

OH
O
NO_2
F
(*R*)-5g
1.87
1.97
0.95
1.00
0.98
0.97
2.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

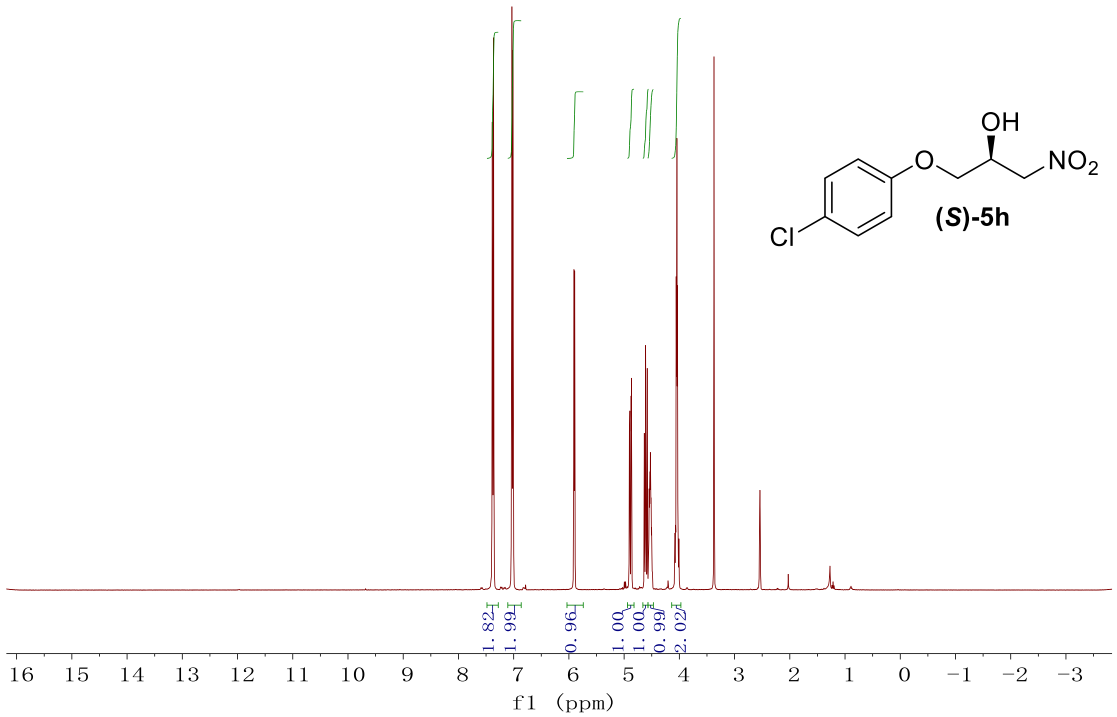

158.3364
155.9895
155.0086
154.9890
116.4369
116.3513
116.2129
79.4772
70.2113
67.2439
OH
O
NO_2
F
(*R*)-5g
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

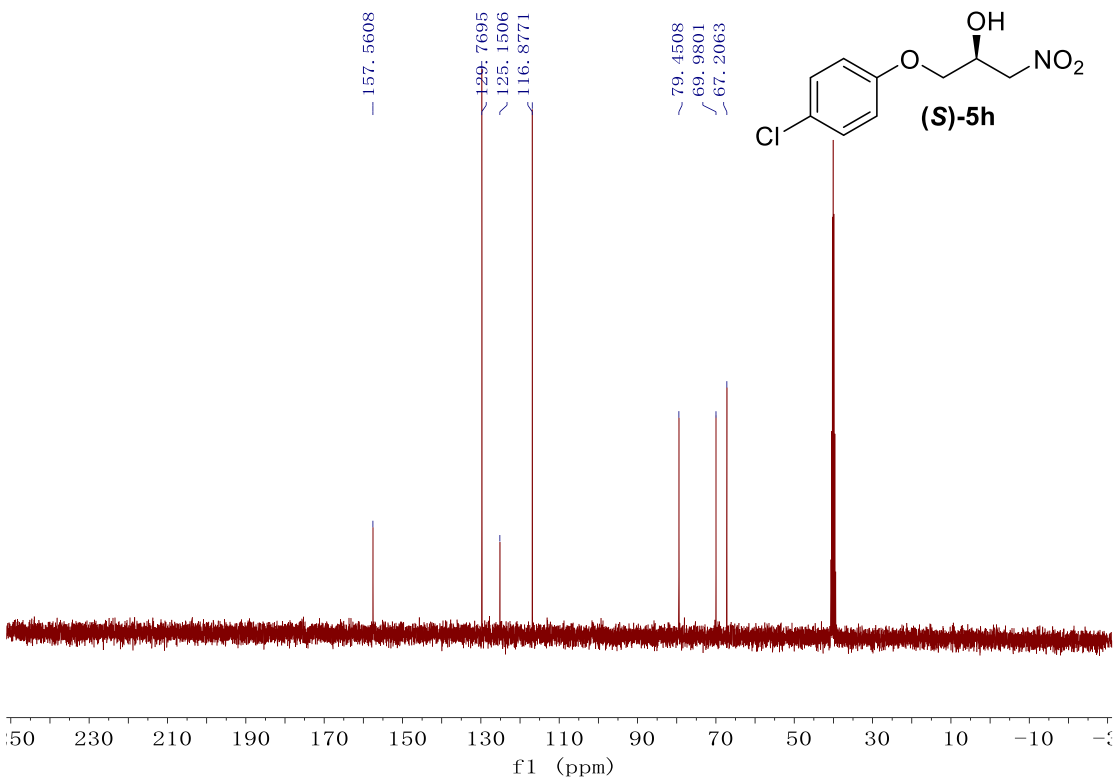

1.76
1.92
0.91
1.00
0.97
0.97
2.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)
OH
O
NO2
F
(S)-5g

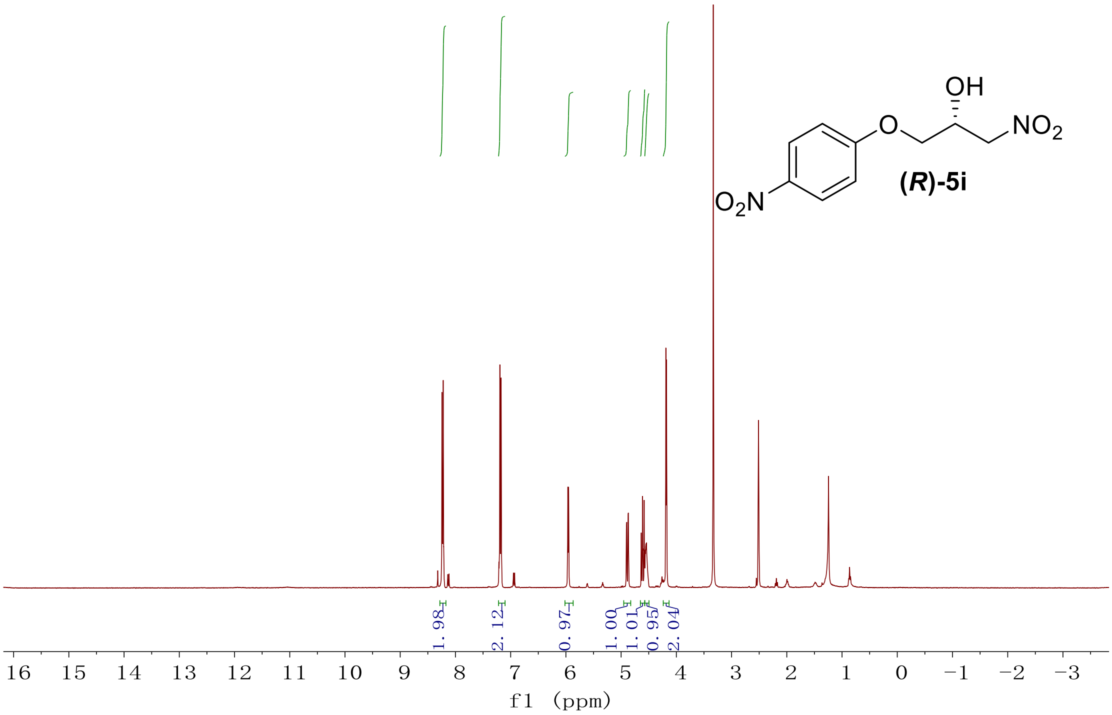

158.3236
155.9784
154.9927
154.9727
116.4508
116.4015
116.3203
116.2217
79.4829
70.1710
67.2427
OH
O
NO2
F
(S)-5g
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

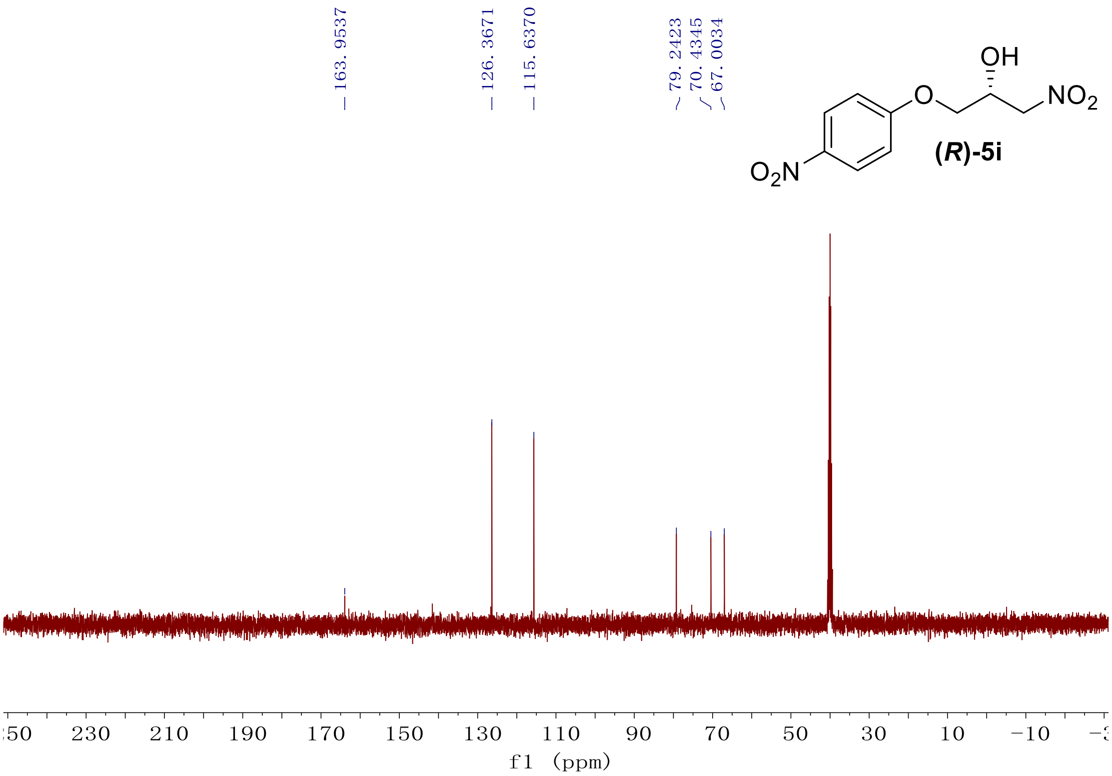

OH
O
NO2
Cl
(R)-5h
1.85
1.99
1.00
0.99
1.01
2.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

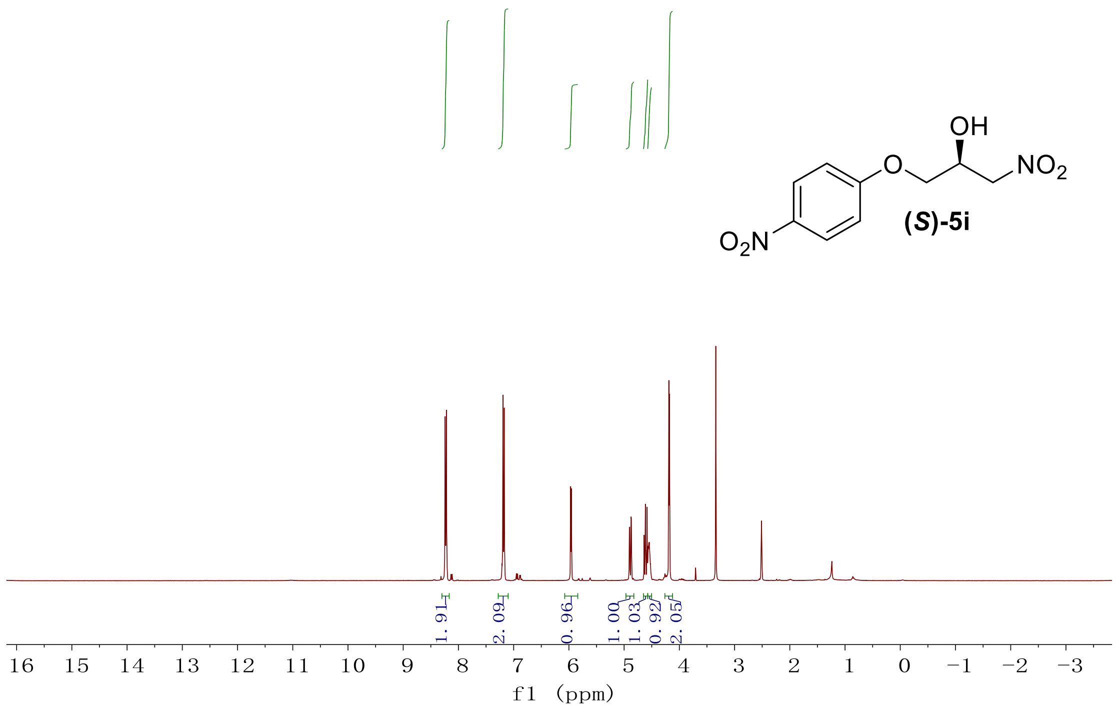

157.5264
129.7473
125.1042
116.8459
79.4228
69.9370
67.1715
OH
O
NO2
Cl
(R)-5h
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

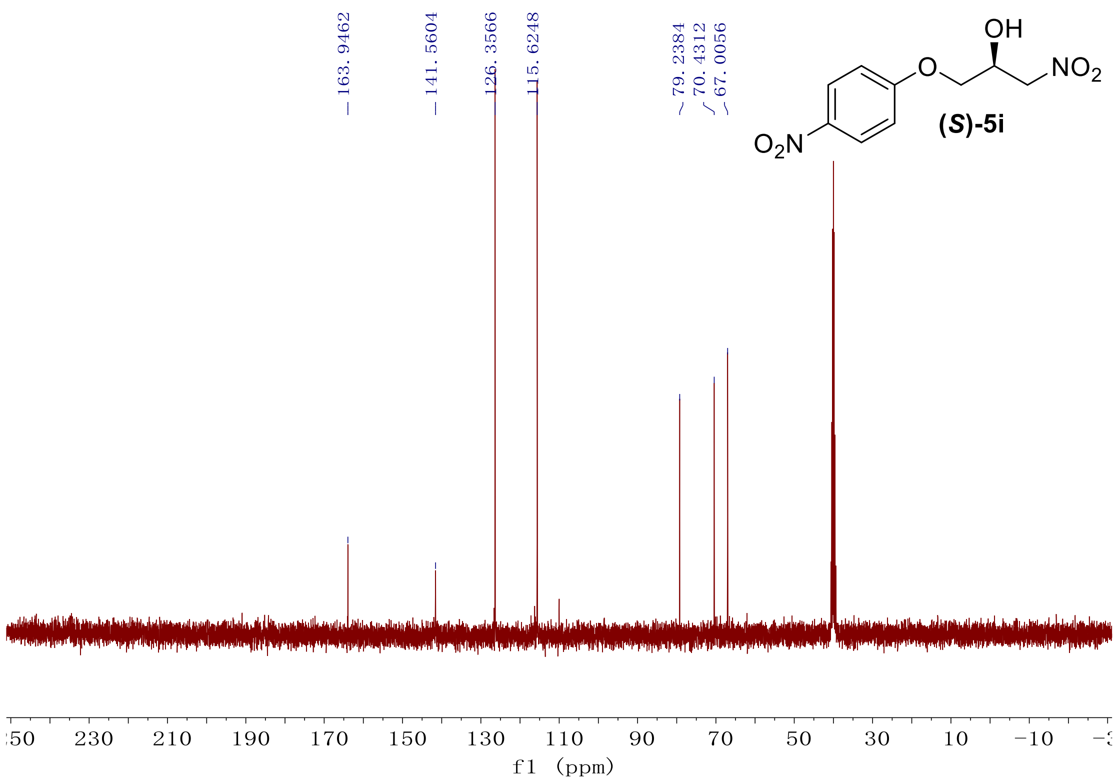

OH
O
NO2
Cl
(S)-5h
1.82
1.99
0.96
1.00
1.00
0.99
2.02
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

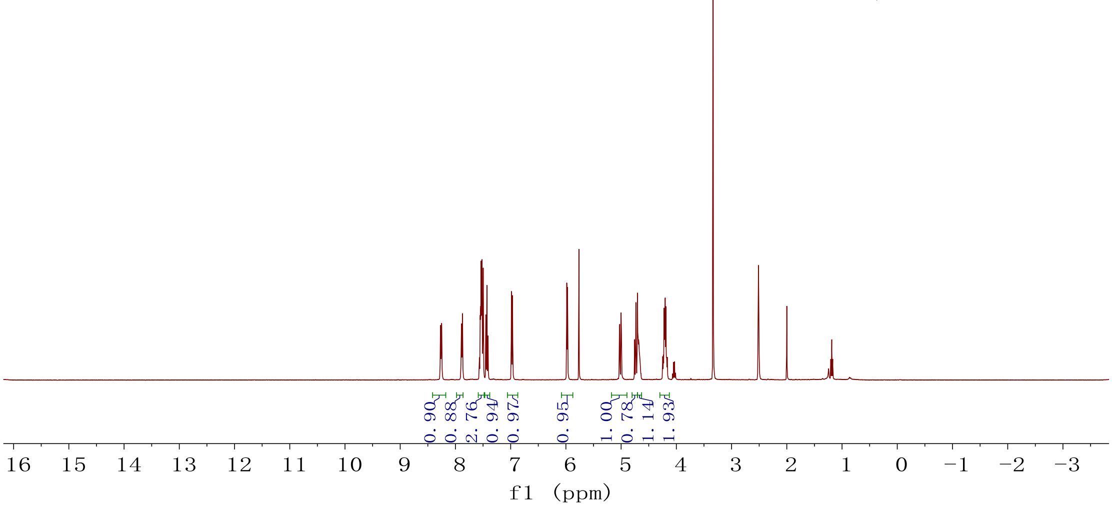

157.5608
129.7695
125.1506
116.8771
79.4508
69.9801
67.2063
OH
O
NO2
Cl
(S)-5h
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

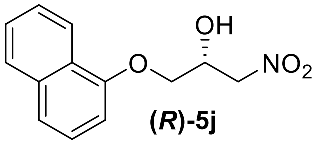

OH
O
NO2
O2N
(R)-5i
1.98
2.12
0.97
1.00
1.01
0.95
2.04
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)


163.9537
126.3671
115.6370
79.2423
70.4345
67.0034
OH
O
NO2
O2N
(R)-5i
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)

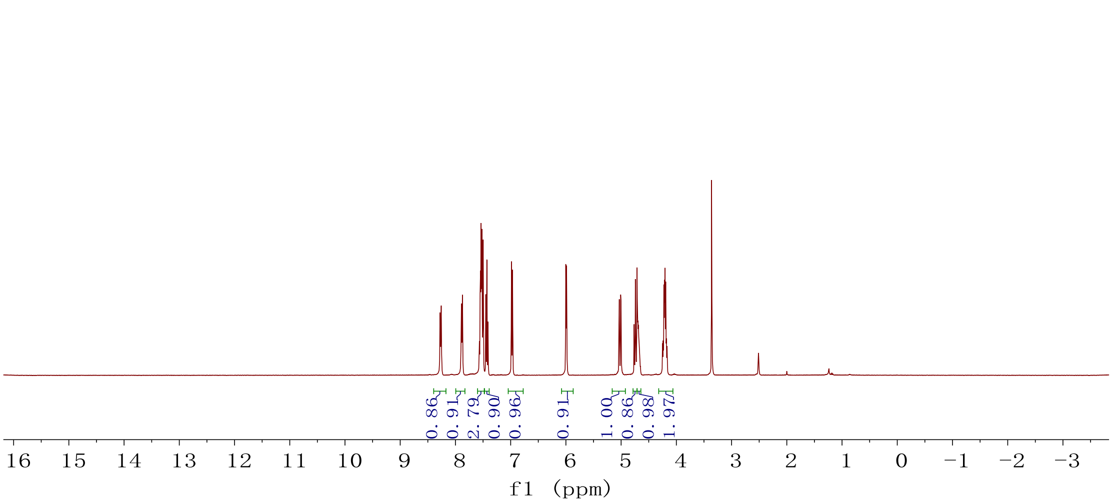

OH
O
NO_2
O_2N
(*S*)-5i
1.91
2.09
0.96
1.00
1.03
0.92
2.05
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)

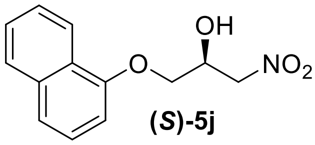

163.9462
141.5604
126.3566
115.6248
79.2384
70.4312
67.0056
OH
O
NO_2
O_2N
(*S*)-5i
230 210 190 170 150 130 110 90 70 50 30 10 −10
f1 (ppm)





(*R*)-5j



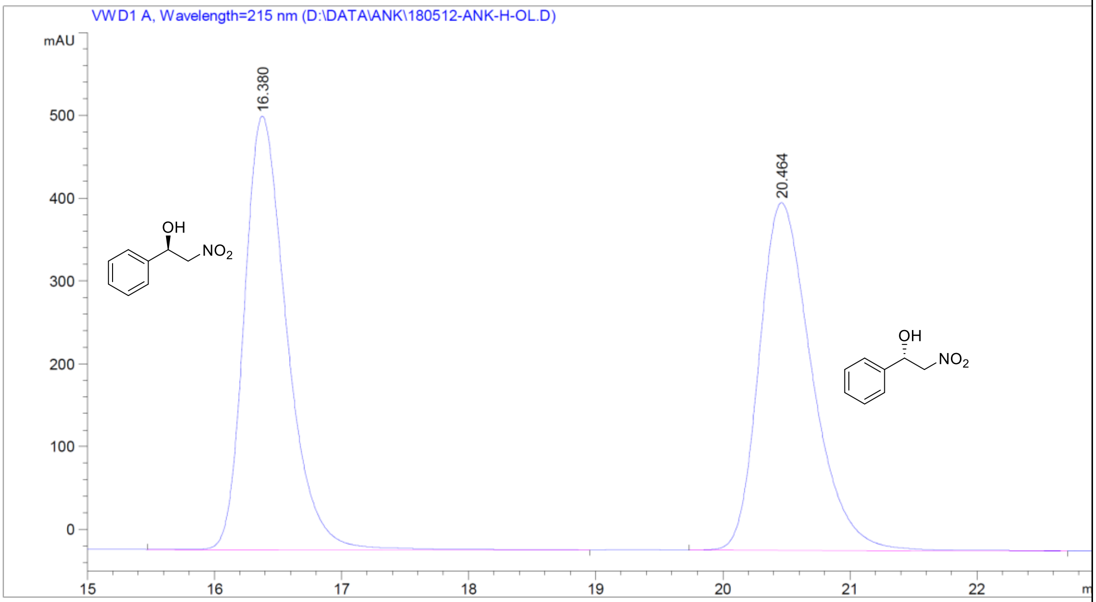


(*S*)-5j

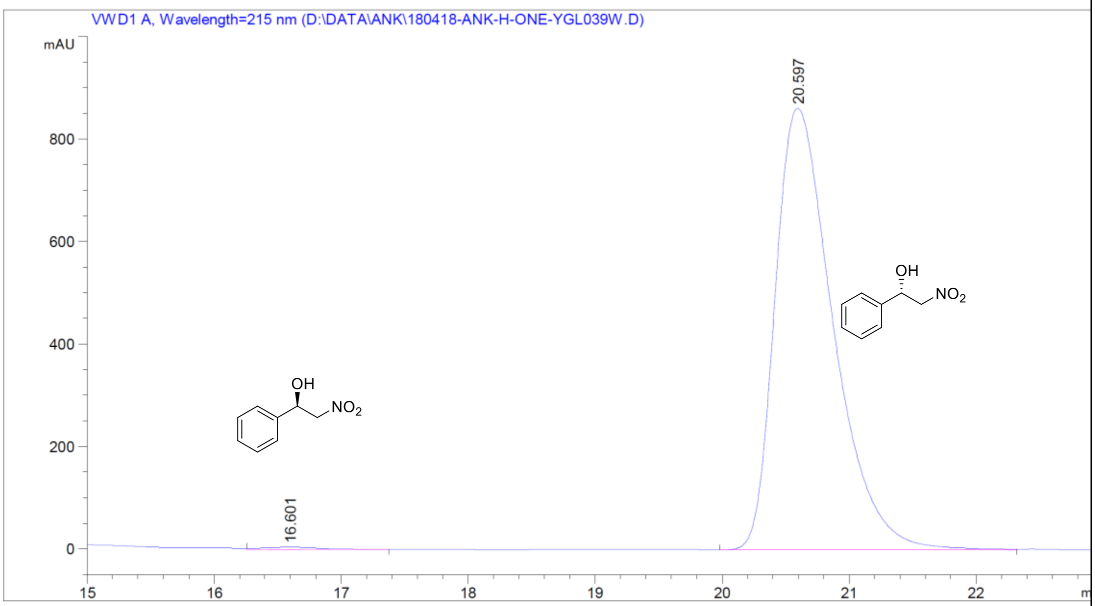
HPLC spectra of the products from analytical scale reactions

***(S)*-2-nitro-1-phenylethanol (2a)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.4 min (minor), t_R'=20.5 min (major)



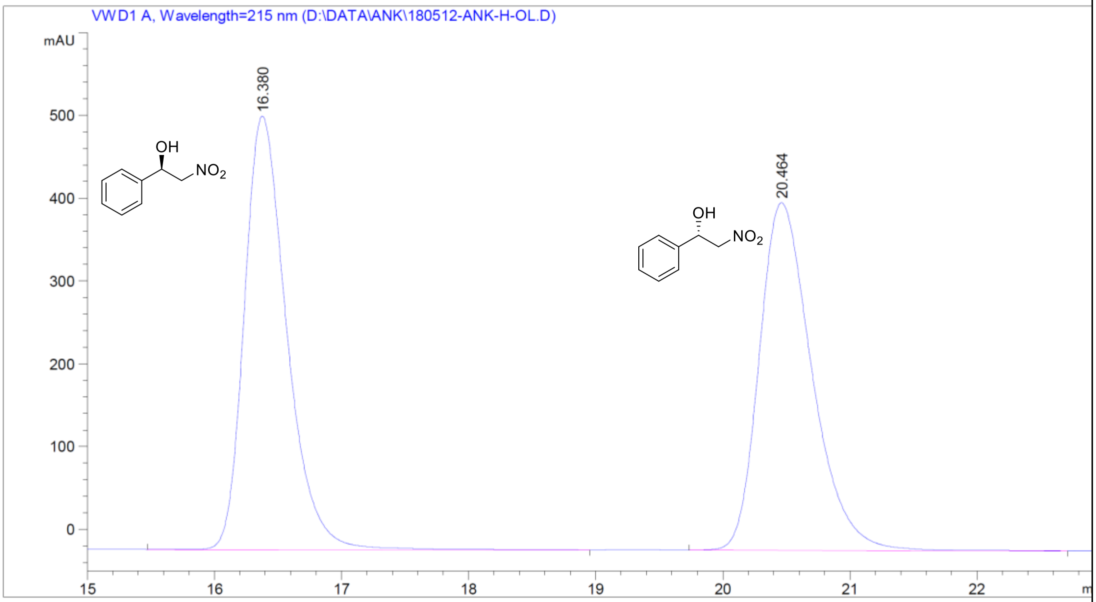
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.380	VB	0.3549	1.21474e4	523.11871	50.1021
2	20.464	BB	0.4403	1.20979e4	419.70804	49.8979



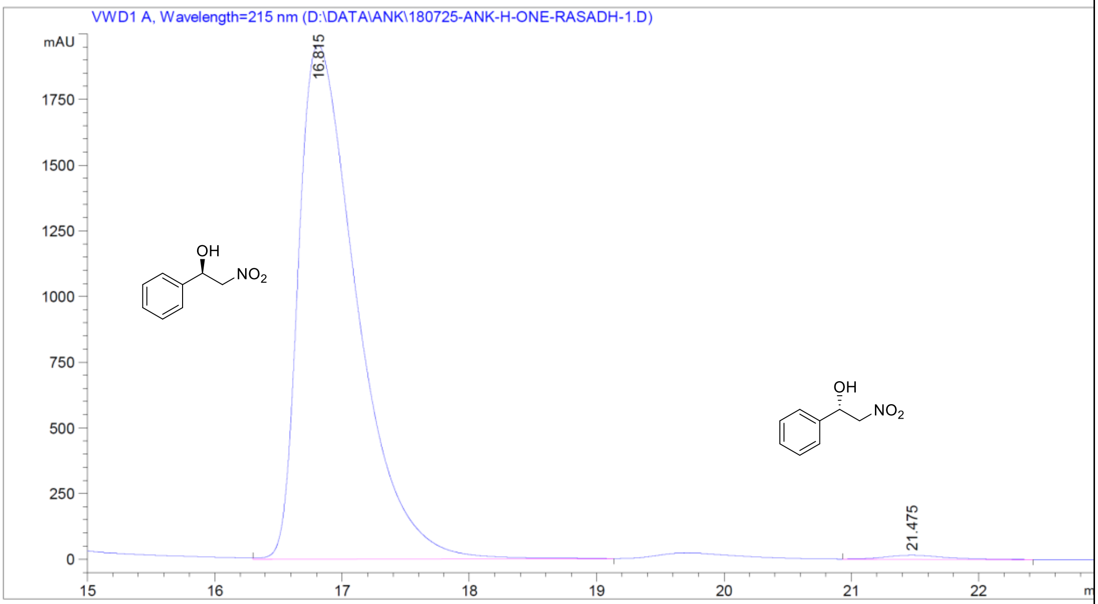
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.601	VB	0.4586	168.09796	5.23552	0.6106
2	20.597	BV	0.4868	2.73634e4	861.05811	99.3894

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-2-nitro-1-phenylethanol (2a)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.4 min (major), t_R'=20.5 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.380	VB	0.3549	1.21474e4	523.11871	50.1021
2	20.464	BB	0.4403	1.20979e4	419.70804	49.8979

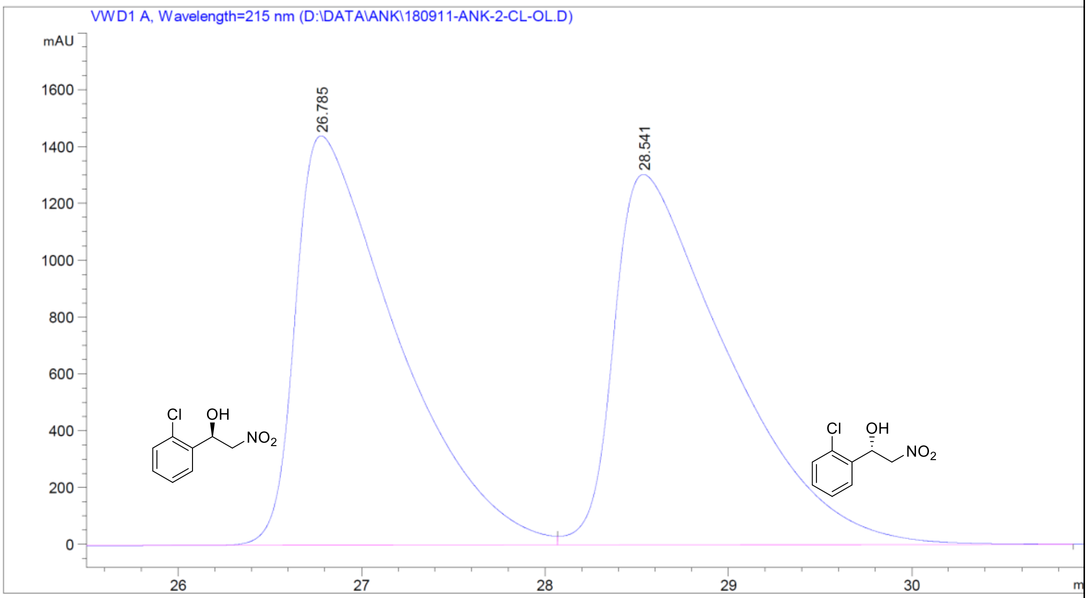


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.815	VB	0.4823	6.20511e4	1955.18005	99.2214
2	21.475	VB	0.4923	486.94031	15.09527	0.7786

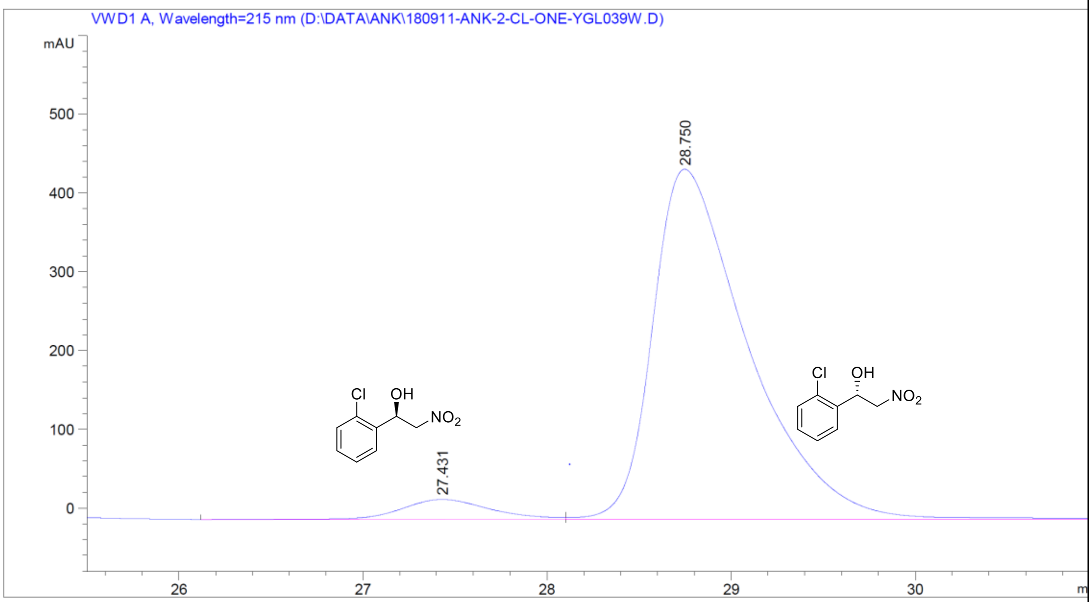
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-1-(2-chlorophenyl)-2-nitroethan-1-ol (2b)

Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 99:1, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=26.8 min (minor), t_R'=28.5 min (major)



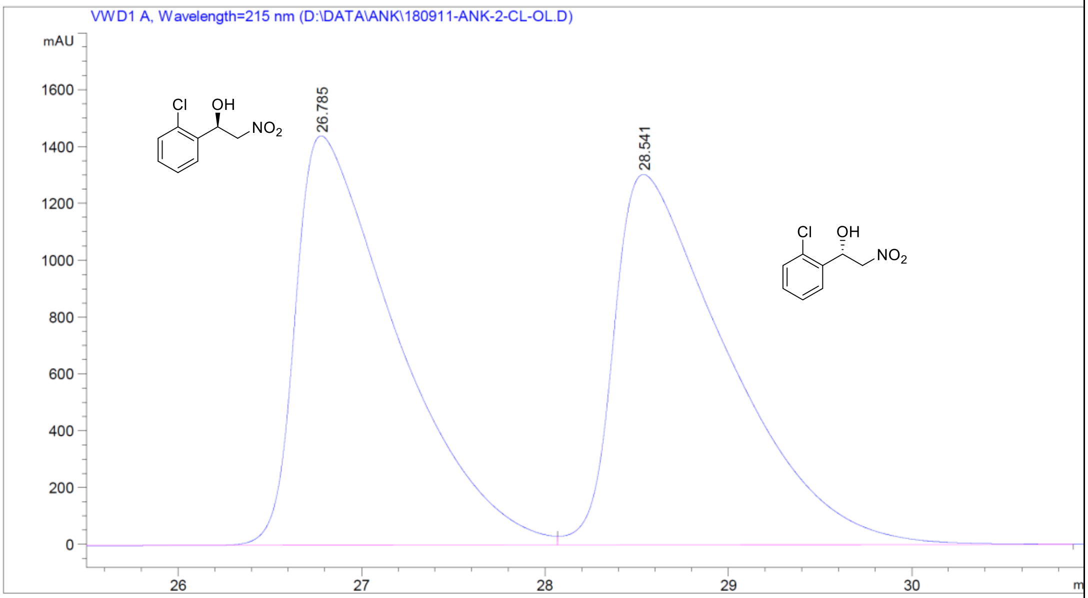
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	26.785	BV	0.5783	5.55586e4	1439.39465	49.6222
2	28.541	VB	0.6254	5.64046e4	1302.04199	50.3778



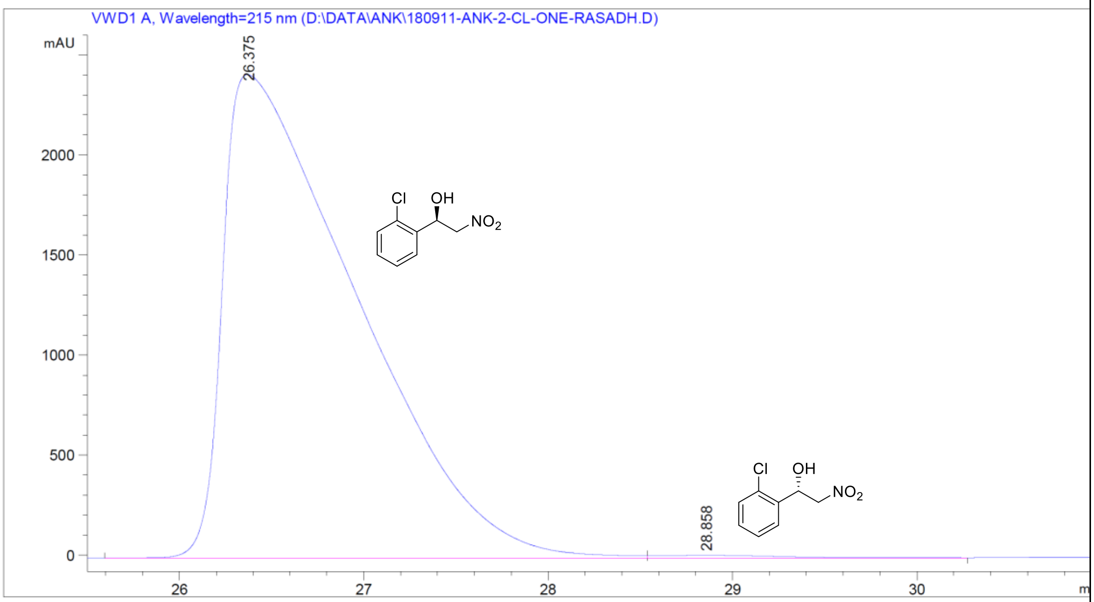
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	27.431	BV	0.5108	848.74939	25.34026	5.0329
2	28.750	VB	0.5332	1.60152e4	443.62631	94.9671

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(2-chlorophenyl)-2-nitroethan-1-ol (2b)**
Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 99:1, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=26.8 min (major), t_R'=28.5 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	26.785	BV	0.5783	5.55586e4	1439.39465	49.6222
2	28.541	VB	0.6254	5.64046e4	1302.04199	50.3778

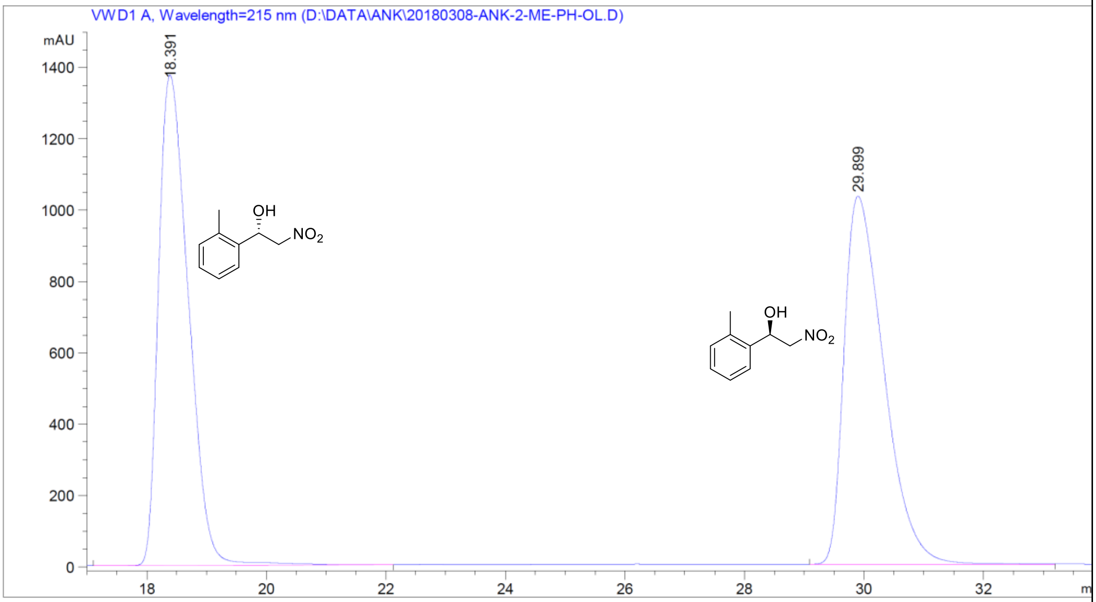


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	26.375	BV	0.7153	1.21404e5	2411.87402	99.5555
2	28.858	VB	0.6569	542.02588	12.32889	0.4445

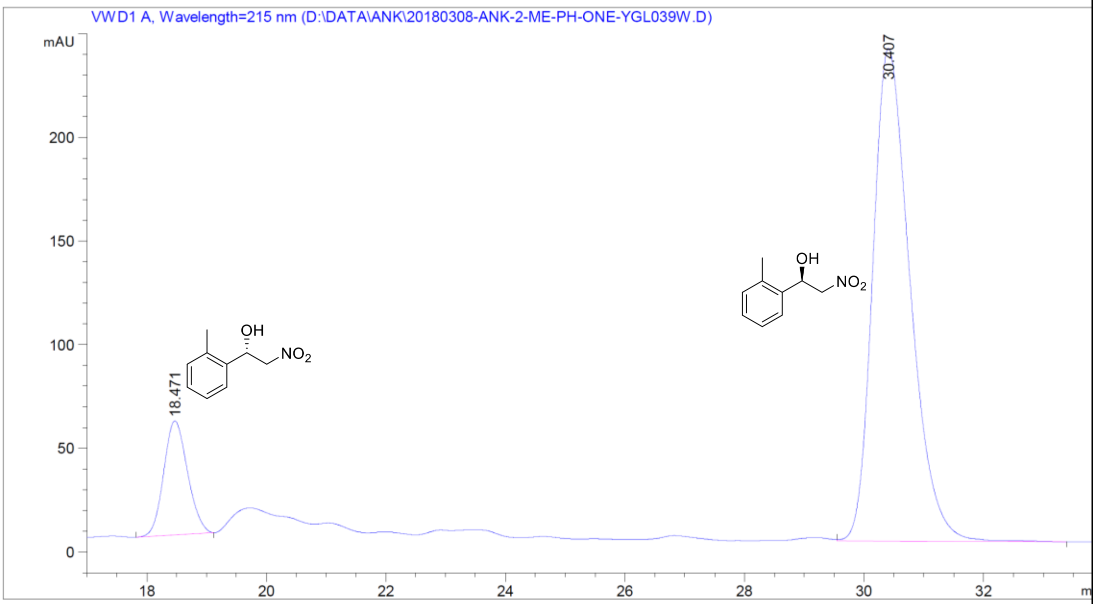
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-2-nitro-1-(o-tolyl)ethan-1-ol (2c)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=18.4 min (minor), t_R'=20.0 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.391	BB	0.5328	4.77175e4	1375.26160	50.0728
2	29.899	BV	0.7383	4.75787e4	1031.16663	49.9272

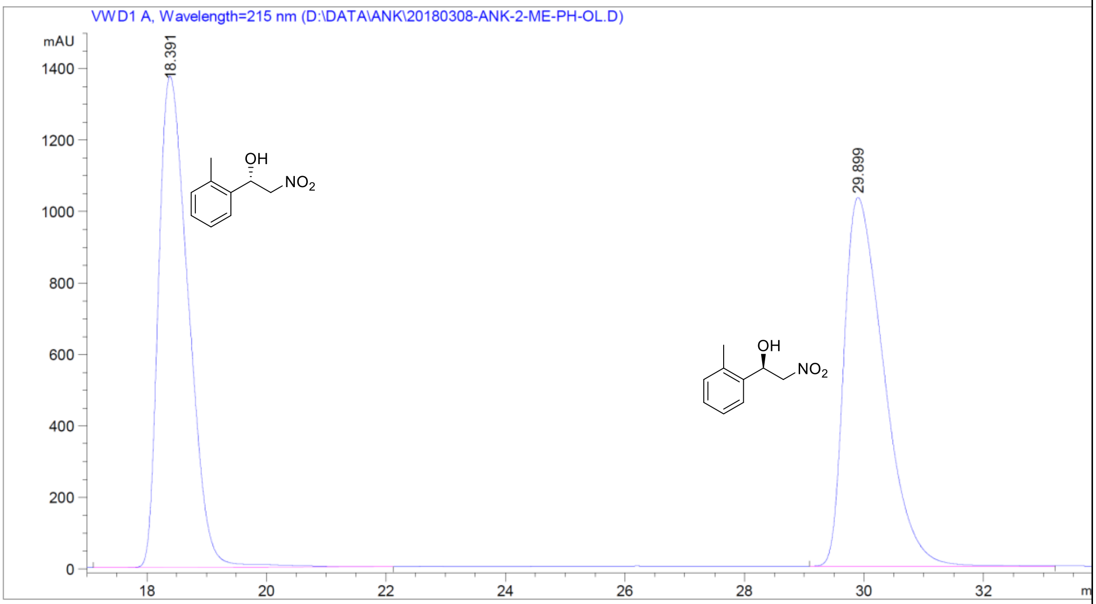


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.471	BB	0.4359	1525.22534	54.93120	12.8802
2	30.407	VB	0.6667	1.03164e4	237.54245	87.1198

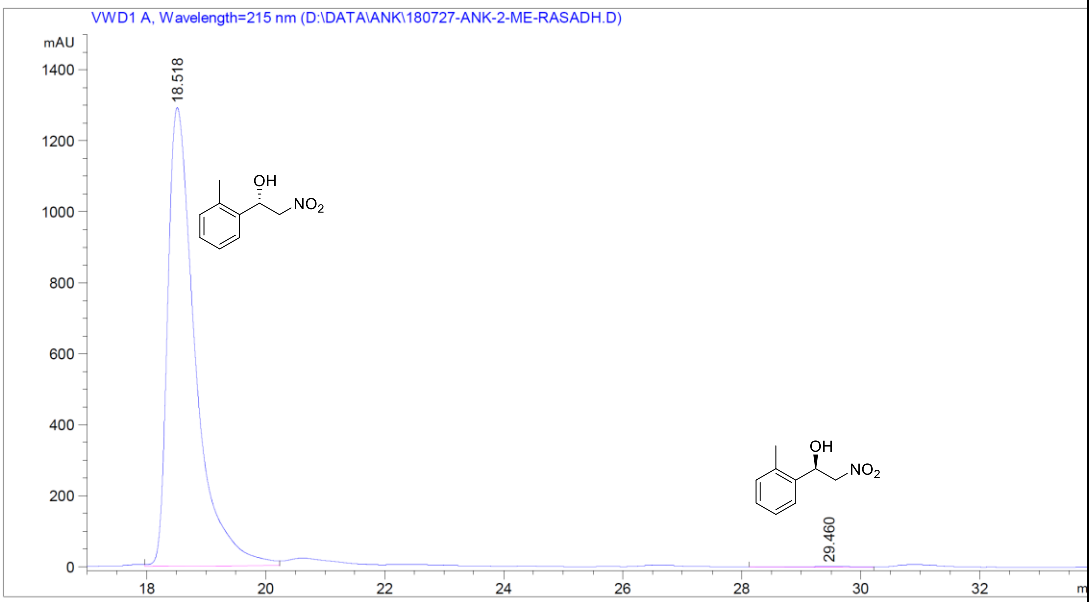
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*R*)-2-nitro-1-(o-tolyl)ethan-1-ol (2c)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=18.4 min (major), t_R'=20.0 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.391	BB	0.5328	4.77175e4	1375.26160	50.0728
2	29.899	BV	0.7383	4.75787e4	1031.16663	49.9272

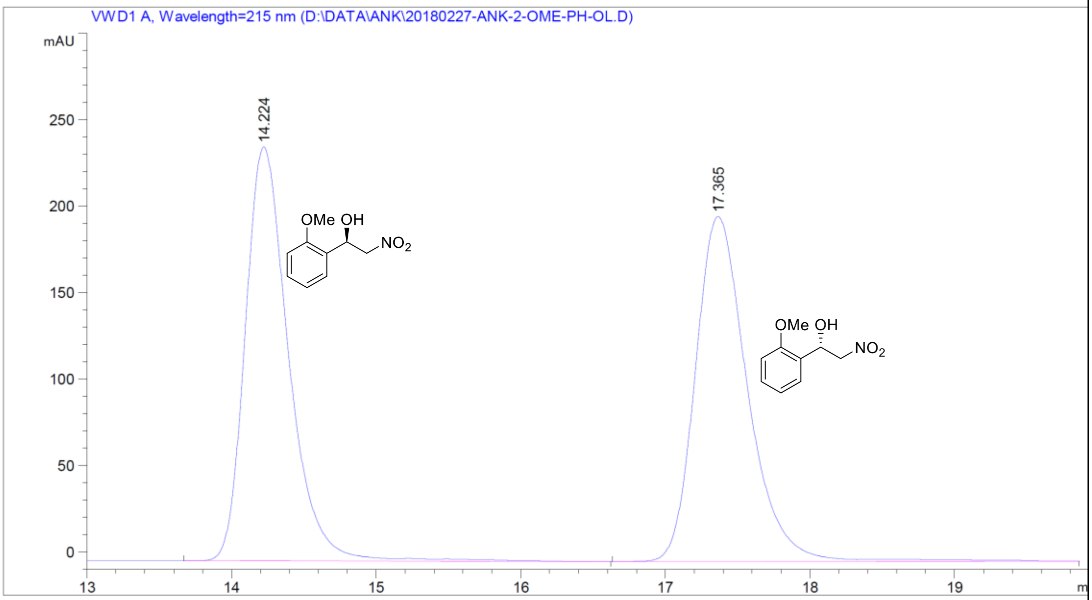


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.518	VV	0.4871	4.15257e4	1291.43127	99.6917
2	29.460	VV	0.8945	128.40529	2.08502	0.3083

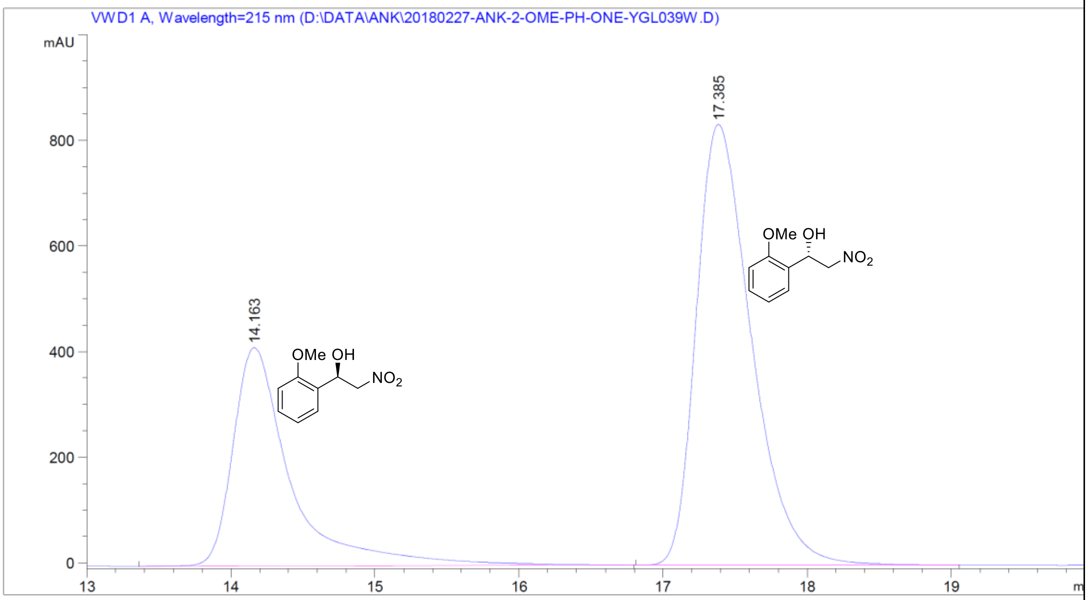
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-1-(2-methoxyphenyl)-2-nitroethan-1-ol (2d)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (minor), t_R'=17.4 min (major)



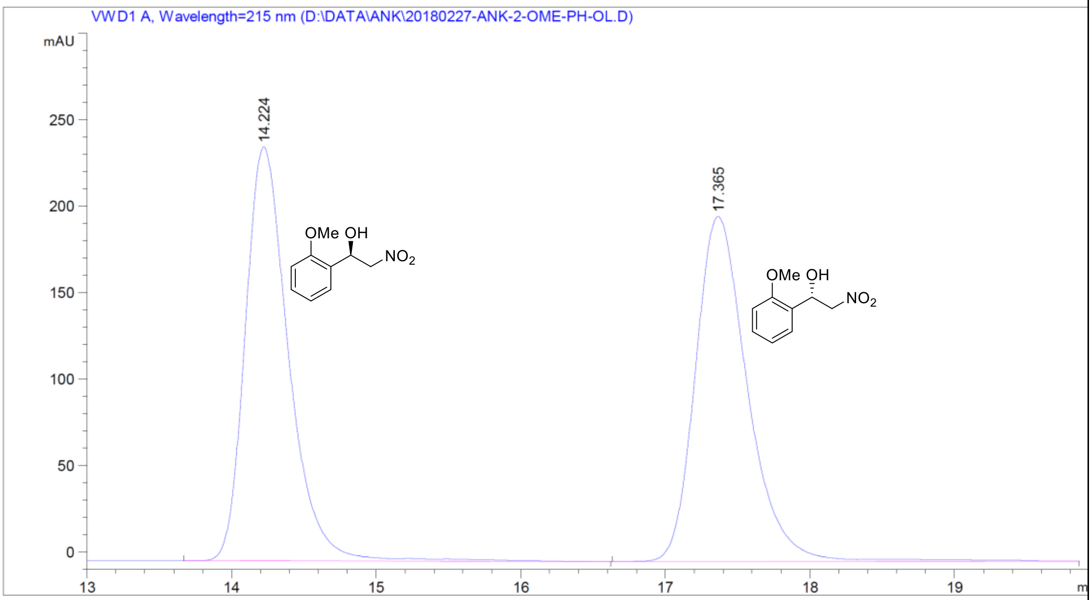
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.224	BB	0.3200	5006.38672	239.39793	49.9782
2	17.365	BBA	0.3851	5010.75098	199.44981	50.0218



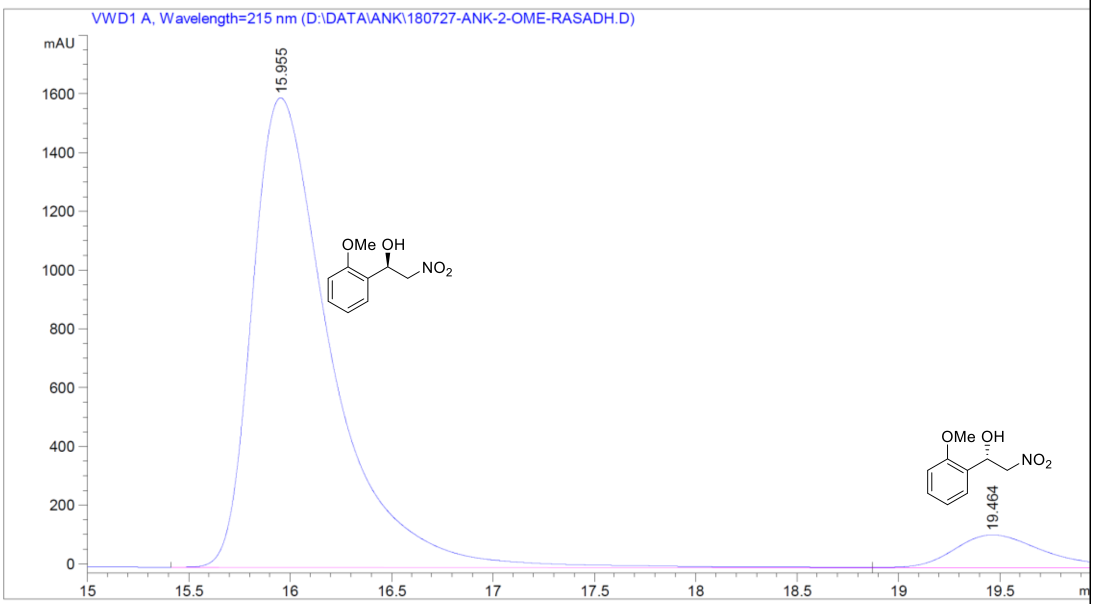
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.163	BB	0.4147	1.15569e4	412.69119	34.3041
2	17.385	BB	0.4101	2.21326e4	832.65906	65.6959

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(2-methoxyphenyl)-2-nitroethan-1-ol (2d)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (major), t_R'=17.4 min (minor)



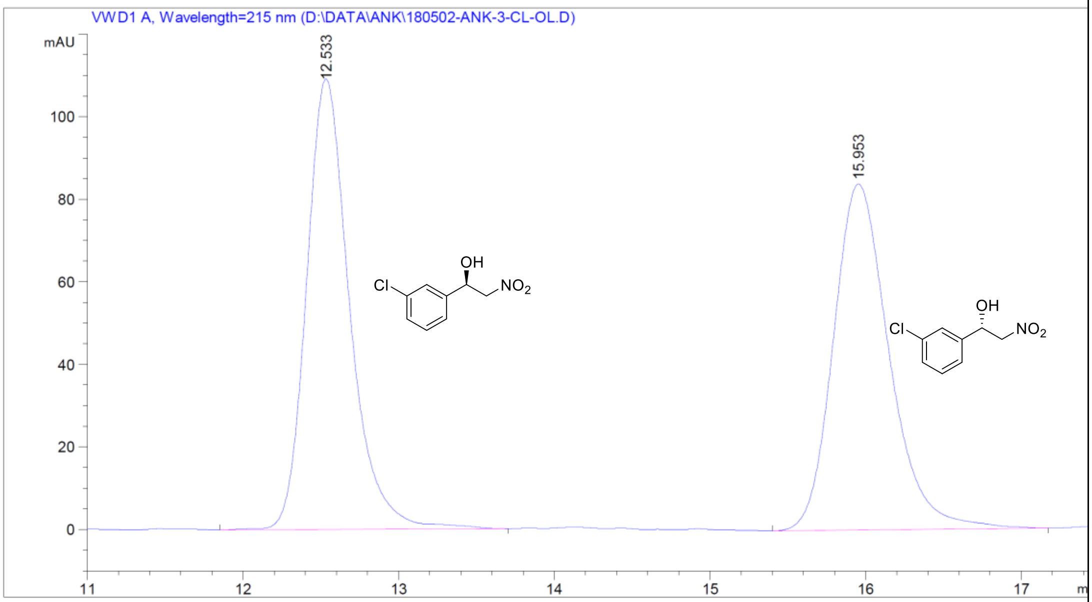
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.224	BB	0.3200	5006.38672	239.39793	49.9782
2	17.365	BBA	0.3851	5010.75098	199.44981	50.0218



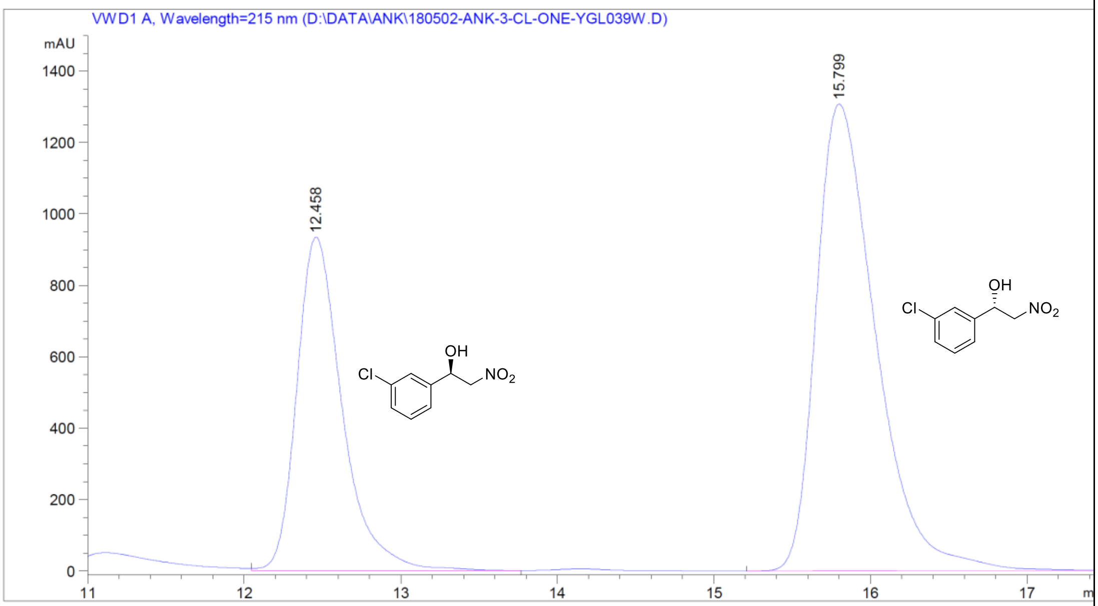
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.955	BV	0.4041	4.32945e4	1598.14014	92.2580
2	19.464	VB	0.4891	3633.15088	112.40070	7.7420

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(3-chlorophenyl)-2-nitroethan-1-ol (2e)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=12.5 min (minor), t_R'=16.0 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.533	BB	0.2933	2107.63501	109.14163	50.1796
2	15.953	BB	0.3822	2092.54541	83.82163	49.8204

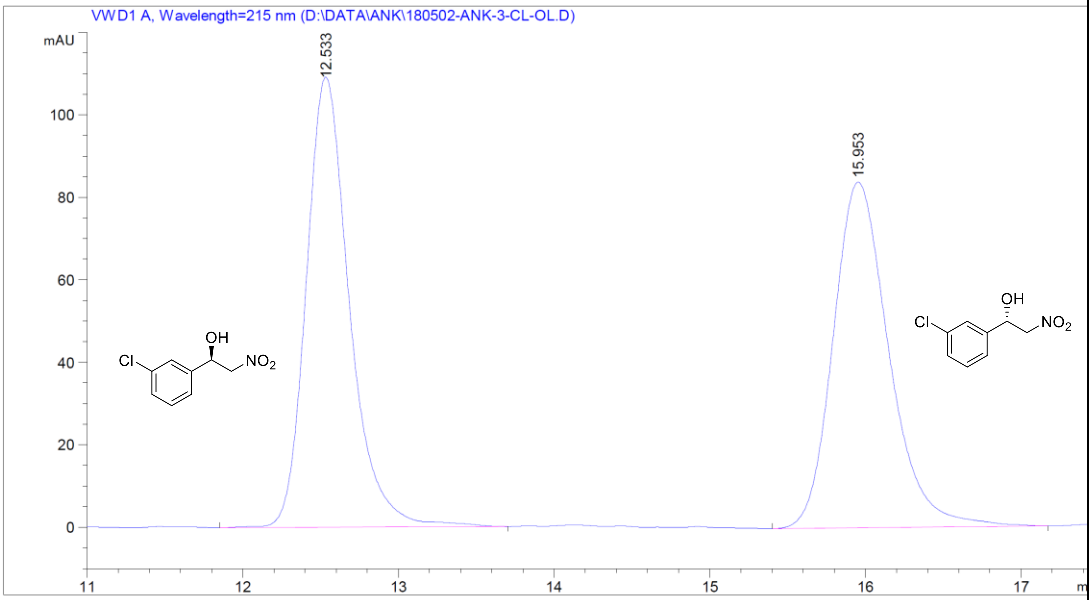


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.458	VB	0.3075	1.88651e4	934.61163	35.3158
2	15.799	BB	0.4043	3.45533e4	1307.62231	64.6842

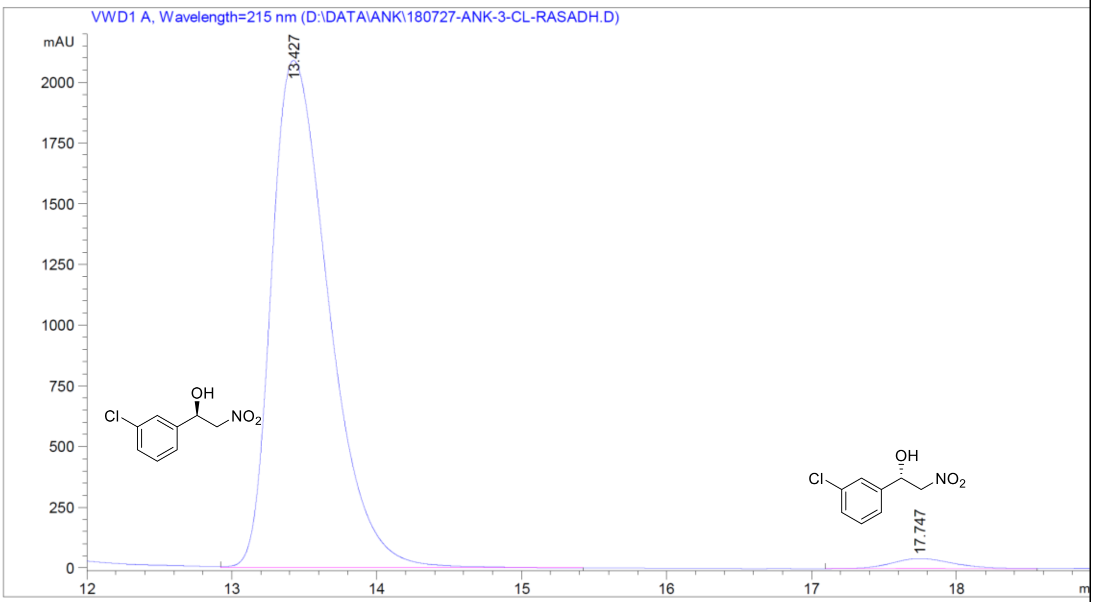
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(3-chlorophenyl)-2-nitroethan-1-ol (2e)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=12.5 min (major), t_R'=16.0 min (minor)



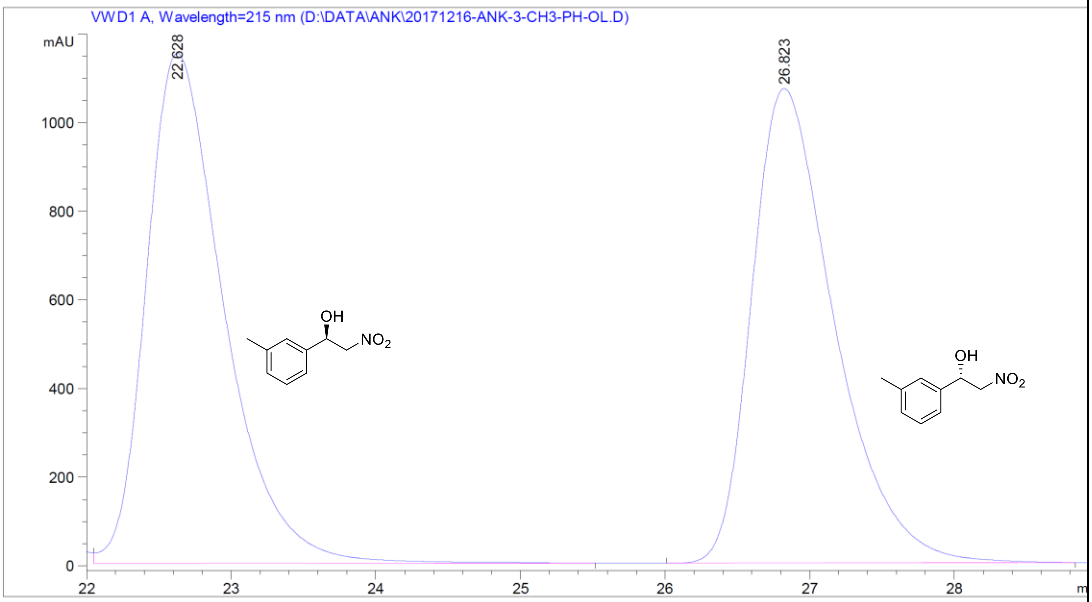
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.533	BB	0.2933	2107.63501	109.14163	50.1796
2	15.953	BB	0.3822	2092.54541	83.82163	49.8204



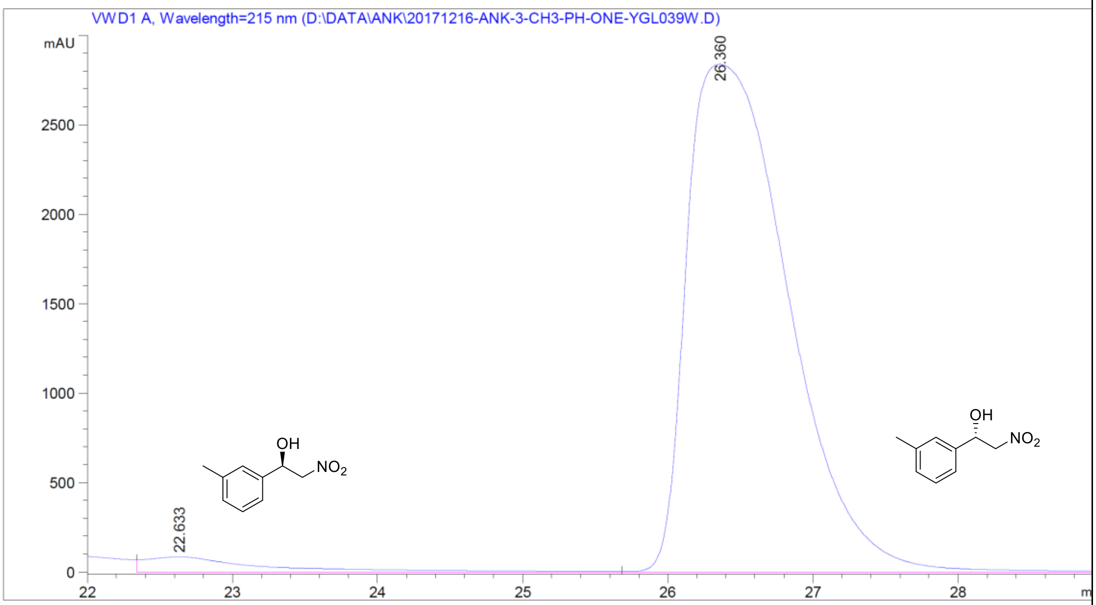
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.427	VV	0.4261	5.75350e4	2090.41211	97.8767
2	17.747	BV	0.4406	1248.13025	41.89462	2.1233

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-2-nitro-1-(m-tolyl)ethan-1-ol (2f)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=22.6 min (minor), t_R'=26.8 min (major)



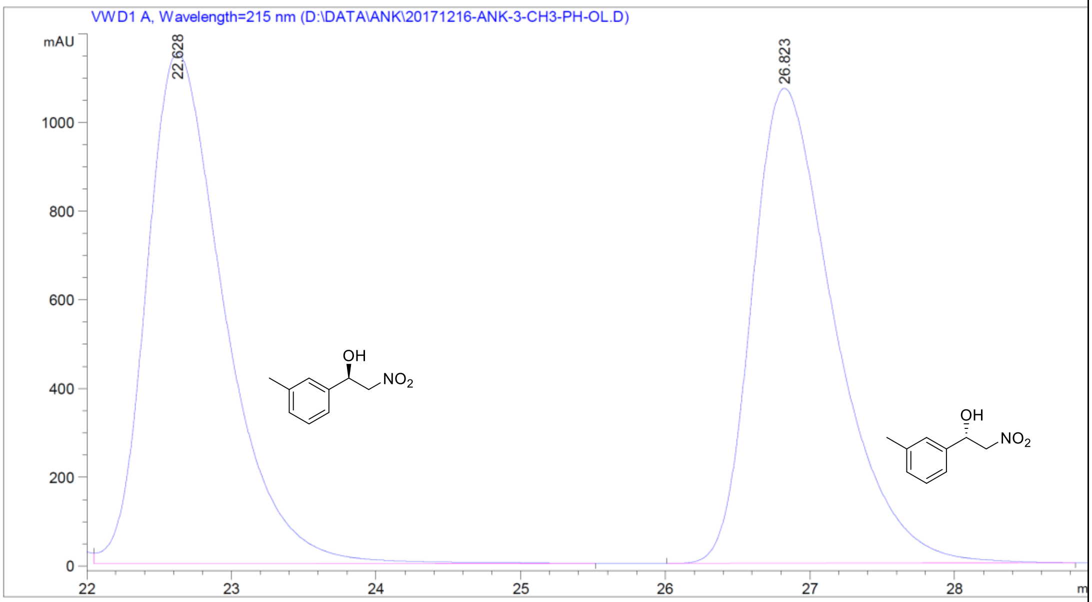
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.628	VB	0.5684	4.29731e4	1151.41504	50.2671
2	26.823	BB	0.6045	4.25164e4	1070.24817	49.7329



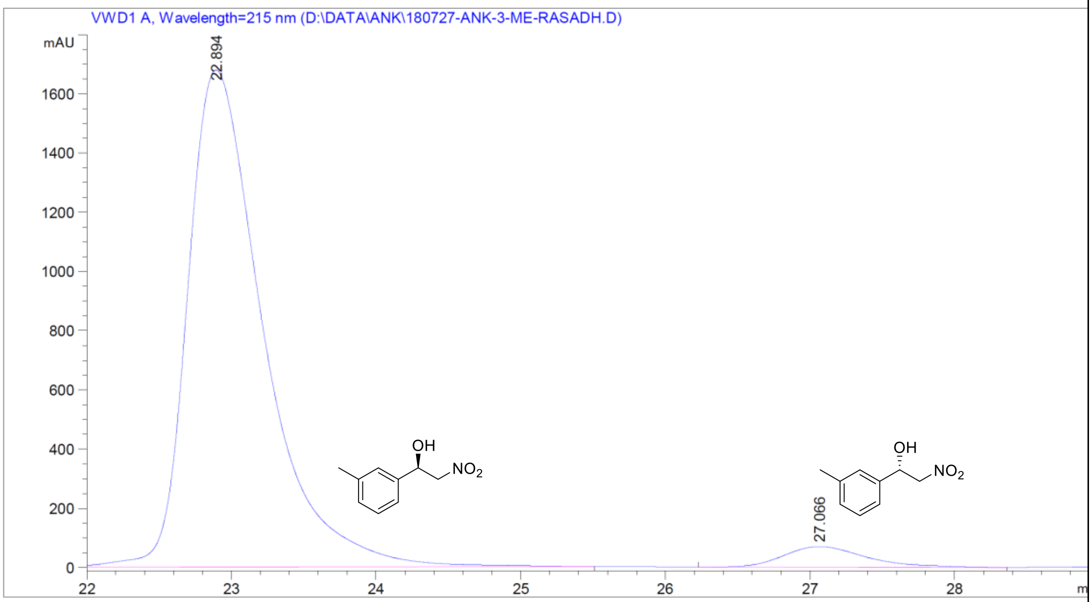
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.633	VV	0.7631	4771.24463	84.32117	3.3549
2	26.360	VB	0.7645	1.37445e5	2835.49634	96.6451

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-2-nitro-1-(m-tolyl)ethan-1-ol (2f)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=22.6 min (major), t_R'=26.8 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.628	VB	0.5684	4.29731e4	1151.41504	50.2671
2	26.823	BB	0.6045	4.25164e4	1070.24817	49.7329

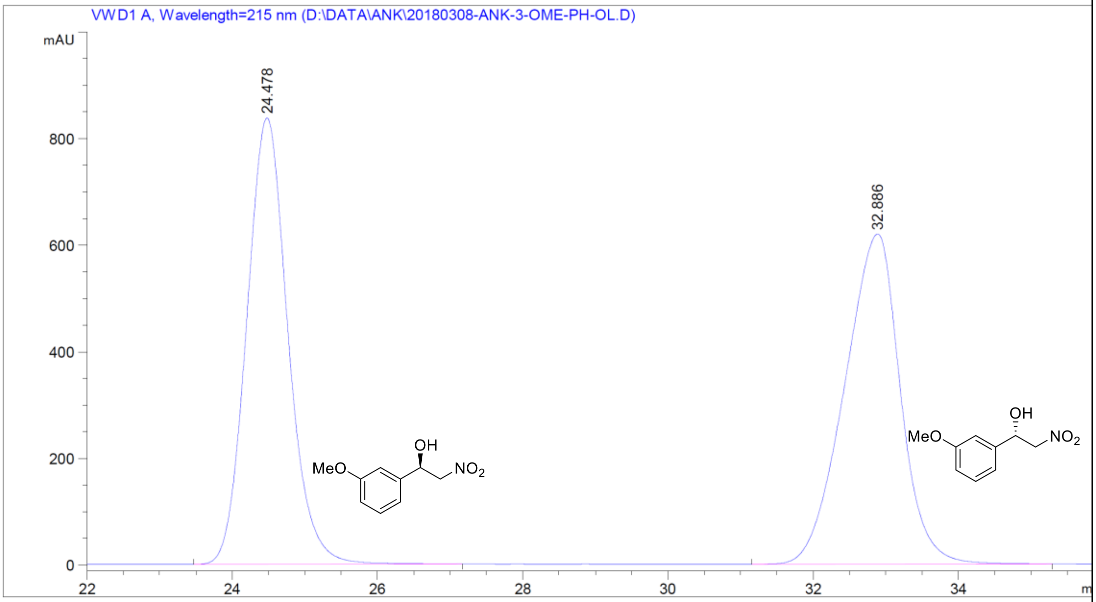


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.894	BB	0.5513	6.10049e4	1679.25049	95.6218
2	27.066	BV	0.5927	2793.20801	70.04702	4.3782

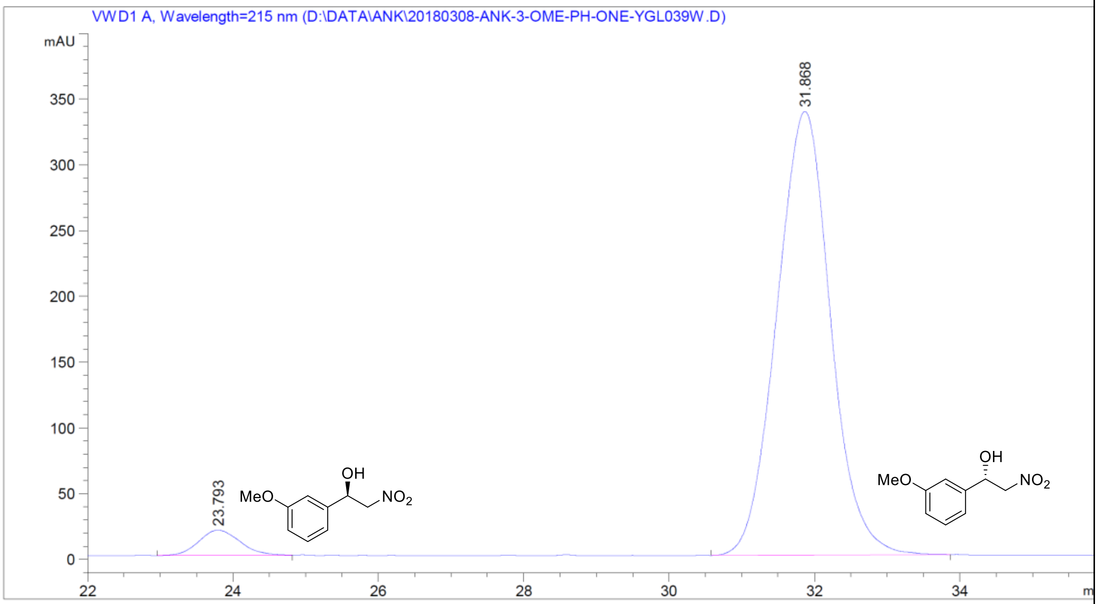
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-1-(3-methoxyphenyl)-2-nitroethan-1-ol (2g)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.5 min (minor), t_R'=32.9 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.478	BB	0.6056	3.29622e4	836.72827	49.9815
2	32.886	BB	0.8149	3.29866e4	618.82013	50.0185

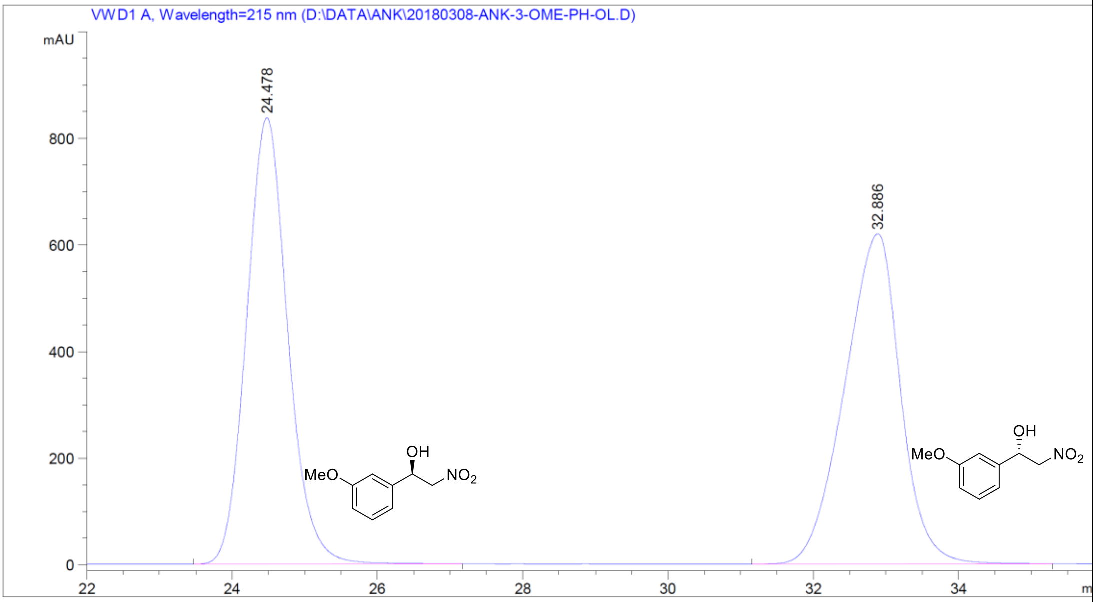


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.793	BV	0.6311	768.98499	19.33037	4.2438
2	31.868	BB	0.8071	1.73513e4	337.35602	95.7562

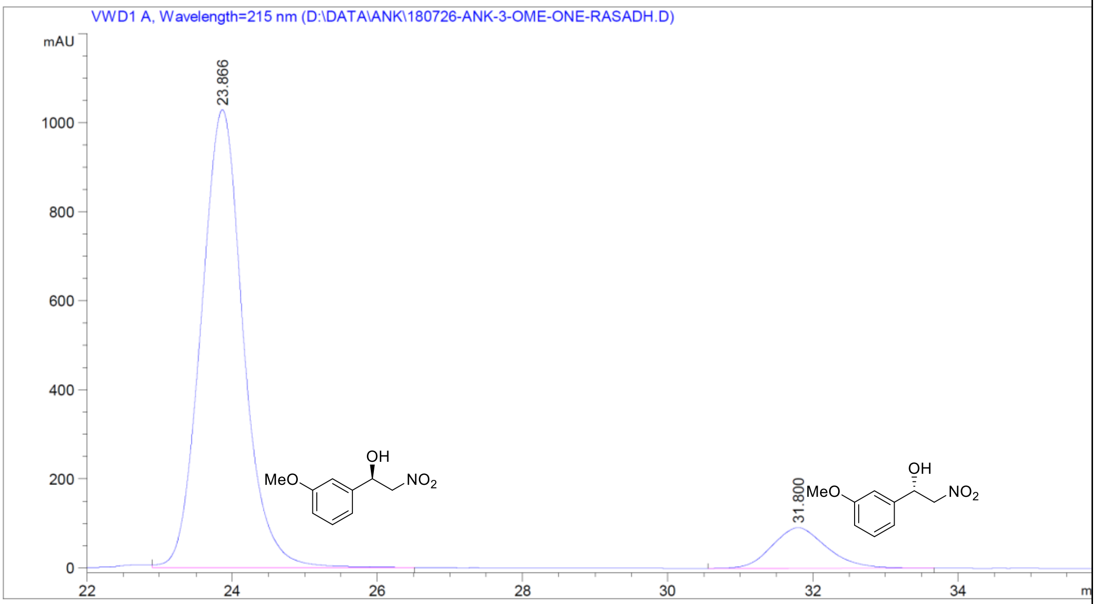
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(R)-1-(3-methoxyphenyl)-2-nitroethan-1-ol (2g)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.5 min (major), t_R'=32.9 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.478	BB	0.6056	3.29622e4	836.72827	49.9815
2	32.886	BB	0.8149	3.29866e4	618.82013	50.0185

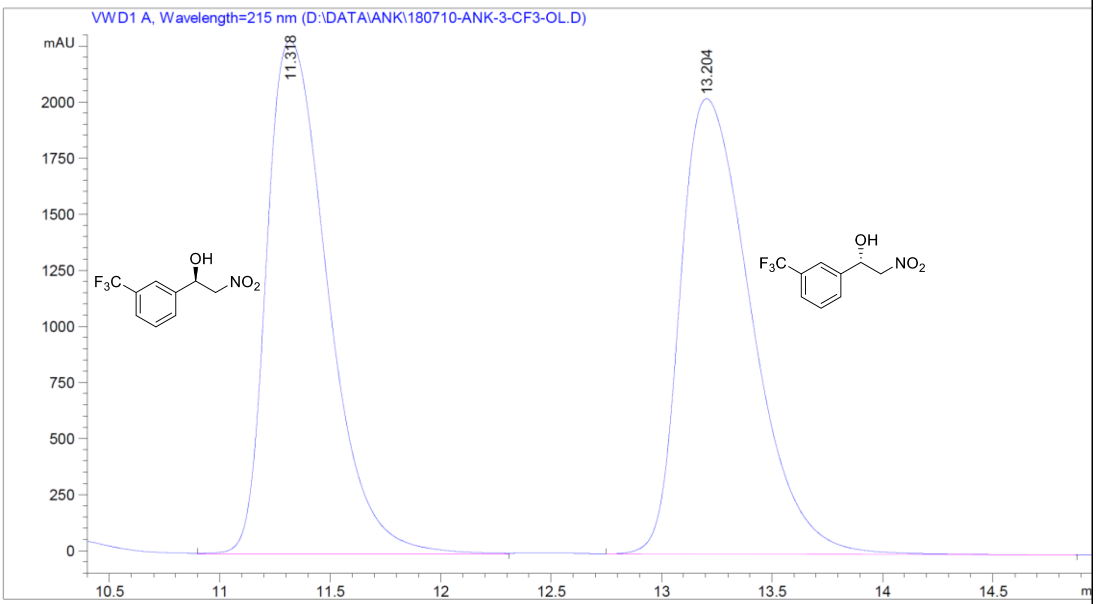


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.866	VB	0.6104	4.13847e4	1027.57959	89.6819
2	31.800	BB	0.7581	4761.42188	91.50236	10.3181

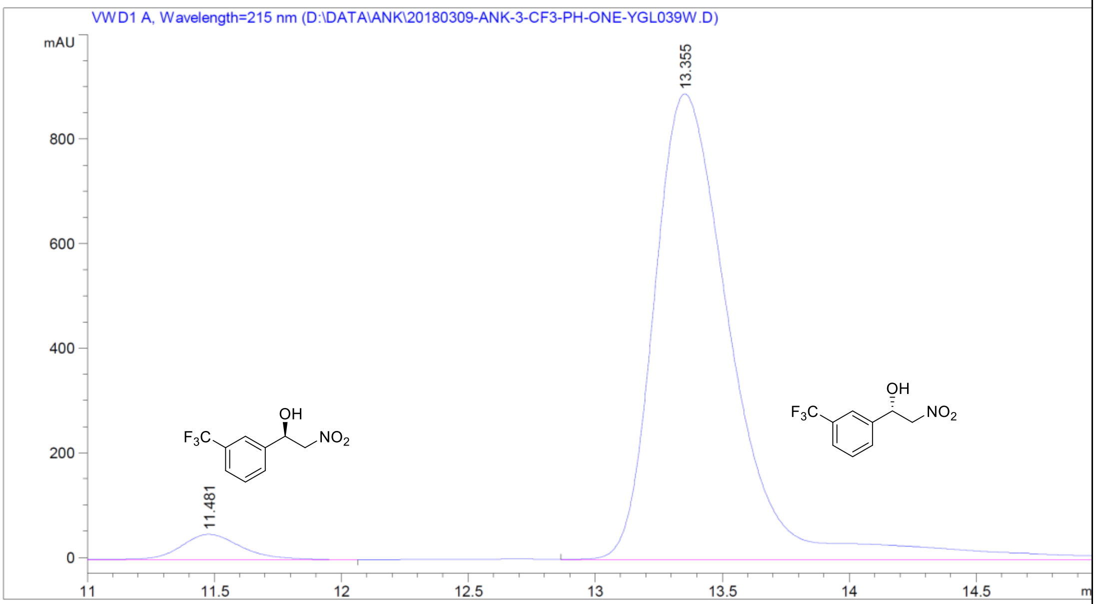
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-2-nitro-1-(3-(trifluoromethyl)phenyl)ethan-1-ol (2h)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.3 min (minor), t_R'=13.2 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.318	VV	0.2984	4.38977e4	2287.25195	49.1150
2	13.204	BB	0.3524	4.54796e4	2029.70337	50.8850

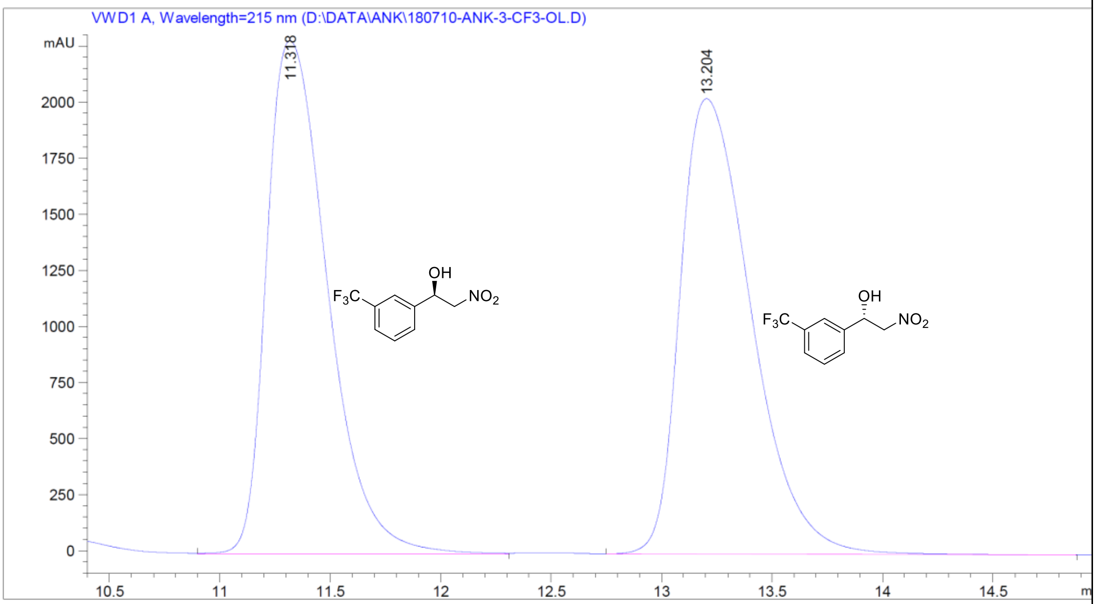


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.481	VB	0.2617	820.04236	48.40012	4.0910
2	13.355	VBA	0.3319	1.92252e4	890.53174	95.9090

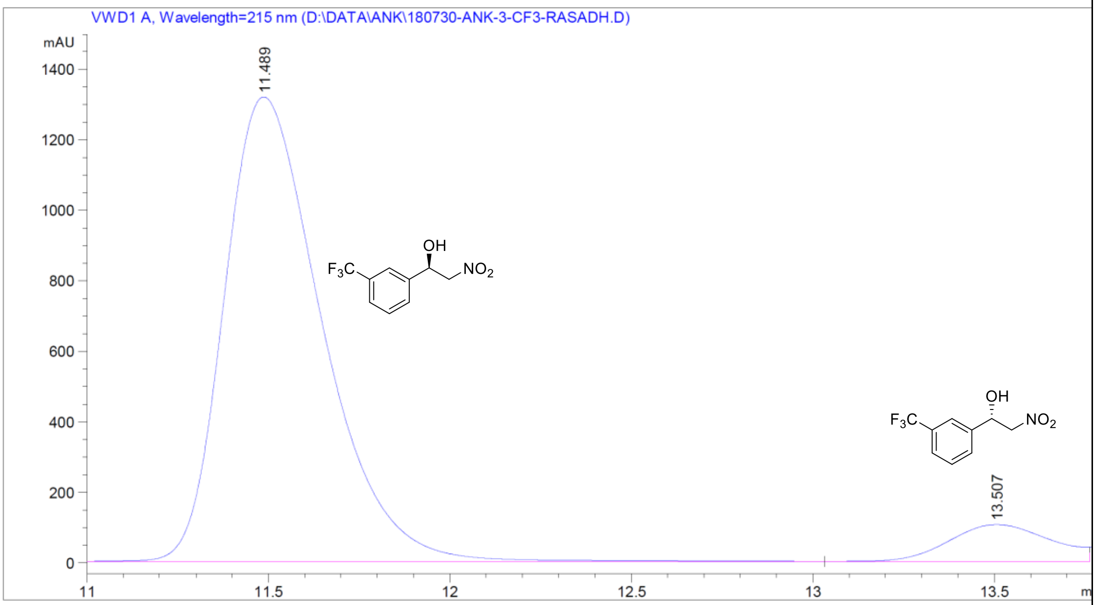
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(R)-2-nitro-1-(3-(trifluoromethyl)phenyl)ethan-1-ol (2h)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.3 min (major), t_R'=13.2 min (minor)



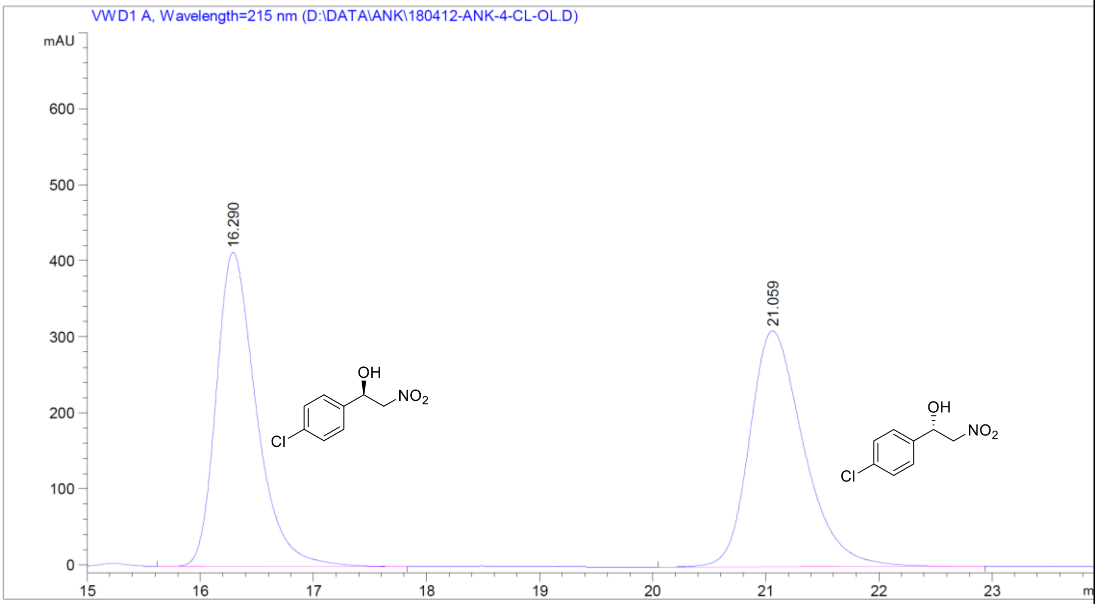
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.318	VV	0.2984	4.38977e4	2287.25195	49.1150
2	13.204	BB	0.3524	4.54796e4	2029.70337	50.8850



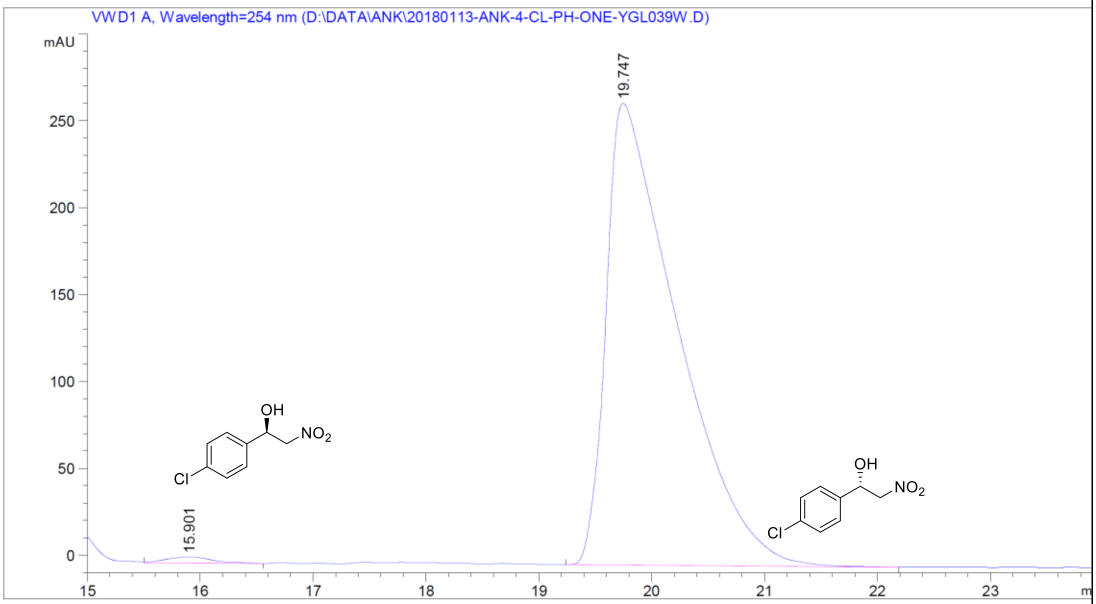
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.489	BV	0.2904	2.46743e4	1318.27087	92.3905
2	13.507	VV	0.3028	2032.22729	104.53981	7.6095

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(4-chlorophenyl)-2-nitroethan-1-ol (2i)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.3 min (minor), t_R'=21.0 min (major)



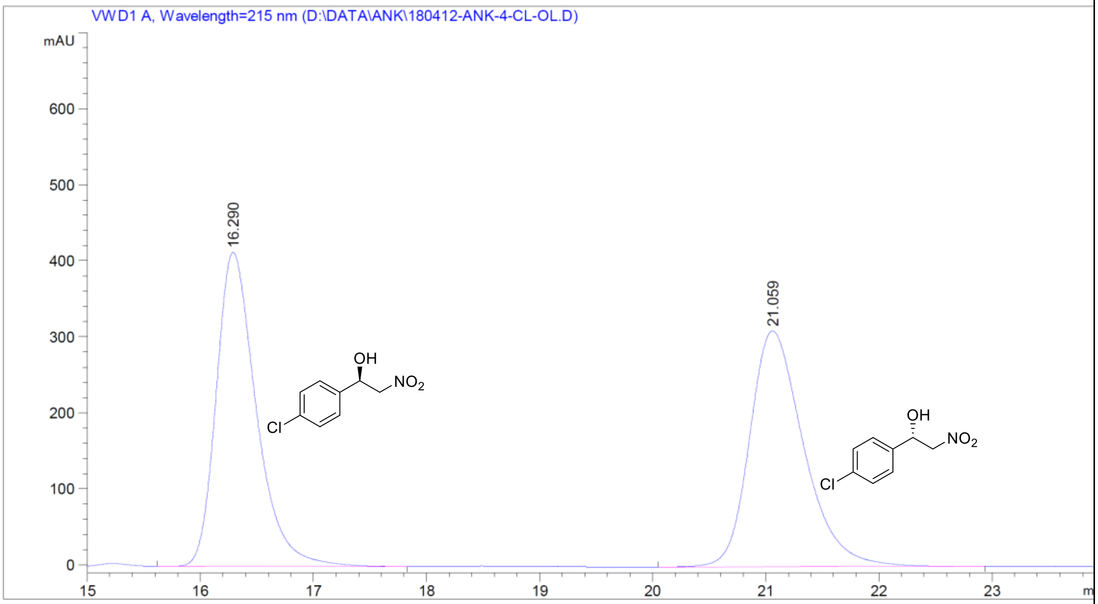
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.290	BB	0.3745	1.01797e4	413.15271	49.6323
2	21.059	BB	0.5072	1.03306e4	310.44525	50.3677



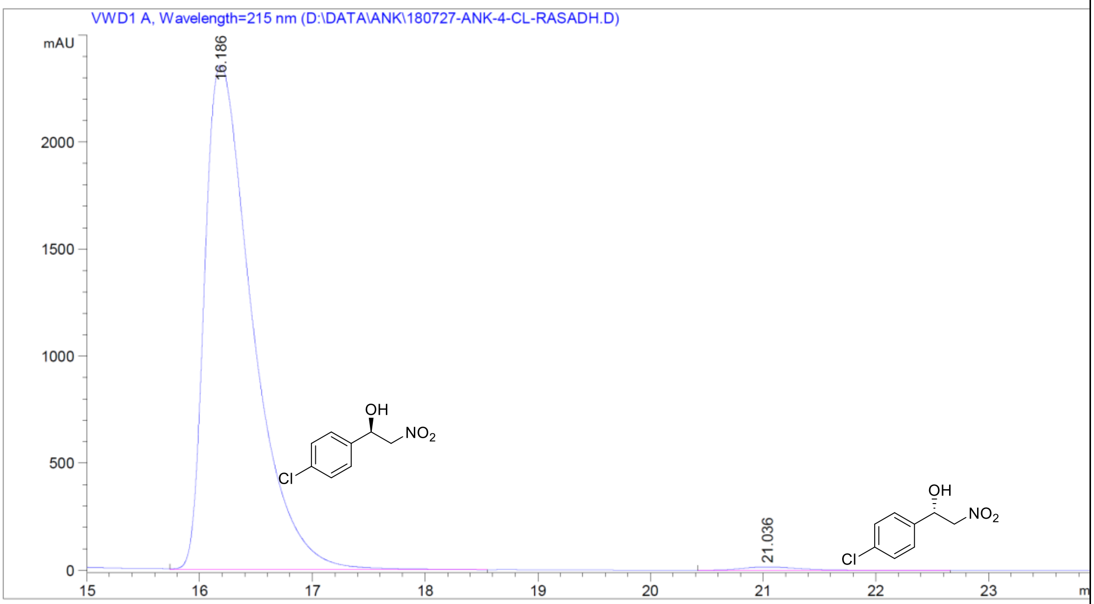
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.901	VB	0.4678	104.61653	3.50953	0.8884
2	19.747	BB	0.6264	1.16715e4	265.73611	99.1116

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(4-chlorophenyl)-2-nitroethan-1-ol (2i)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.3 min (major), t_R'=21.0 min (minor)



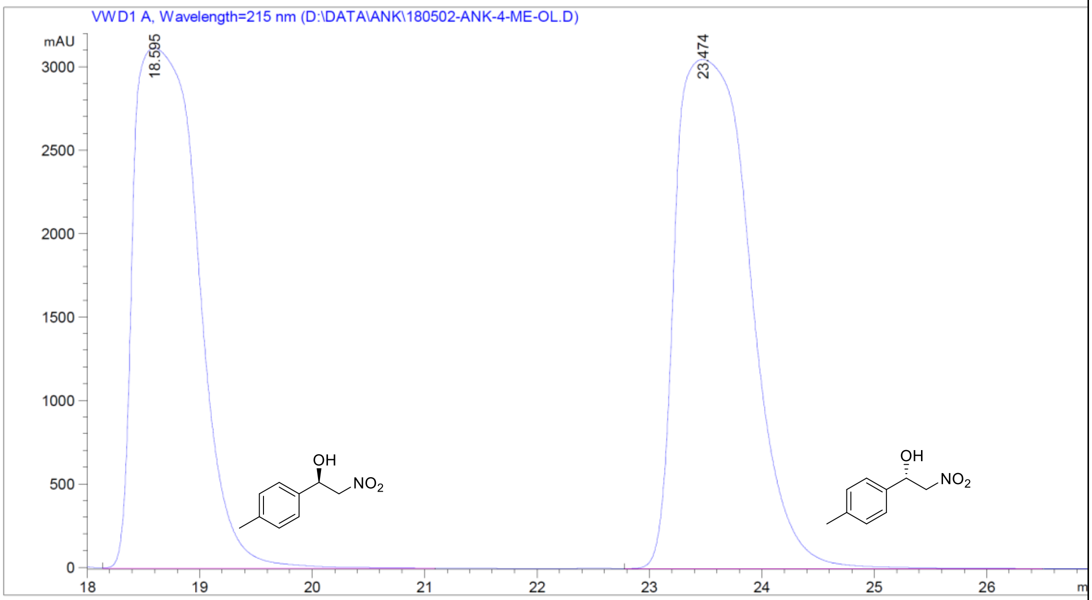
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.290	BB	0.3745	1.01797e4	413.15271	49.6323
2	21.059	BB	0.5072	1.03306e4	310.44525	50.3677



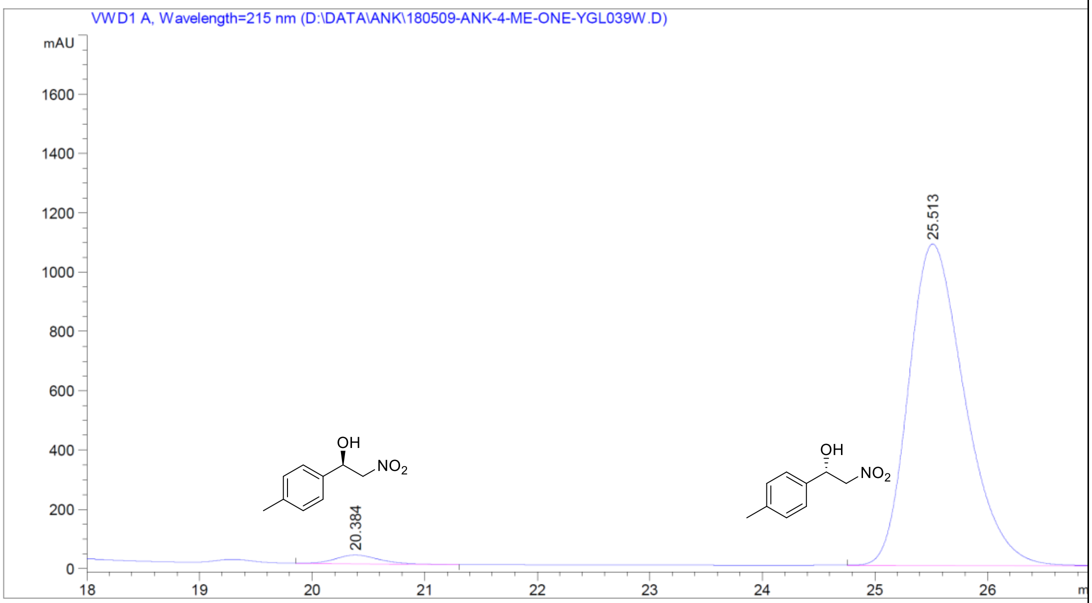
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.186	VB	0.4430	6.92892e4	2356.96899	99.2151
2	21.036	BB	0.4735	548.18646	15.71519	0.7849

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-2-nitro-1-(p-tolyl)ethan-1-ol (2j)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=18.6 min (minor), t_R'=23.5 min (major)



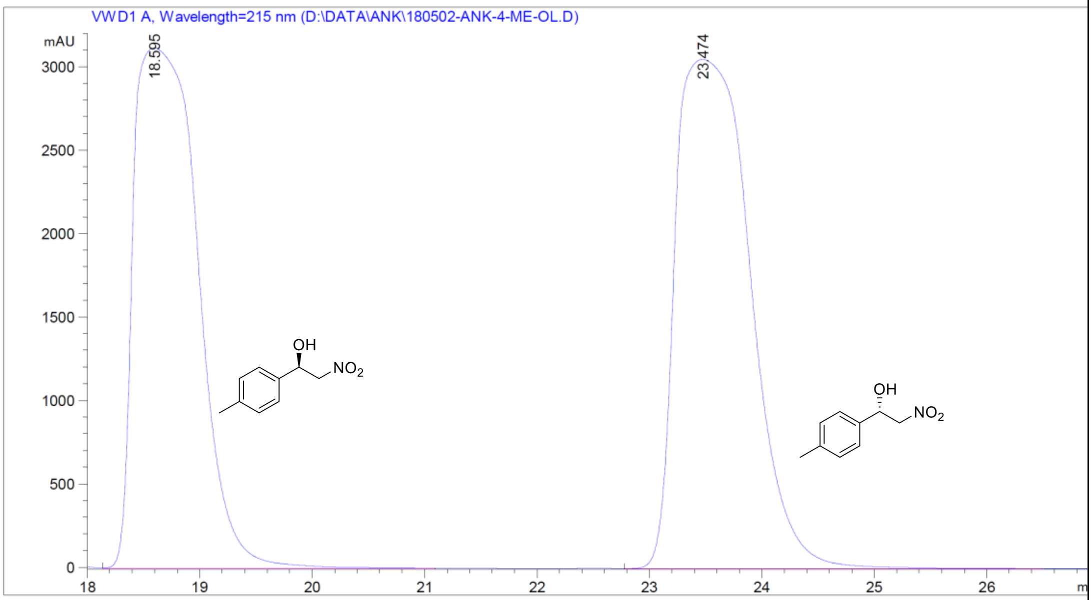
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.595	VB	0.6367	1.23685e5	3118.48682	46.7423
2	23.474	BB	0.7349	1.40925e5	3050.94507	53.2577



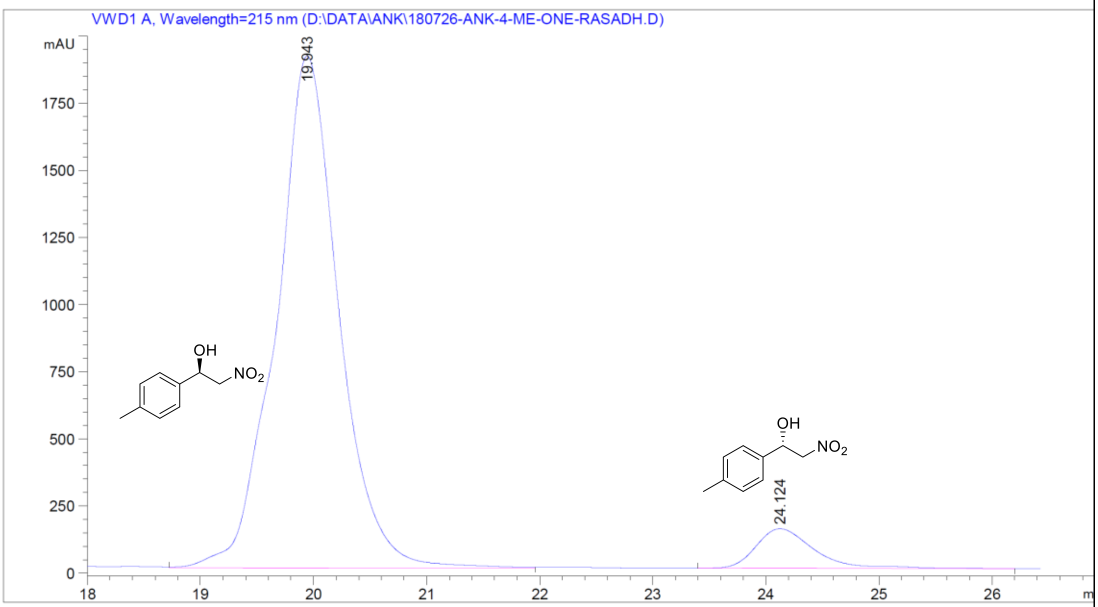
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.384	VB	0.4252	862.83160	30.57942	2.2334
2	25.513	VB	0.5350	3.77707e4	1085.32849	97.7666

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-2-nitro-1-(p-tolyl)ethan-1-ol (2j)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=18.6 min (major), t_R'=23.5 min (minor)



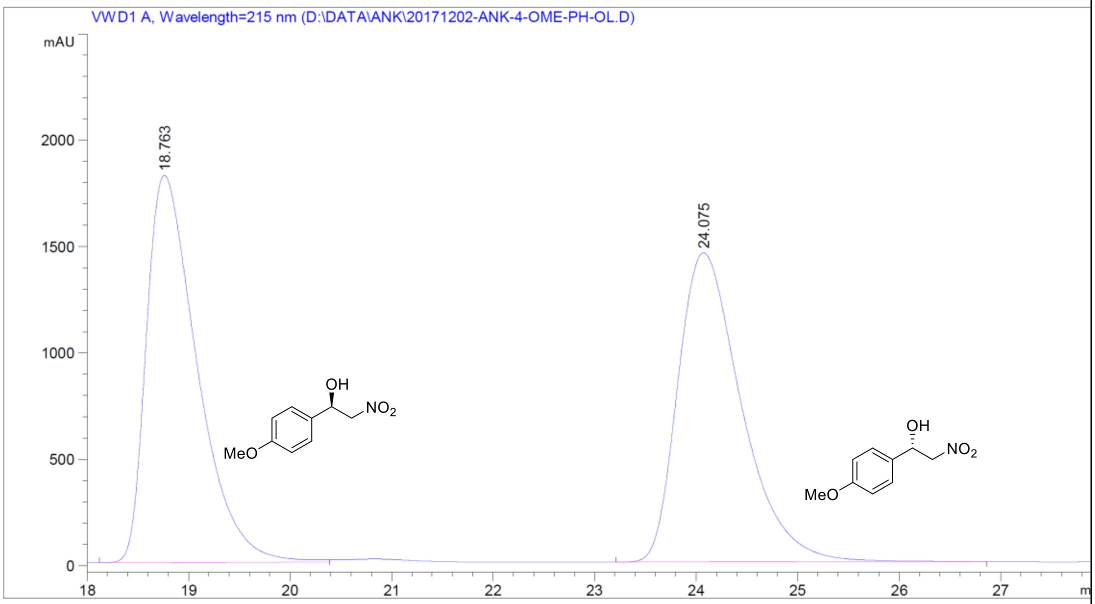
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.595	VB	0.6367	1.23685e5	3118.48682	46.7423
2	23.474	BB	0.7349	1.40925e5	3050.94507	53.2577



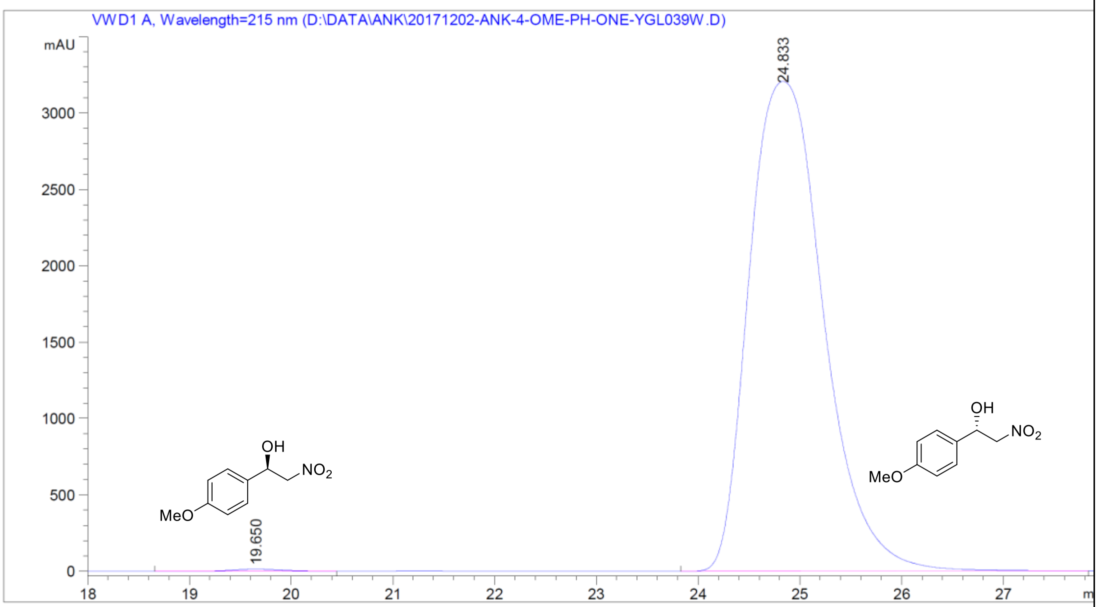
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.943	VV	0.5591	7.29983e4	1904.78662	93.2681
2	24.124	BB	0.5408	5268.90381	146.95996	6.7319

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(4-methoxyphenyl)-2-nitroethan-1-ol (2k)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=18.8 min (minor), t_R'=24.1 min (major)



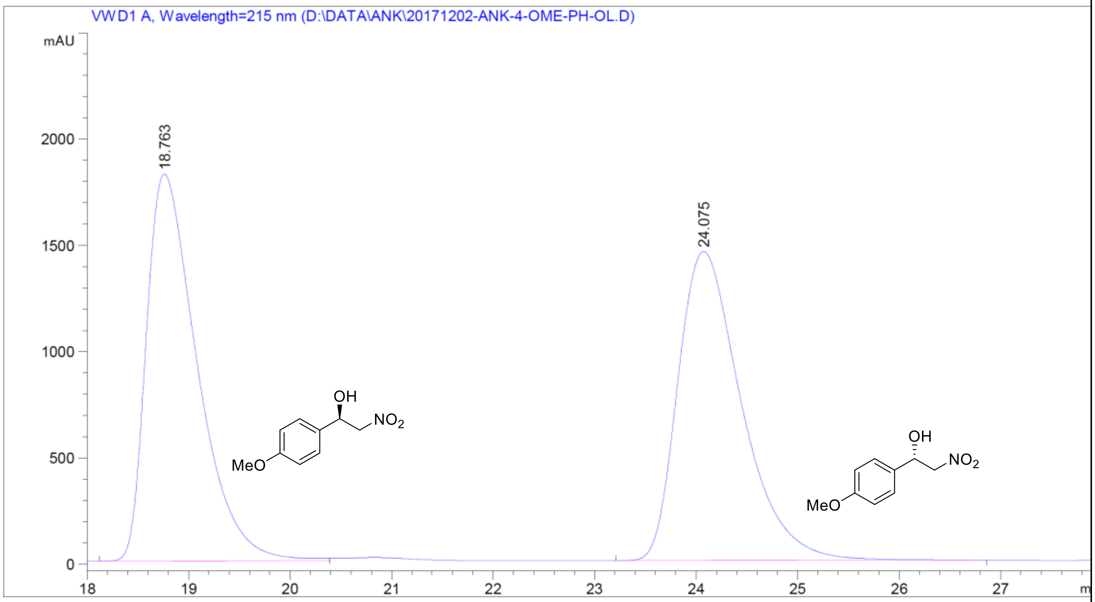
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.763	BV	0.5293	6.30614e4	1819.79443	49.9132
2	24.075	BB	0.6718	6.32808e4	1453.74915	50.0868



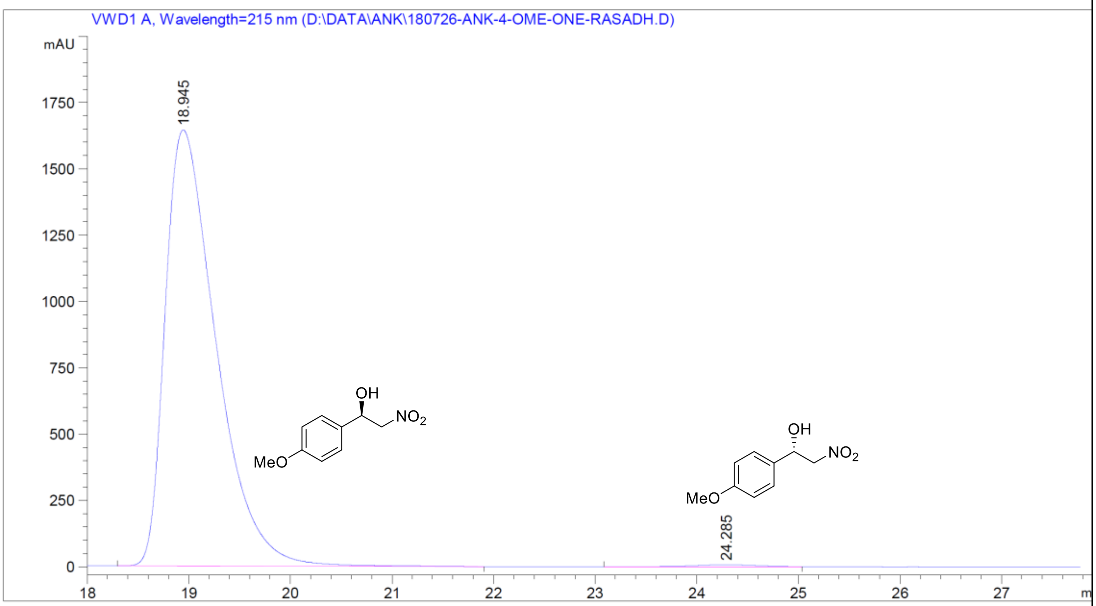
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.650	BB	0.5204	527.85754	15.42077	0.3222
2	24.833	BB	0.8017	1.63282e5	3208.38989	99.6778

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(4-methoxyphenyl)-2-nitroethan-1-ol (2k)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=18.8 min (major), t_R'=24.1 min (minor)



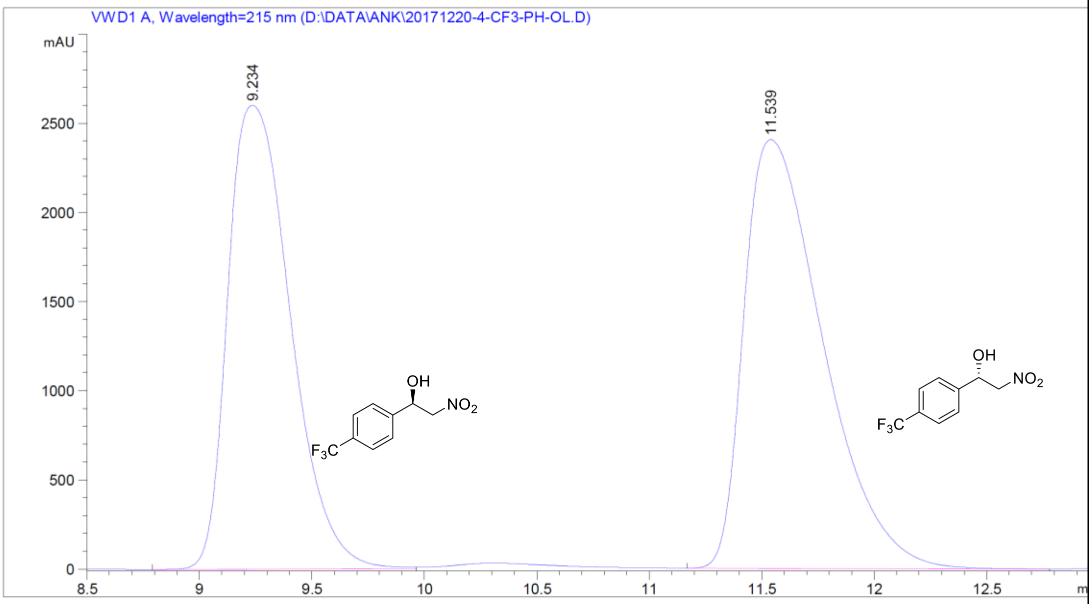
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.763	BV	0.5293	6.30614e4	1819.79443	49.9132
2	24.075	BB	0.6718	6.32808e4	1453.74915	50.0868



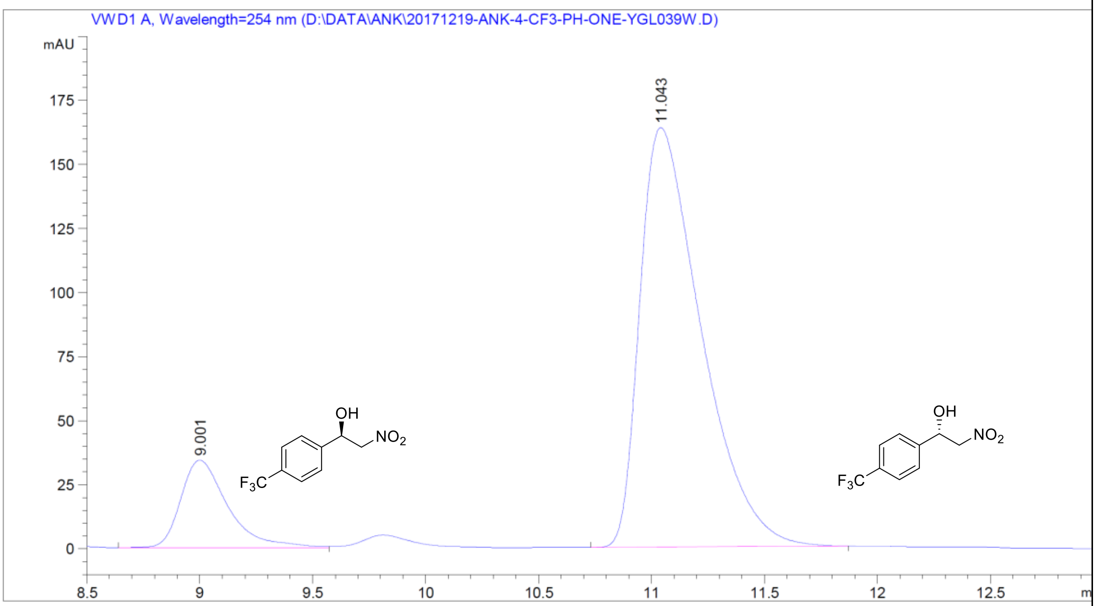
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.945	BV	0.5259	5.72397e4	1643.32092	99.4543
2	24.285	BB	0.5097	314.07745	7.31848	0.5457

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-2-nitro-1-(4-(trifluoromethyl)phenyl)ethan-1-ol (2l)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R=9.2 min (minor), t_R'=11.5 min (major)



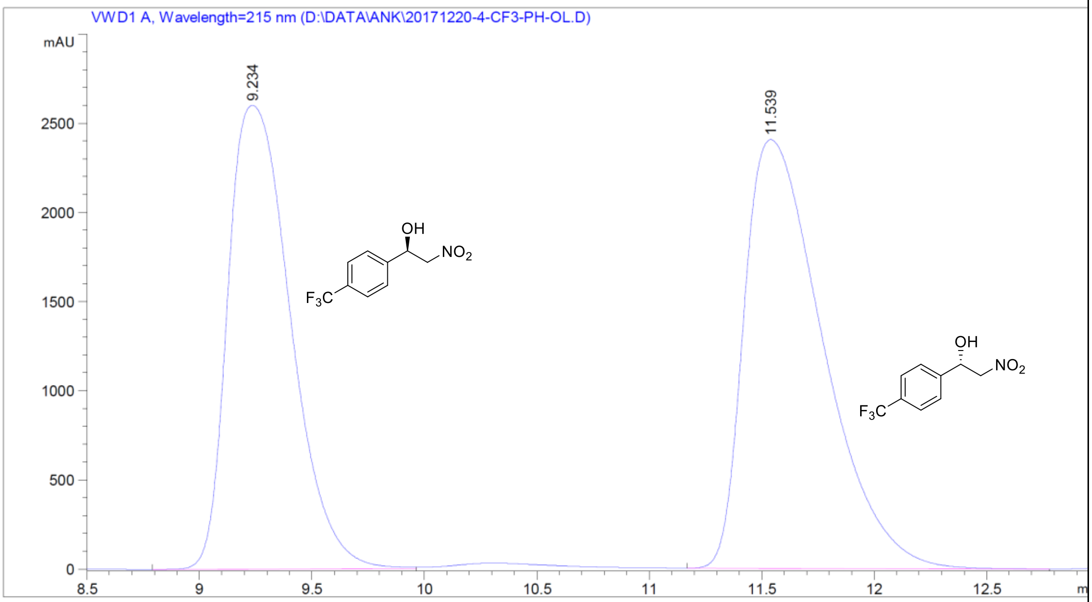
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.234	BV	0.3040	5.03843e4	2600.71362	46.2108
2	11.539	BB	0.3766	5.86471e4	2403.83960	53.7892



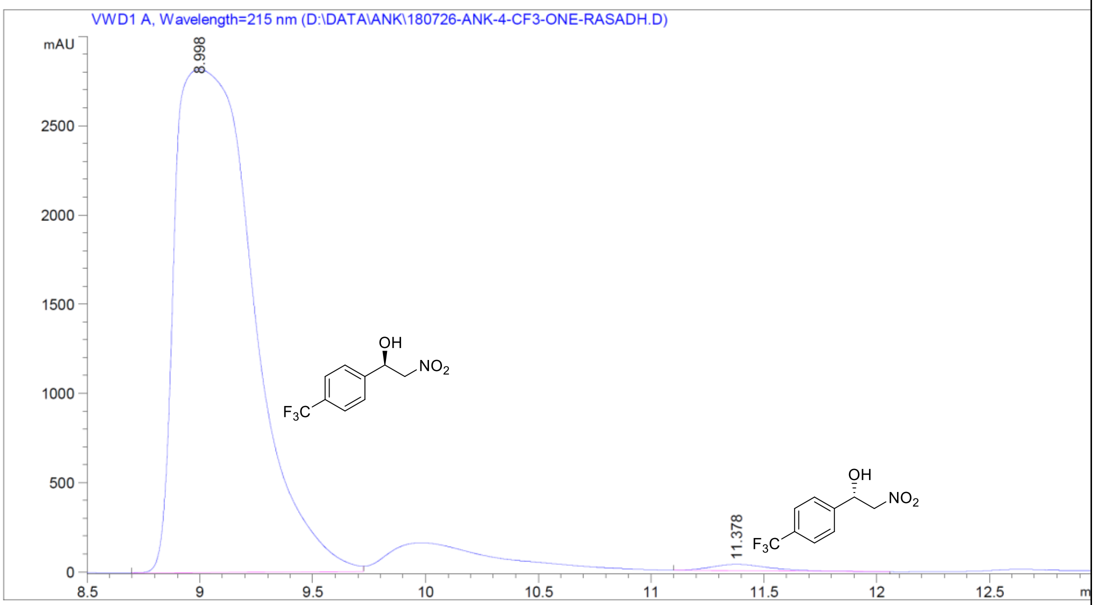
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.001	BV	0.2193	499.68204	34.23344	13.9044
2	11.043	BB	0.2865	3094.01733	163.71184	86.0956

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-2-nitro-1-(4-(trifluoromethyl)phenyl)ethan-1-ol (2l)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R=9.2 min (major), t_R'=11.5 min (minor)



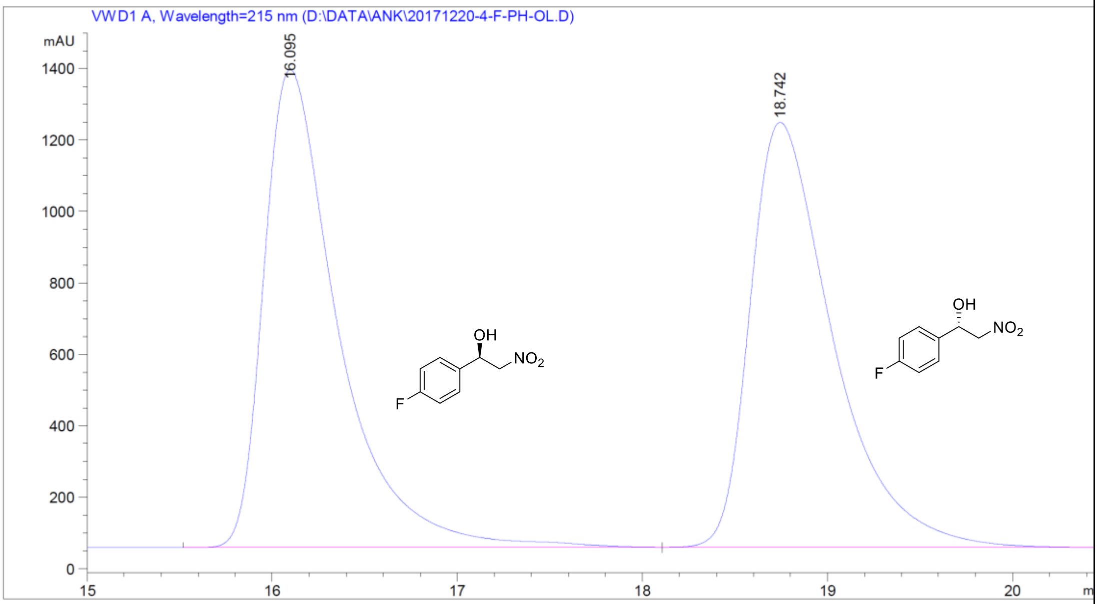
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.234	BV	0.3040	5.03843e4	2600.71362	46.2108
2	11.539	BB	0.3766	5.86471e4	2403.83960	53.7892



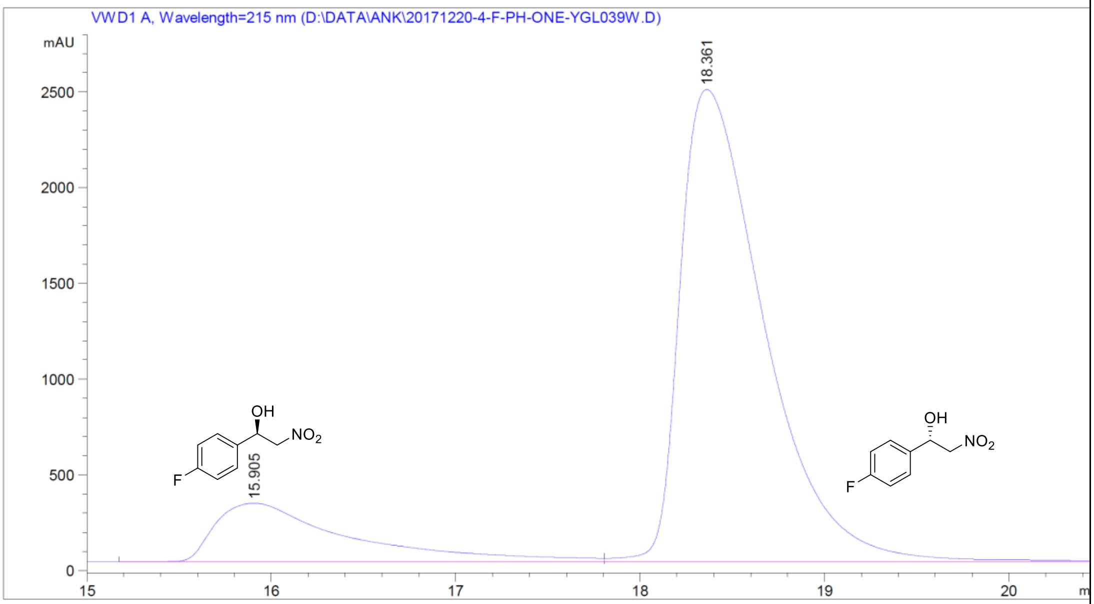
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.998	BV	0.3285	6.82199e4	2817.41479	99.0585
2	11.378	BB	0.2731	648.40070	35.74675	0.9415

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(4-fluorophenyl)-2-nitroethan-1-ol (2m)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R=16.1 min (minor), t_R'=18.7 min (major)



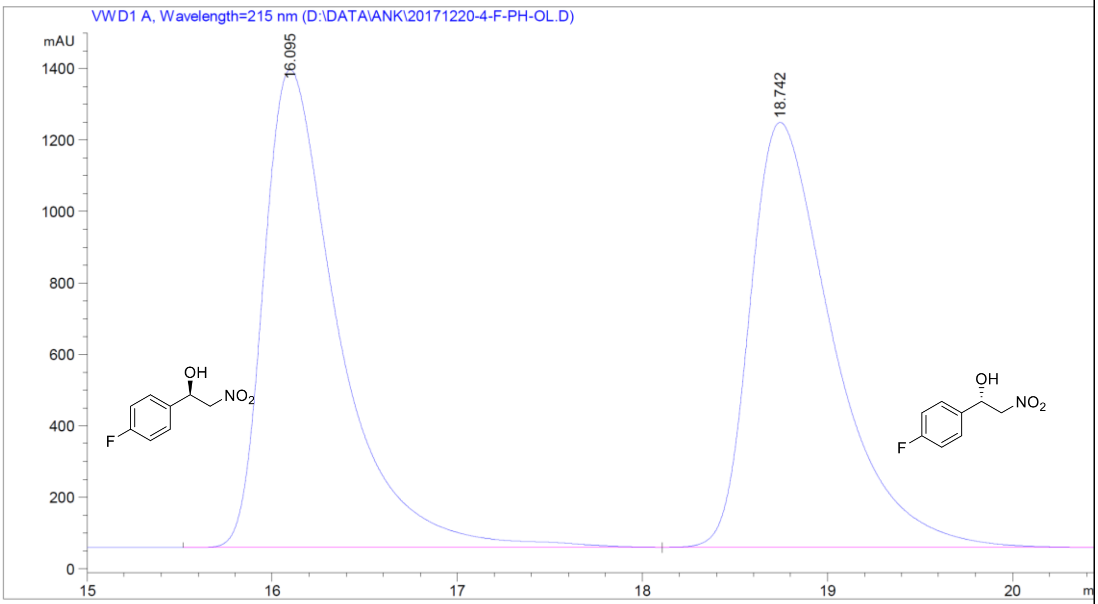
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.095	BB	0.4174	3.74493e4	1338.56348	50.1719
2	18.742	BV	0.4725	3.71927e4	1190.28674	49.8281



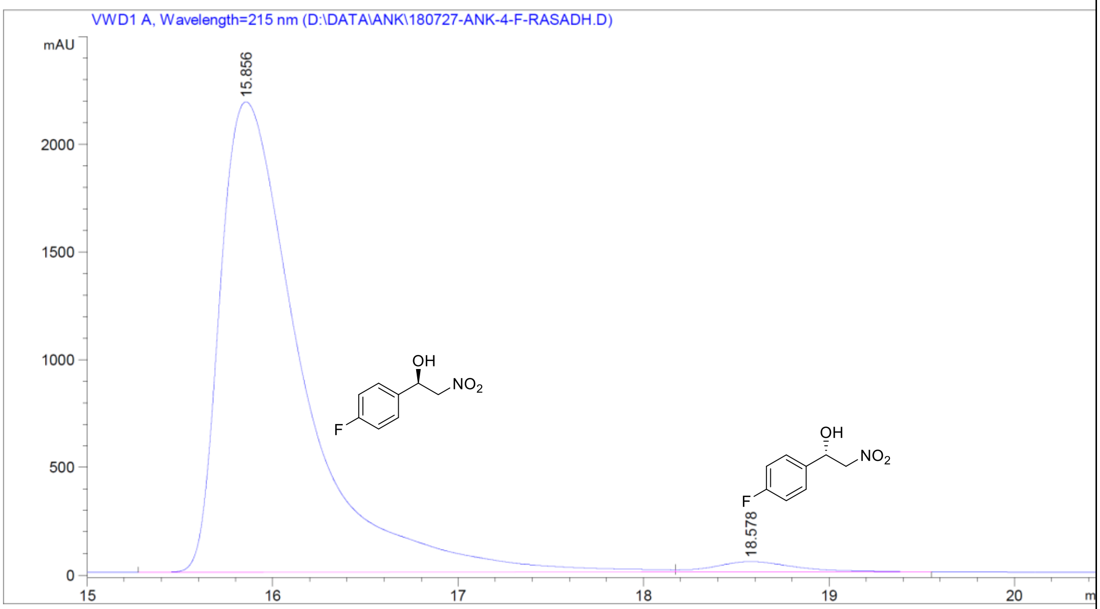
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.905	BV	0.7145	1.51495e4	304.46948	16.2450
2	18.361	VV	0.4846	7.81068e4	2465.36426	83.7550

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(4-fluorophenyl)-2-nitroethan-1-ol (2m)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 215 nm UV lamp, 26 °C, t_R=16.1 min (major), t_R'=18.7 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.095	BB	0.4174	3.74493e4	1338.56348	50.1719
2	18.742	BV	0.4725	3.71927e4	1190.28674	49.8281

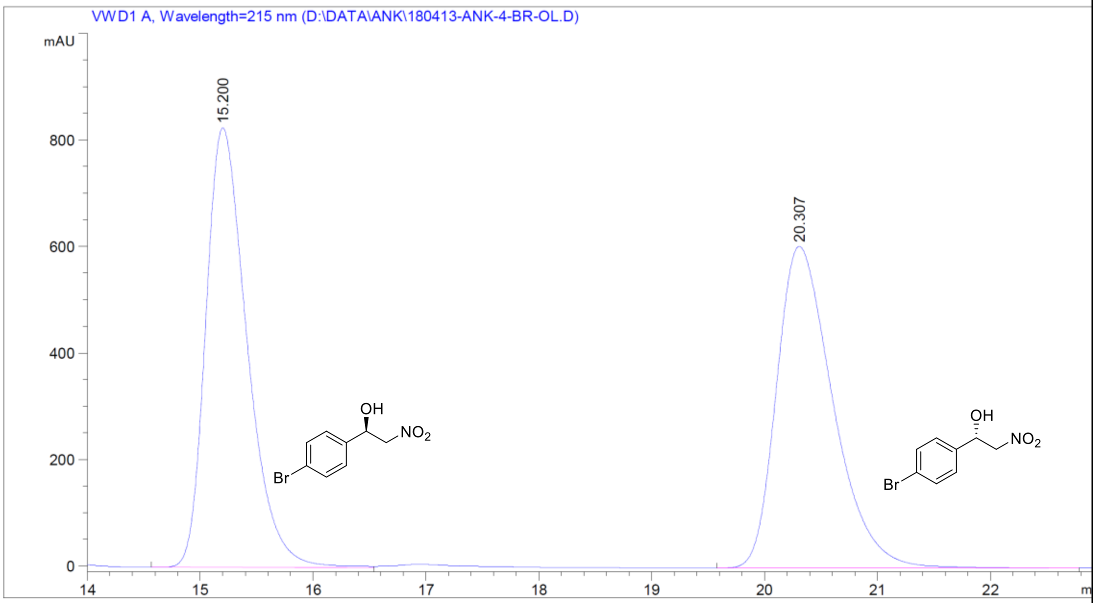


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.856	BV	0.4619	6.72981e4	2184.49292	97.8435
2	18.578	VB	0.4552	1483.26001	48.24824	2.1565

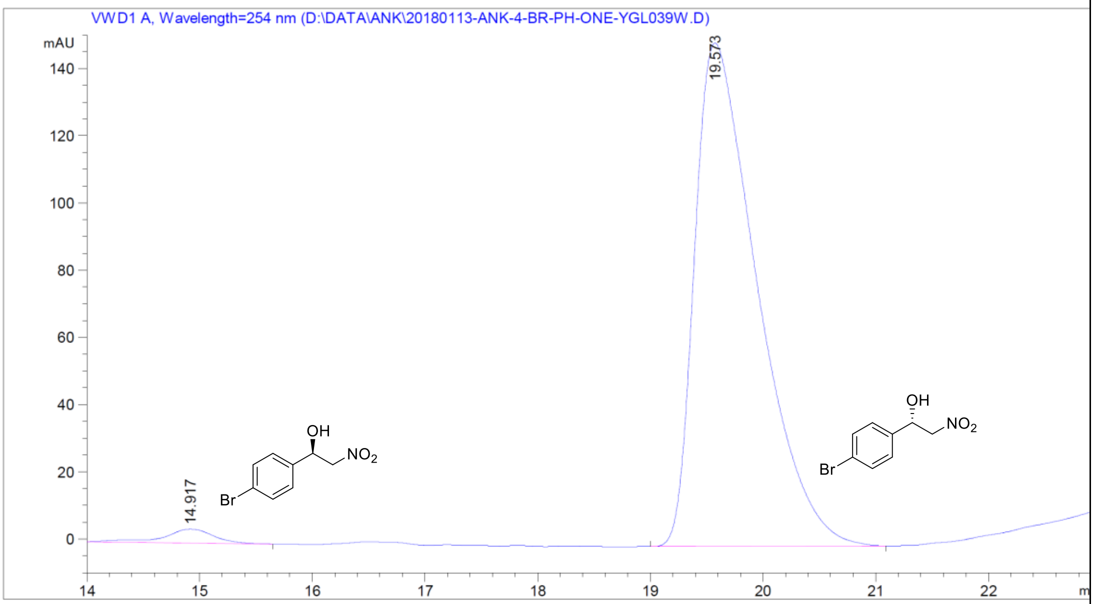
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-1-(4-bromophenyl)-2-nitroethan-1-ol (2n)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=15.2 min (minor), t_R'=20.3 min (major)



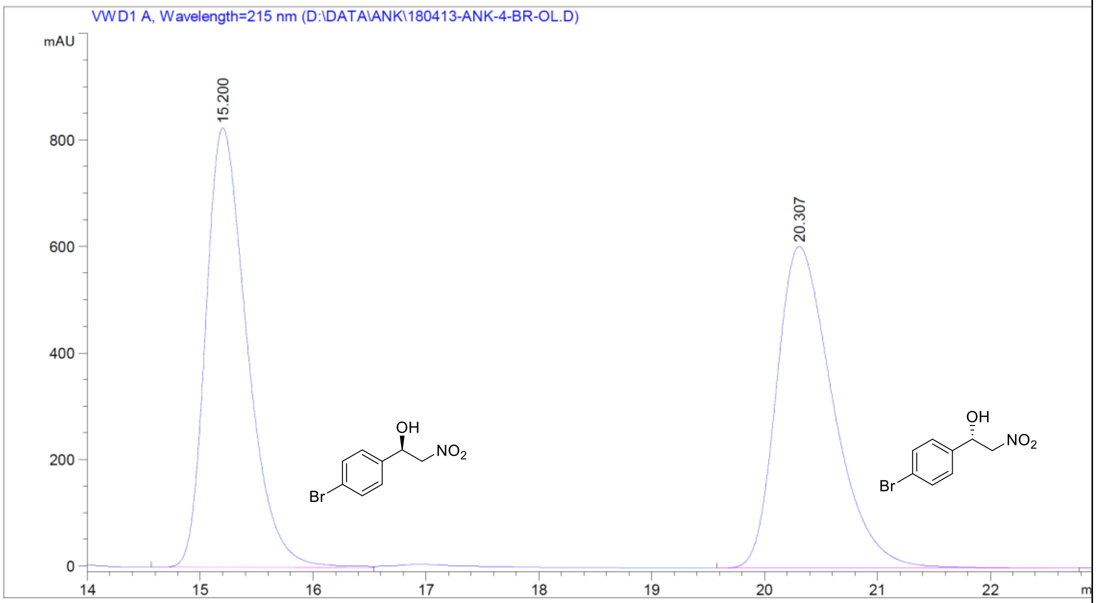
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.200	BV	0.3893	2.09426e4	824.67712	50.0133
2	20.307	BB	0.5357	2.09315e4	603.35590	49.9867



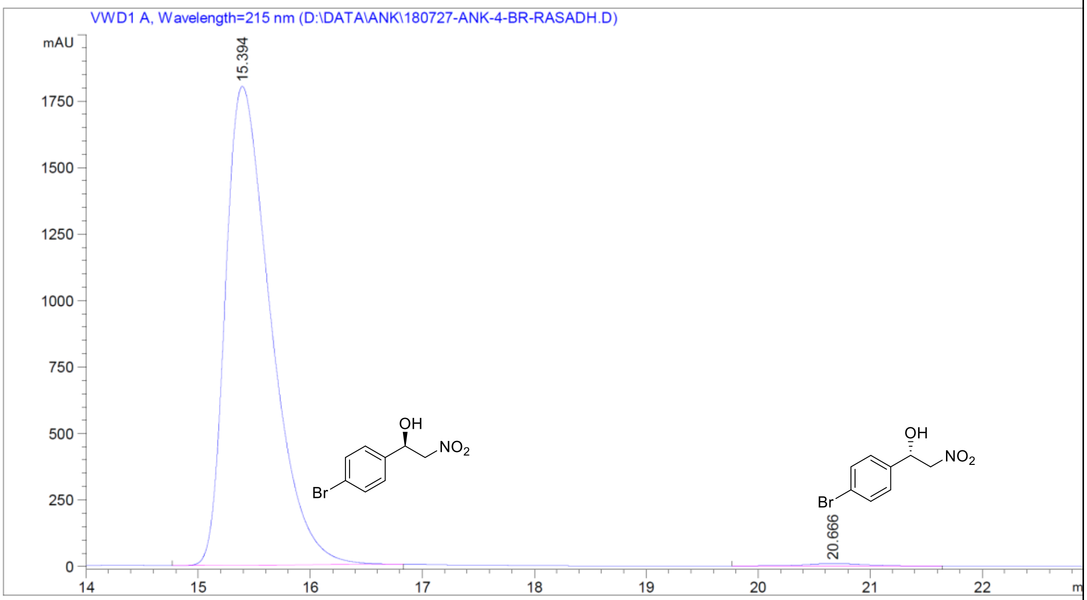
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.917	BB	0.4558	127.00278	4.13002	2.1567
2	19.573	BB	0.5948	5761.78076	149.77921	97.8433

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(4-bromophenyl)-2-nitroethan-1-ol (2n)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=15.2 min (major), t_R'=20.3 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.200	BV	0.3893	2.09426e4	824.67712	50.0133
2	20.307	BB	0.5357	2.09315e4	603.35590	49.9867

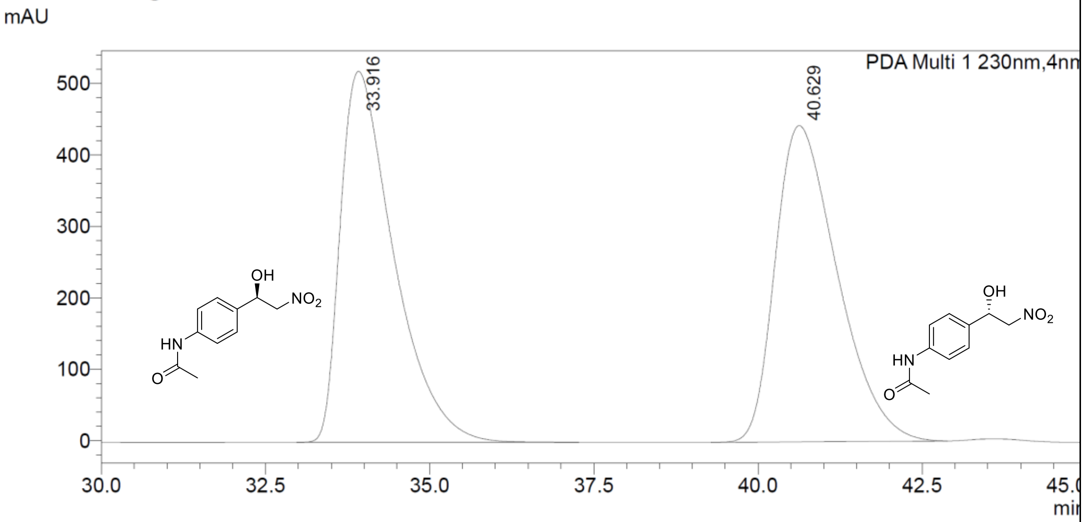


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.394	BB	0.4260	5.05389e4	1800.50500	99.2964
2	20.666	BB	0.4654	358.13092	9.10520	0.7036

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-N-(4-(1-hydroxy-2-nitroethyl)phenyl)acetamide (2o)**
Chiracel® IC, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 230 nm UV lamp, 24 °C, t_R=33.9 min (minor), t_R’=40.6 min (major)

<Chromatogram>

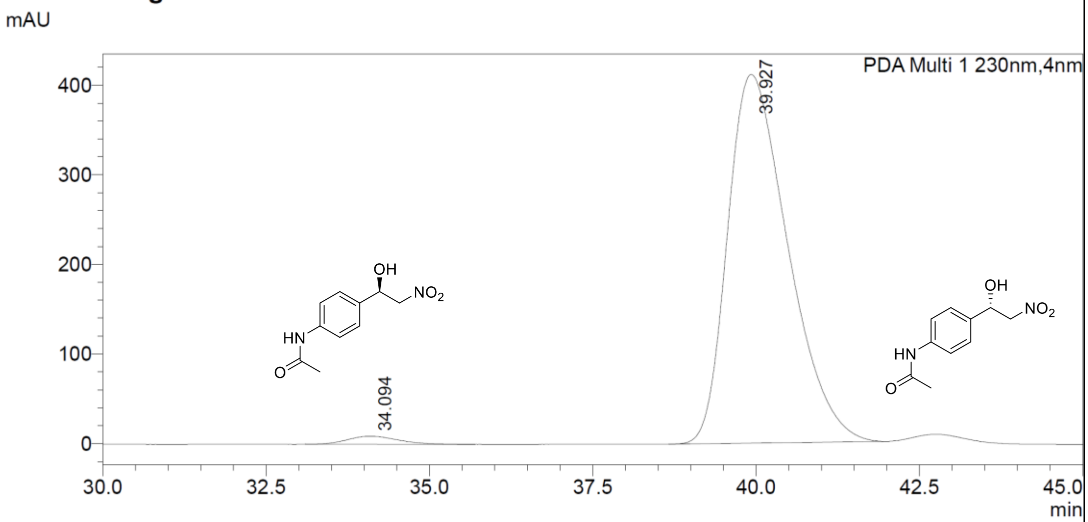


<Peak Table>

PDA Ch1 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	33.916	29440002	519496	50.211			
2	40.629	29192300	442772	49.789			
Total		58632302	962267				

<Chromatogram>



<Peak Table>

PDA Ch1 230nm

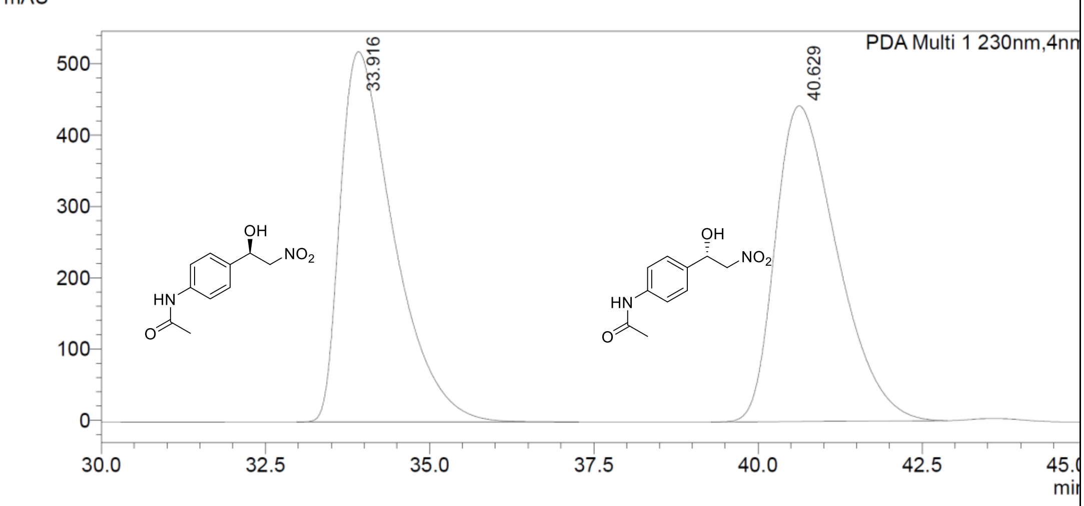
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	34.094	482716	8989	1.796			
2	39.927	26398071	411381	98.204			
Total		26880787	420370				

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-N-(4-(1-hydroxy-2-nitroethyl)phenyl)acetamide (2o)**

Chiracel® IC, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 230 nm UV lamp, 24 °C, t_R=33.9 min (major), t_R'=40.6 min (minor)

<Chromatogram>

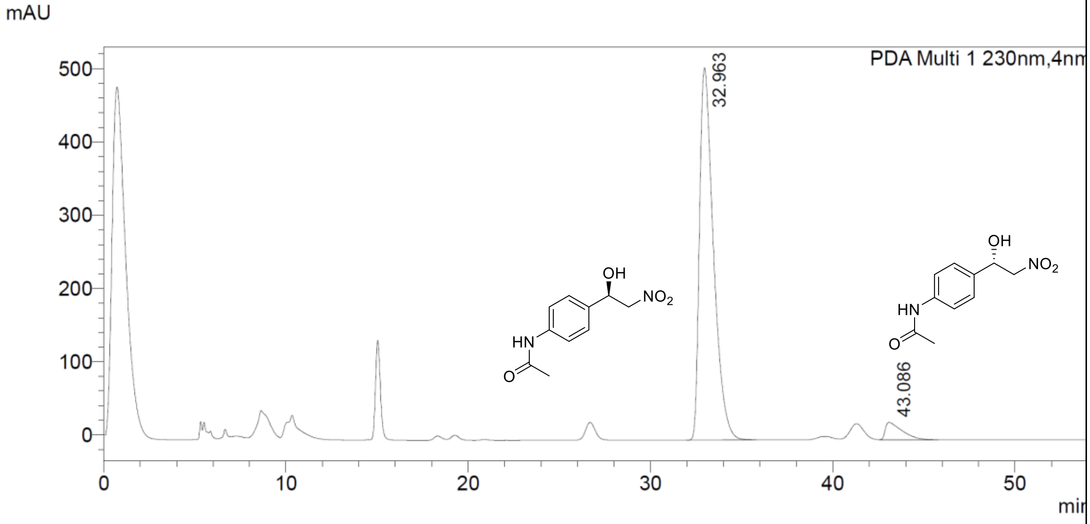


<Peak Table>

PDA Ch1 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	33.916	29440002	519496	50.211			
2	40.629	29192300	442772	49.789			
Total		58632302	962267				

<Chromatogram>



<Peak Table>

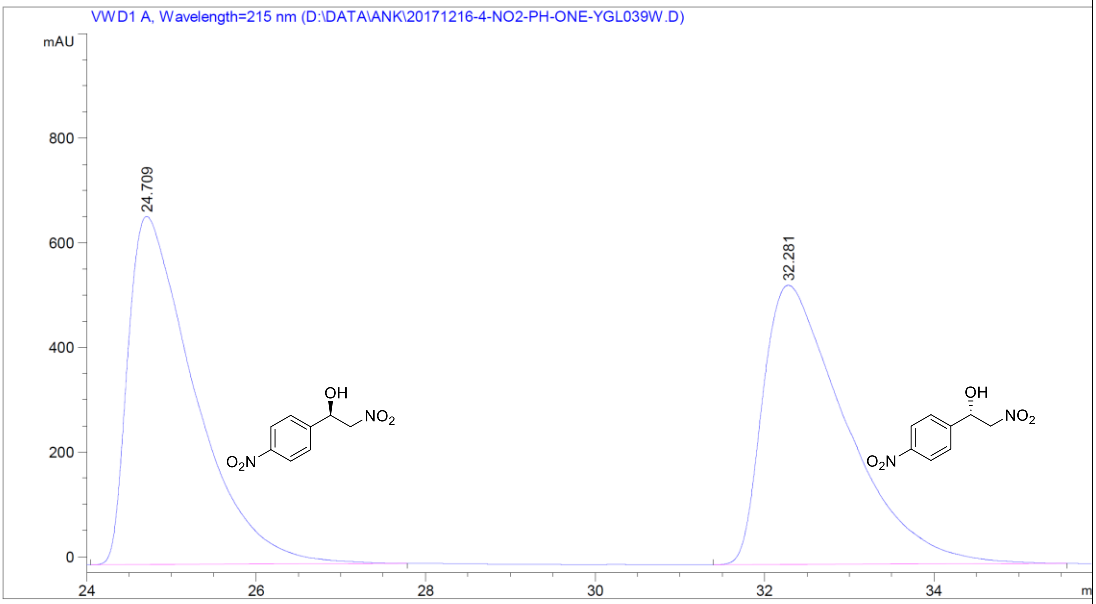
PDA Ch1 230nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	32.963	27029865	508402	94.694			
2	43.086	1514705	23668	5.306			
Total		28544570	532070				

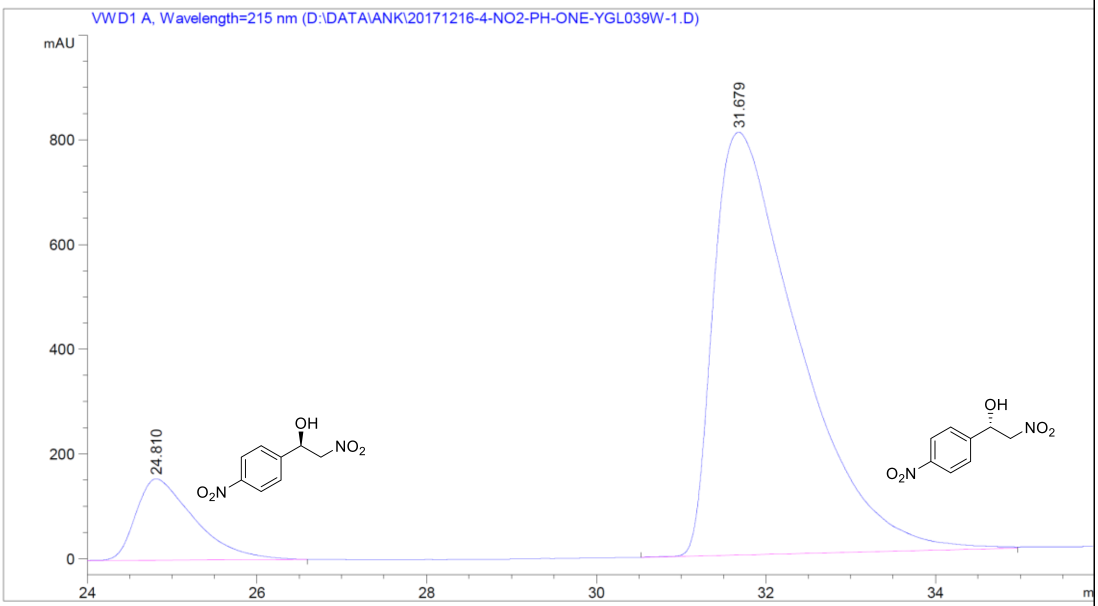
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-2-nitro-1-(4-nitrophenyl)ethan-1-ol (2p)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=24.7 min (minor), t_R'=32.3 min (major)



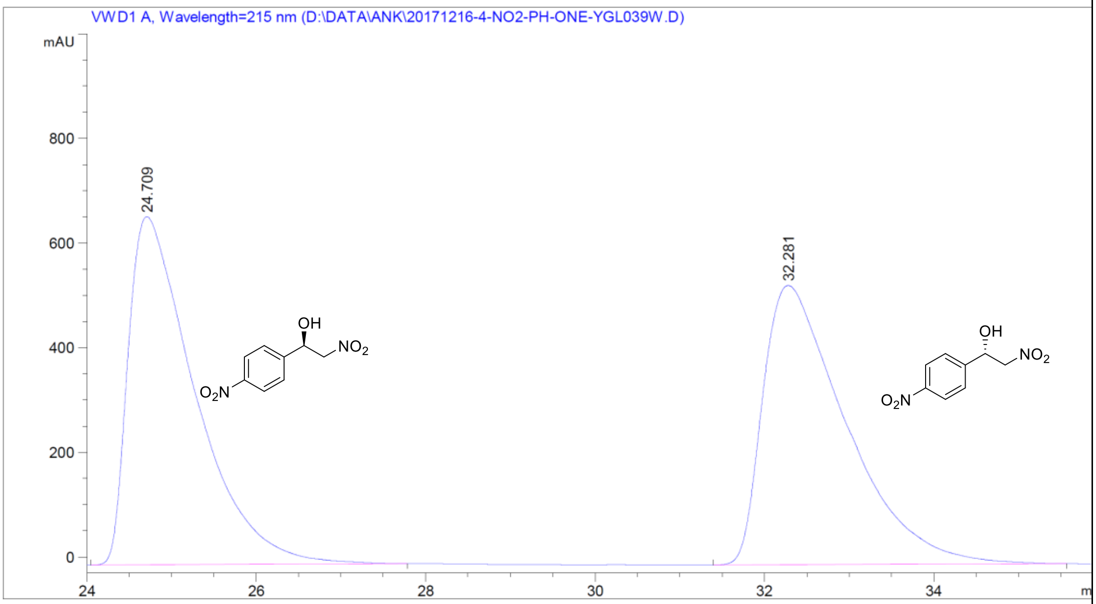
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.709	BB	0.7812	3.63517e4	665.58405	49.9804
2	32.281	BB	0.9810	3.63803e4	533.87085	50.0196



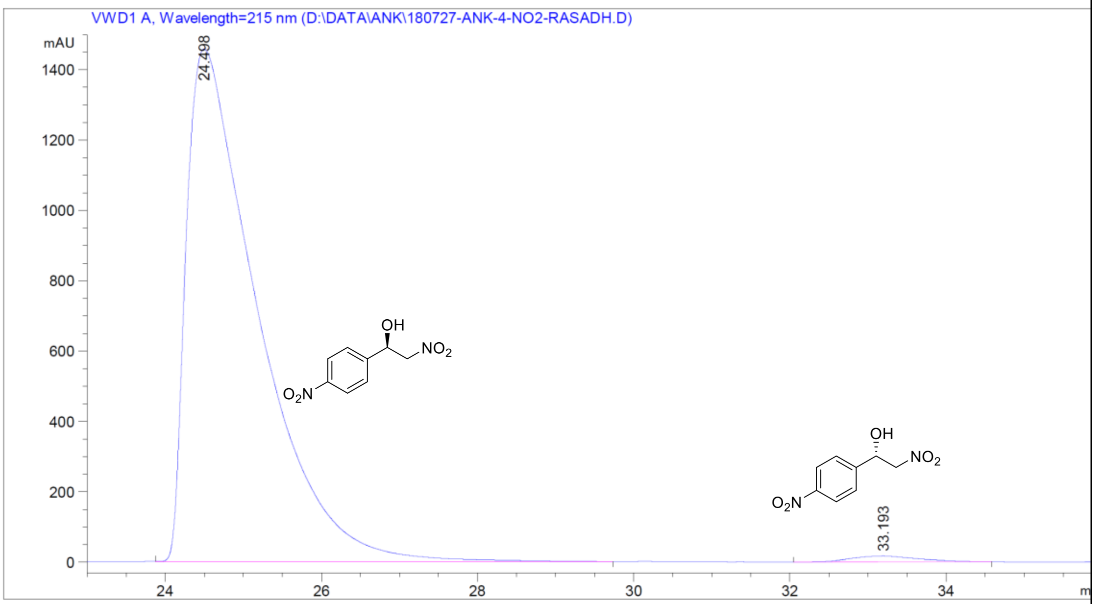
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.810	BB	0.7071	7406.49023	155.38113	11.6047
2	31.679	BV	1.0102	5.64167e4	807.40222	88.3953

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-2-nitro-1-(4-nitrophenyl)ethan-1-ol (2p)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=24.7 min (major), t_R'=32.3 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.709	BB	0.7812	3.63517e4	665.58405	49.9804
2	32.281	BB	0.9810	3.63803e4	533.87085	50.0196

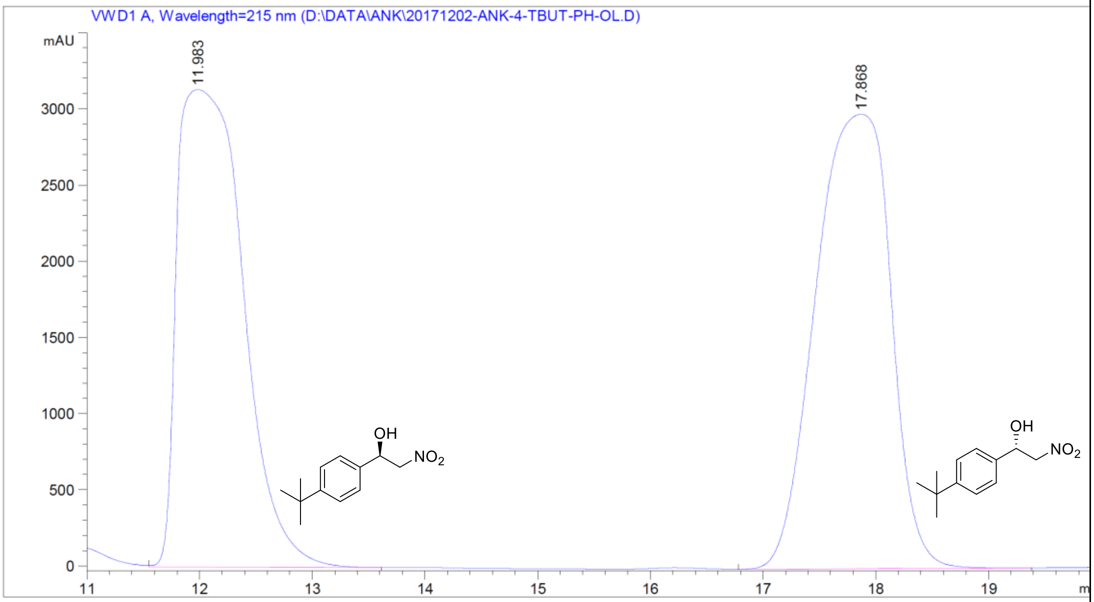


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.498	VB	0.8850	9.23436e4	1458.82251	98.8951
2	33.193	BB	0.7261	1031.74976	17.30431	1.1049

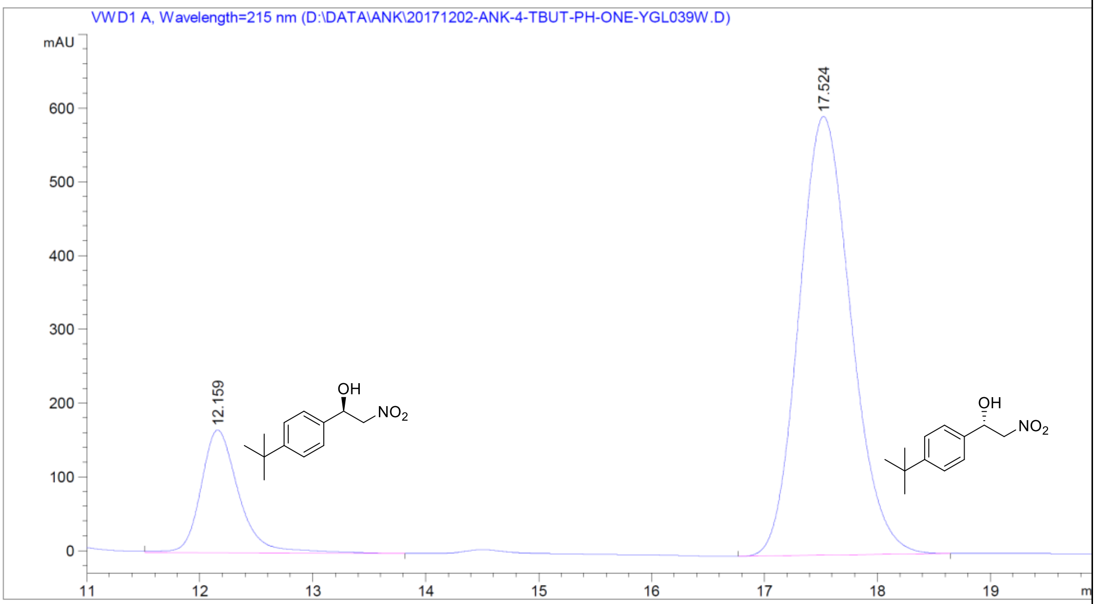
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*S*)-1-(4-(tert-butyl)phenyl)-2-nitroethan-1-ol (2q)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=12.0 min (minor), t_R'=17.9 min (major)



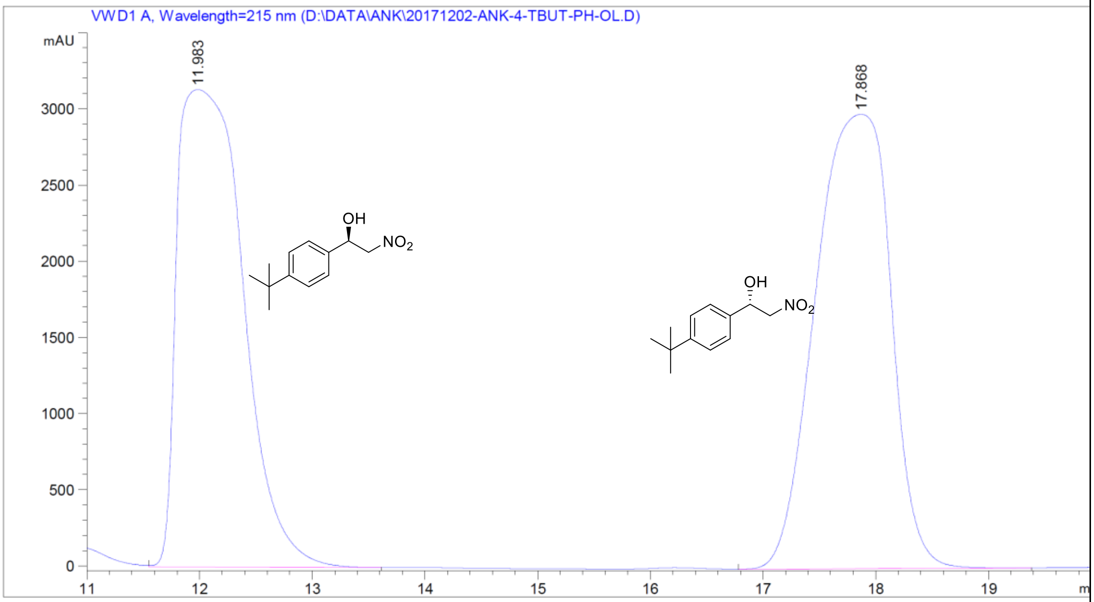
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.983	VB	0.6511	1.27908e5	3134.18164	48.0361
2	17.868	BB	0.7463	1.38367e5	2982.42456	51.9639



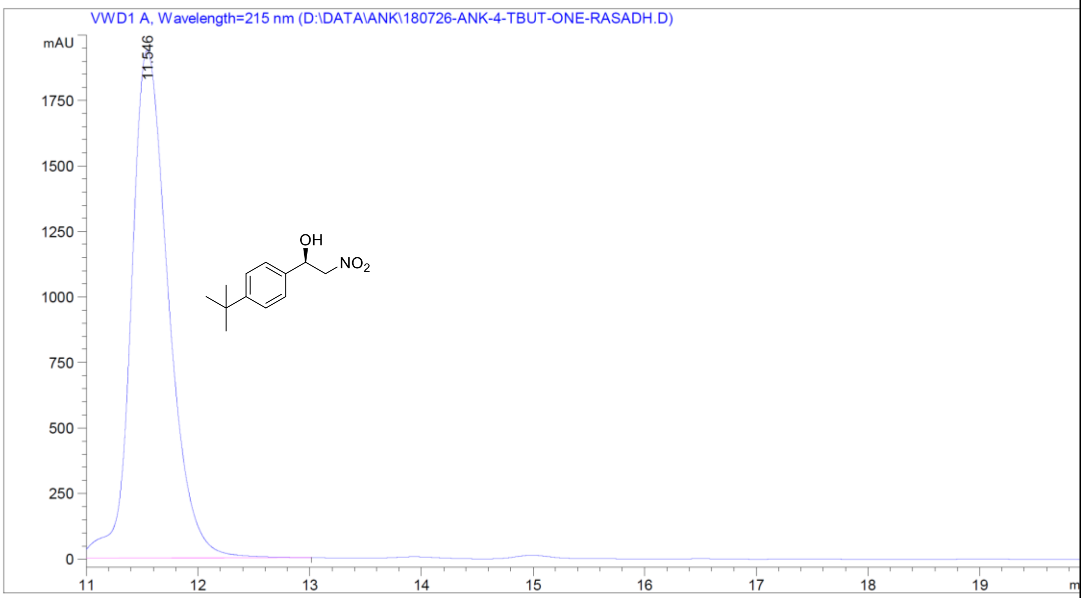
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.159	VB	0.3555	3901.23169	166.43982	16.9747
2	17.524	BB	0.4993	1.90814e4	594.79913	83.0253

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(4-(tert-butyl)phenyl)-2-nitroethan-1-ol (2q)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=12.0 min (major), t_R'=17.9 min (minor)



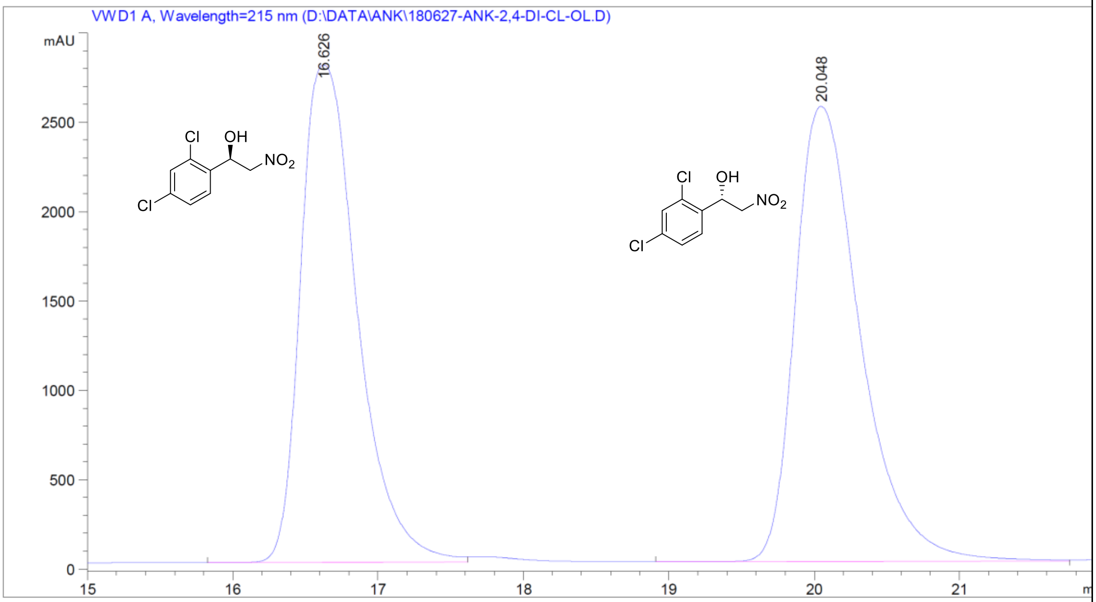
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.983	VB	0.6511	1.27908e5	3134.18164	48.0361
2	17.868	BB	0.7463	1.38367e5	2982.42456	51.9639



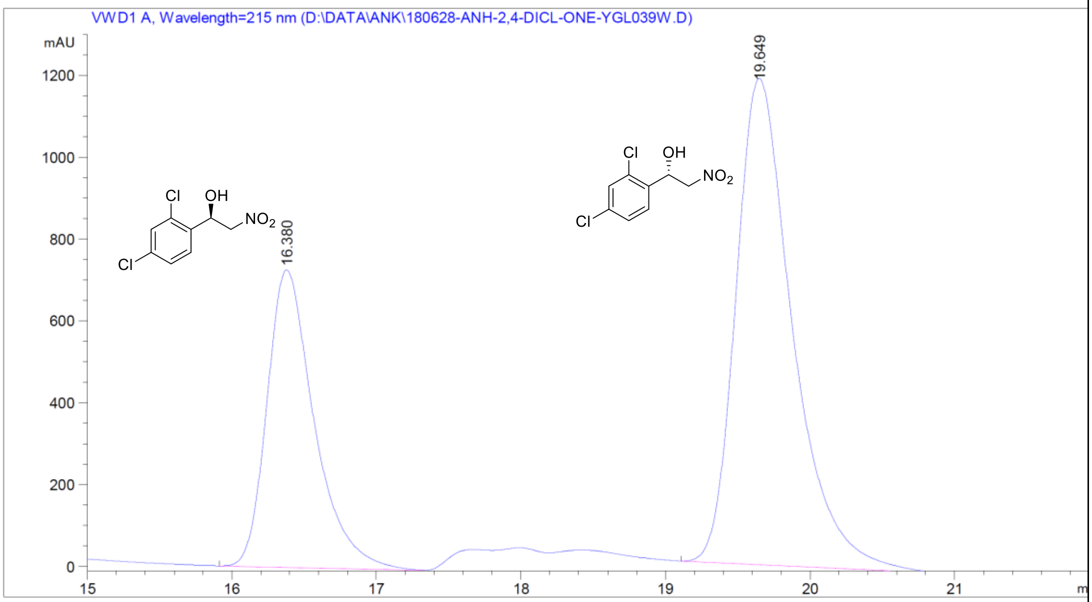
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.546	VB	0.3534	4.48393e4	1938.04541	100.0000

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(2,4-Dichlorophenyl)-2-nitroethanol (2r)**
Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=16.6 min (minor), t_R'=20.0 min (major)



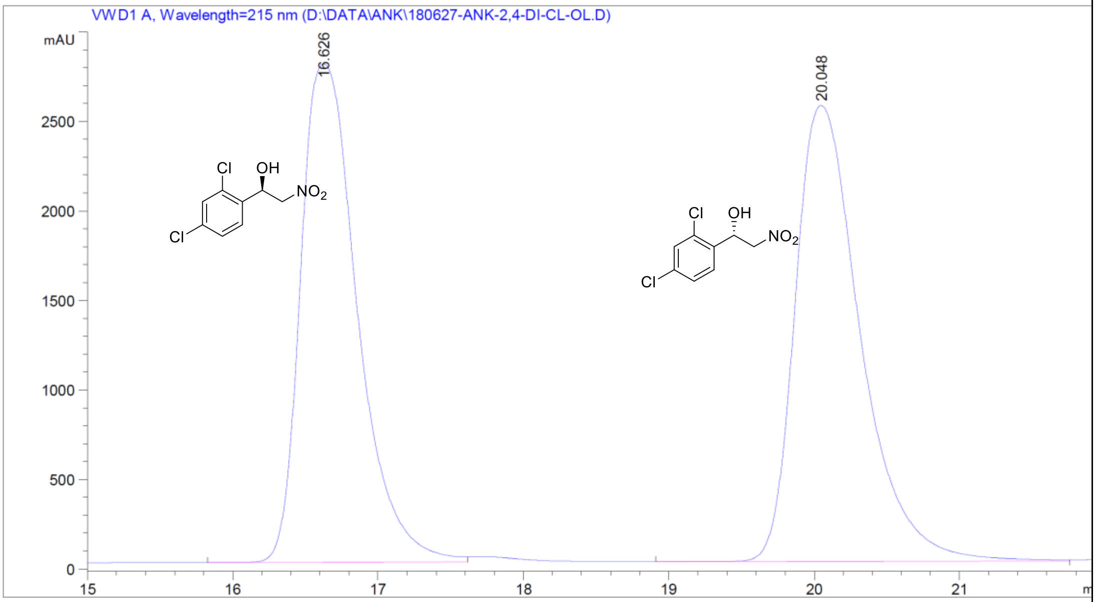
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.626	BV	0.4162	7.53754e4	2781.08545	48.7087
2	20.048	BV	0.4759	7.93721e4	2544.58569	51.2913



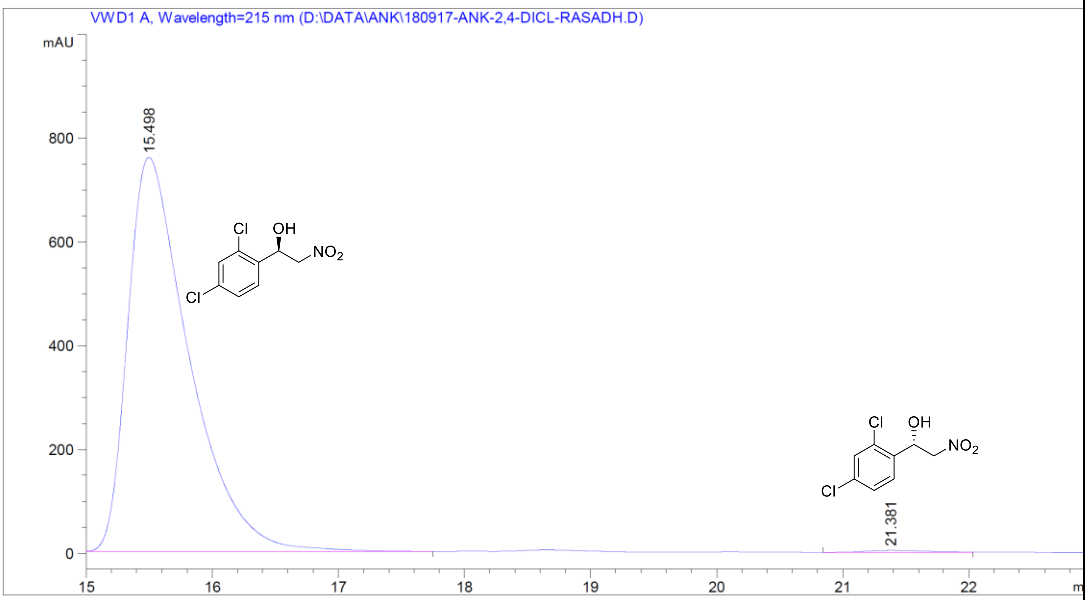
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.380	BB	0.3444	1.64745e4	726.91077	33.7647
2	19.649	BB	0.4094	3.23175e4	1187.88062	66.2353

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(2,4-Dichlorophenyl)-2-nitroethanol (2r)**
Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.5 mL/min flow rate, 215 nm UV lamp, 25 °C, t_R=16.6 min (major), t_R'=20.0 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.626	BV	0.4162	7.53754e4	2781.08545	48.7087
2	20.048	BV	0.4759	7.93721e4	2544.58569	51.2913

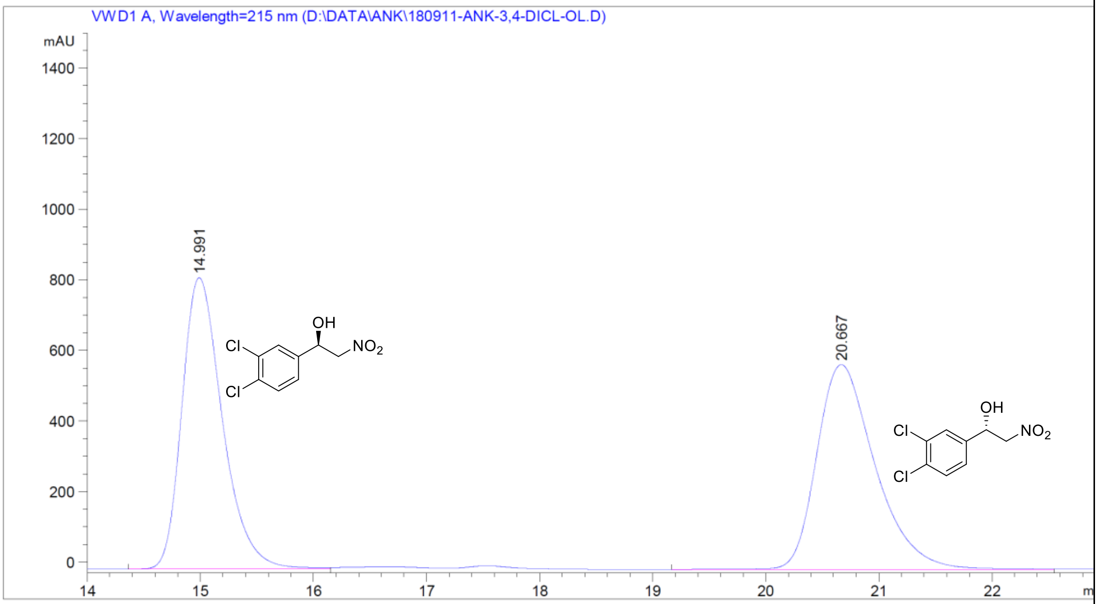


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.498	BB	0.5015	2.56593e4	759.73352	99.4344
2	21.381	BV	0.4443	145.94740	3.87626	0.5656

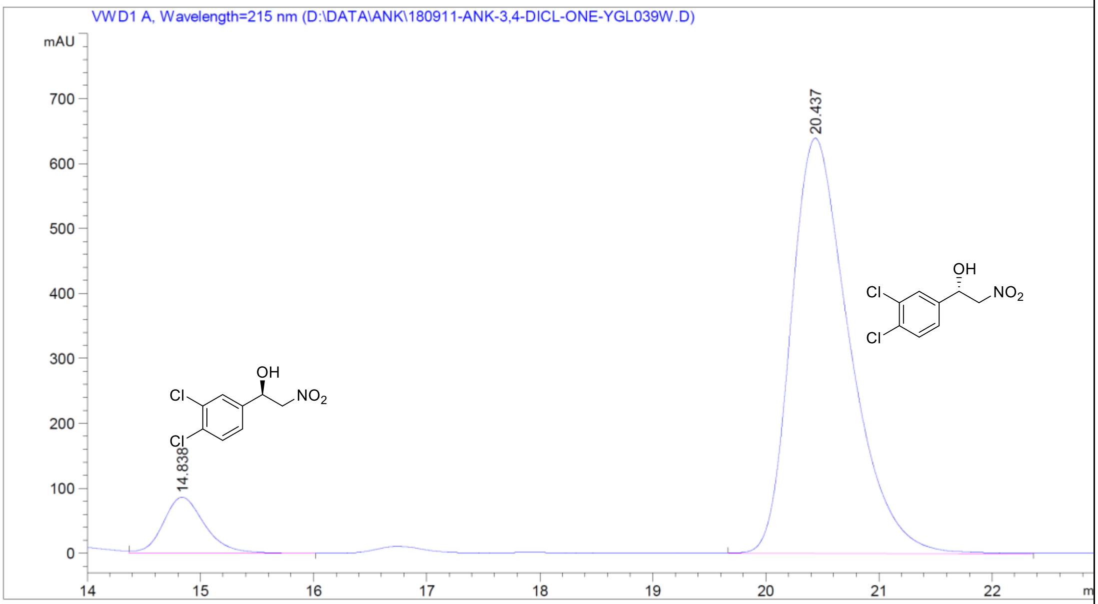
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(3,4-dichlorophenyl)-2-nitroethan-1-ol (2s)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=15.0 min (minor), t_R'=20.7 min (major)



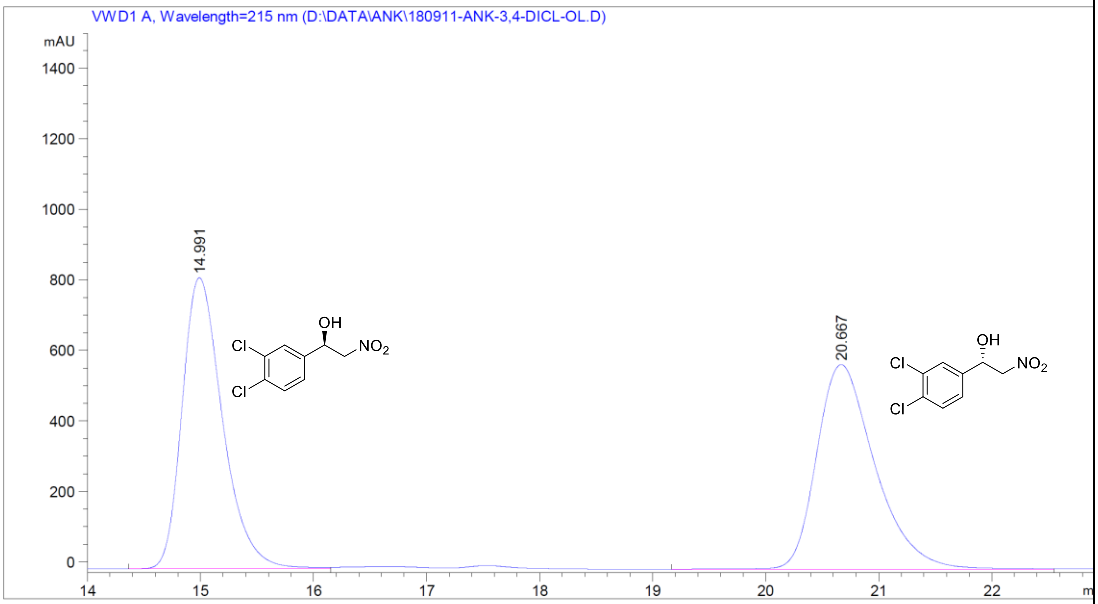
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.991	BV	0.3829	2.05965e4	826.09167	49.5847
2	20.667	BV	0.5484	2.09415e4	581.10333	50.4153



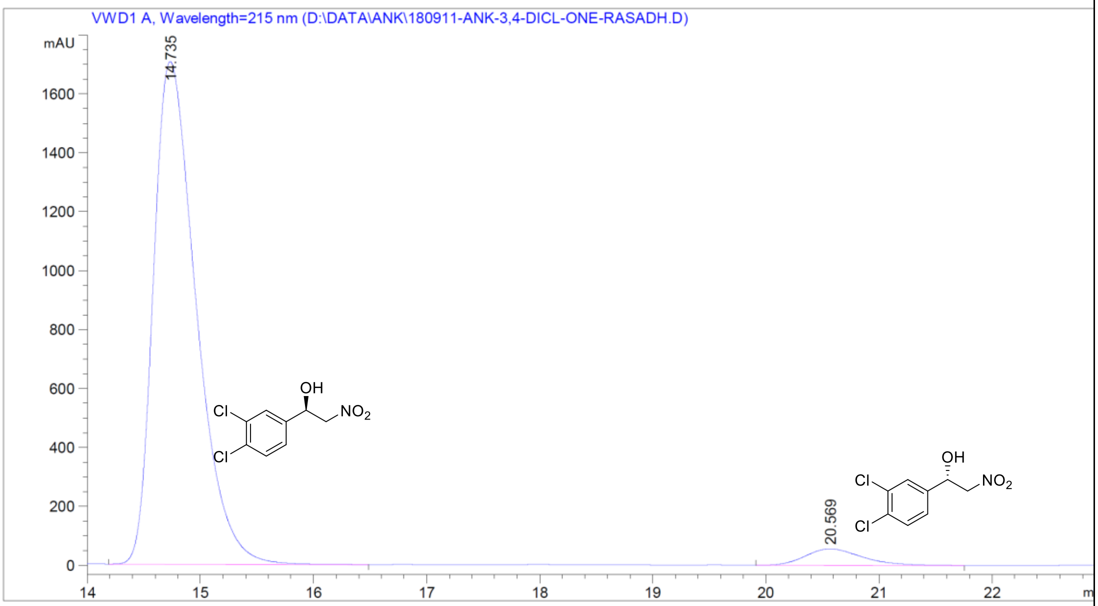
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.838	VB	0.3921	2225.00879	86.51270	8.8173
2	20.437	VV	0.5479	2.30096e4	639.36481	91.1827

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(3,4-dichlorophenyl)-2-nitroethan-1-ol (2s)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=15.0 min (major), t_R'=20.7 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.991	BV	0.3829	2.05965e4	826.09167	49.5847
2	20.667	BV	0.5484	2.09415e4	581.10333	50.4153

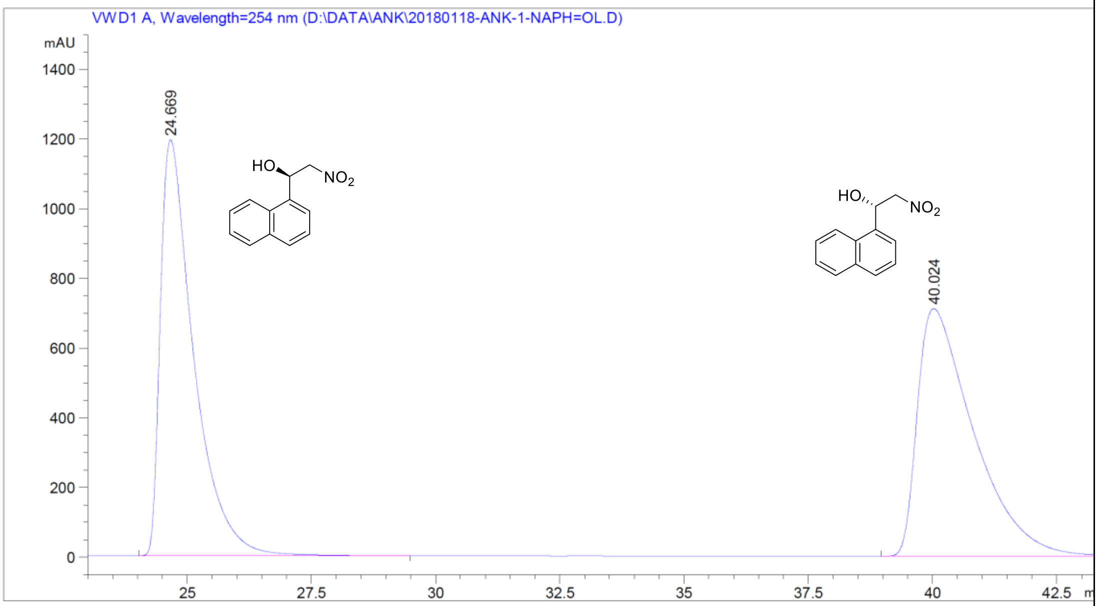


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.735	VV	0.4059	4.47203e4	1705.68335	95.8059
2	20.569	VB	0.5372	1957.71277	55.81910	4.1941

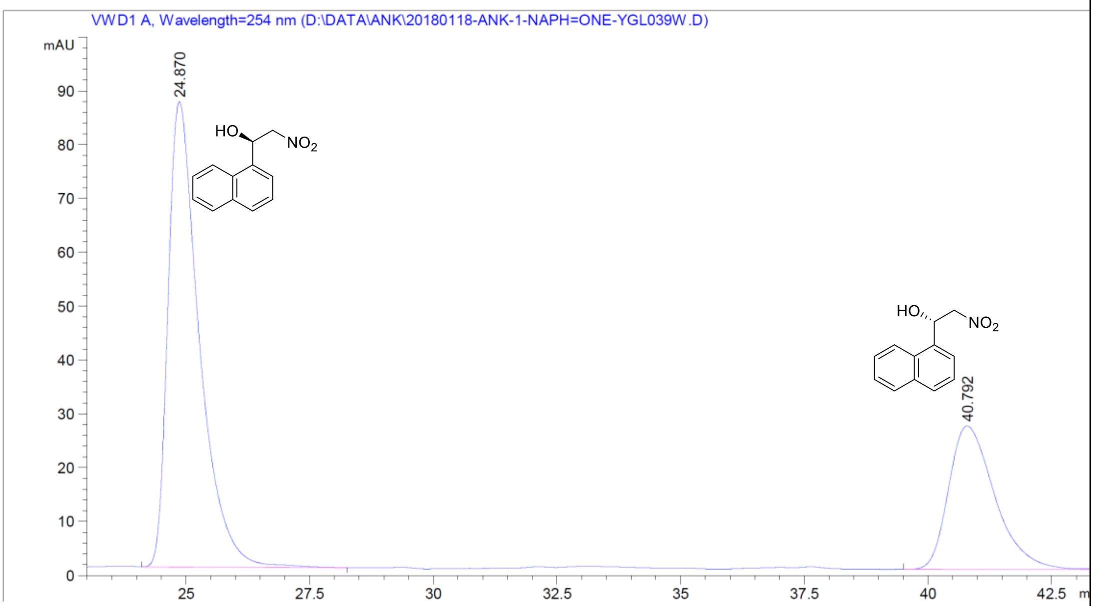
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(R)-1-(1-Naphthyl)-2-nitroethanol (2t)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 254 nm UV lamp, 26 °C, t_R=24.7 min (major), t_R'=40.0 min (minor)



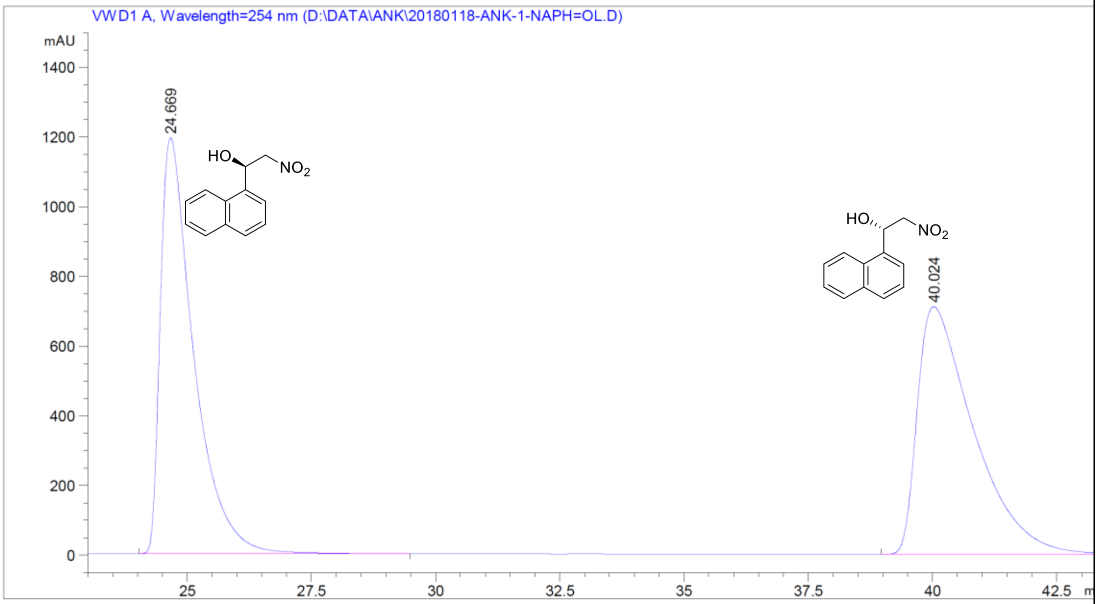
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.669	BB	0.6866	5.55244e4	1193.82434	49.8607
2	40.024	BV	1.1647	5.58346e4	710.57660	50.1393



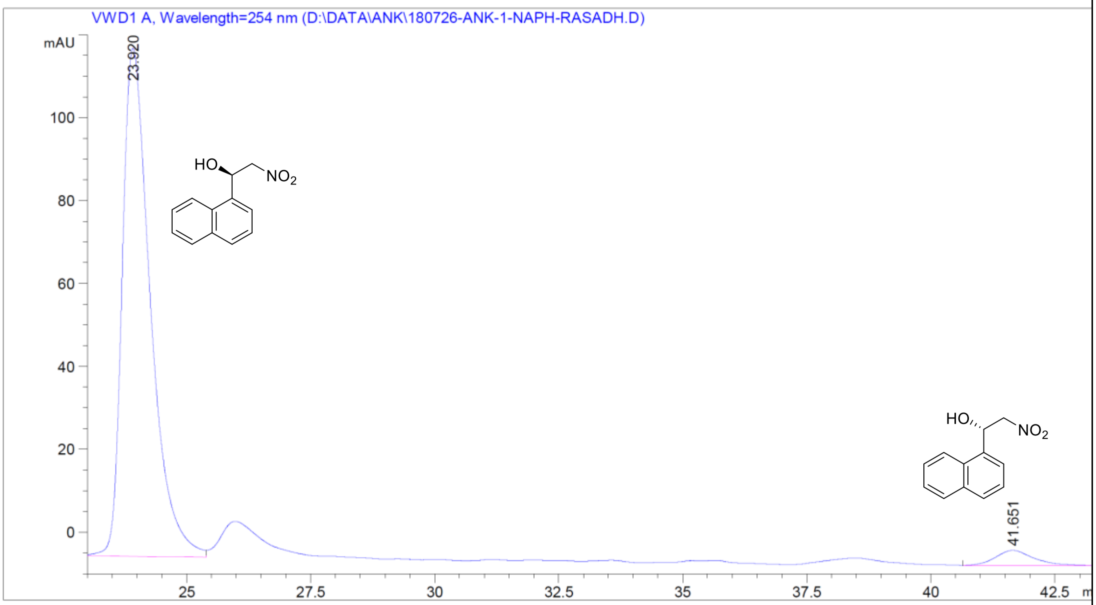
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.870	BB	0.6613	3803.26855	86.43652	68.5910
2	40.792	BV	1.0183	1741.58447	26.65335	31.4090

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(R)*-1-(1-Naphthyl)-2-nitroethanol (2t)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.5 mL/min flow rate, 254 nm UV lamp, 26 °C, t_R=24.7 min (major), t_R'=40.0 min (minor)



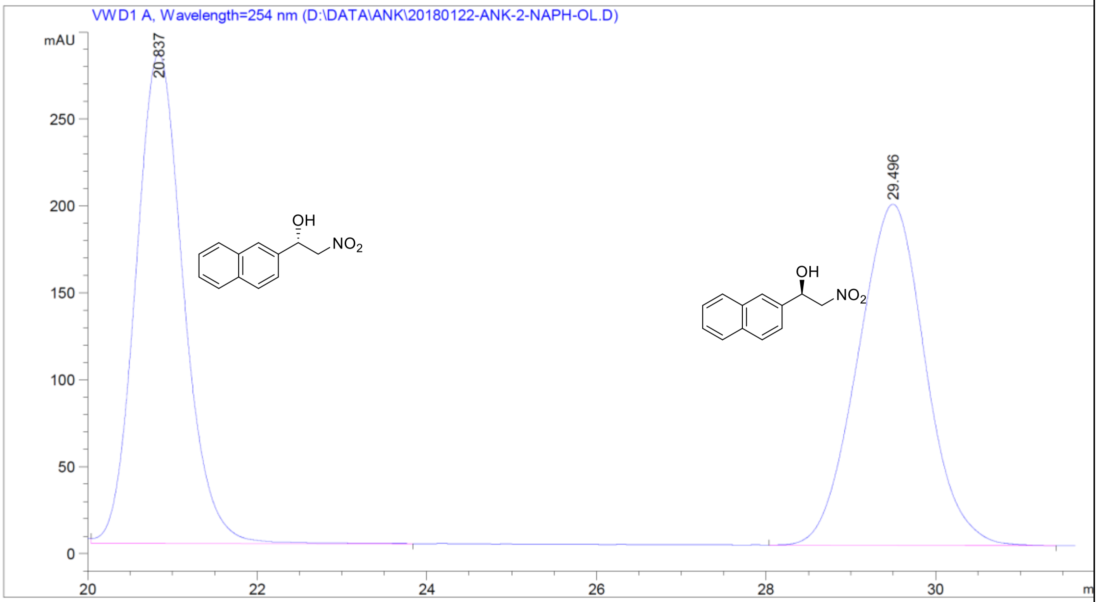
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.669	BB	0.6866	5.55244e4	1193.82434	49.8607
2	40.024	BV	1.1647	5.58346e4	710.57660	50.1393



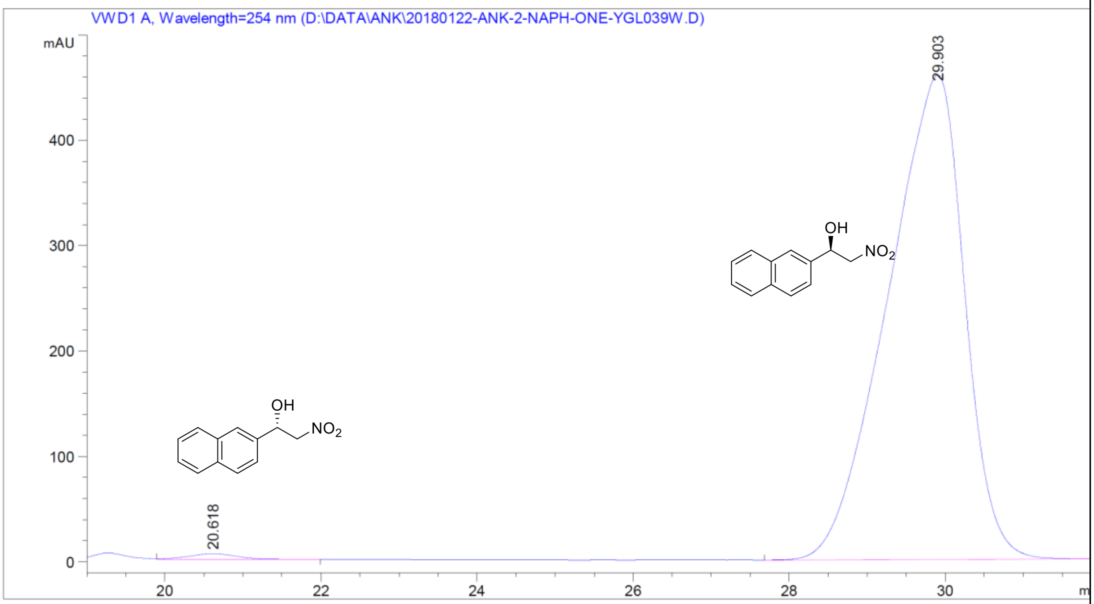
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.920	VV	0.5970	4837.31543	122.43050	95.9986
2	41.651	BBA	0.8087	201.63011	3.67147	4.0014

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(S)*-1-(naphthalen-2-yl)-2-nitroethan-1-ol (2u)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 254 nm UV lamp, 24 °C, t_R=20.8 min (minor), t_R'=29.5 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.837	VB	0.5991	1.09844e4	281.60336	50.2624
2	29.496	BBA	0.8583	1.08697e4	196.22868	49.7376

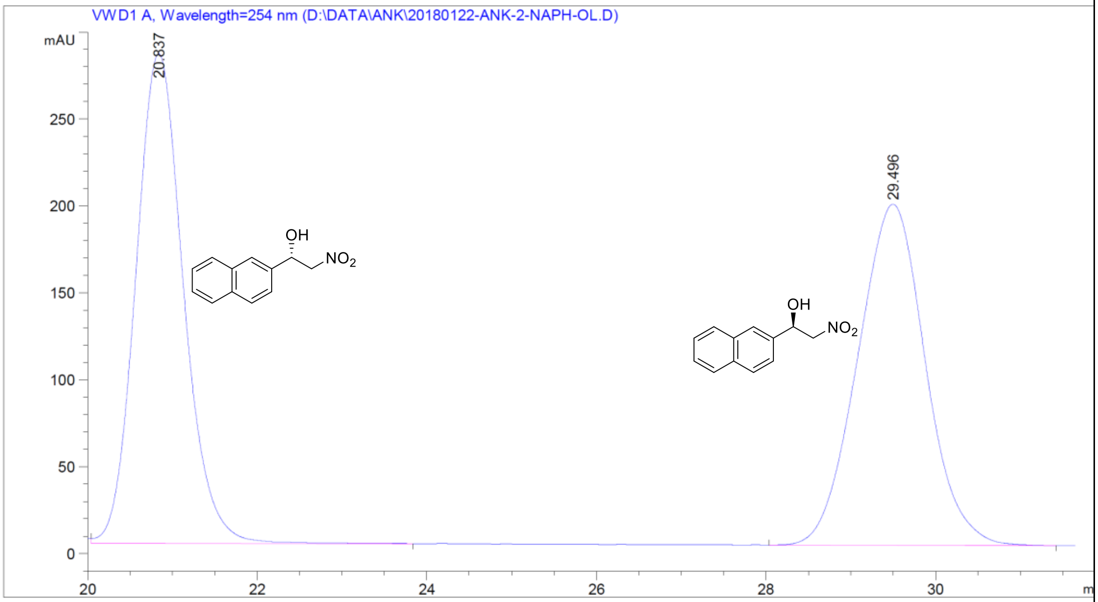


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.618	VB	0.6054	221.09911	5.35850	0.6997
2	29.903	BB	1.0321	3.13773e4	459.84543	99.3003

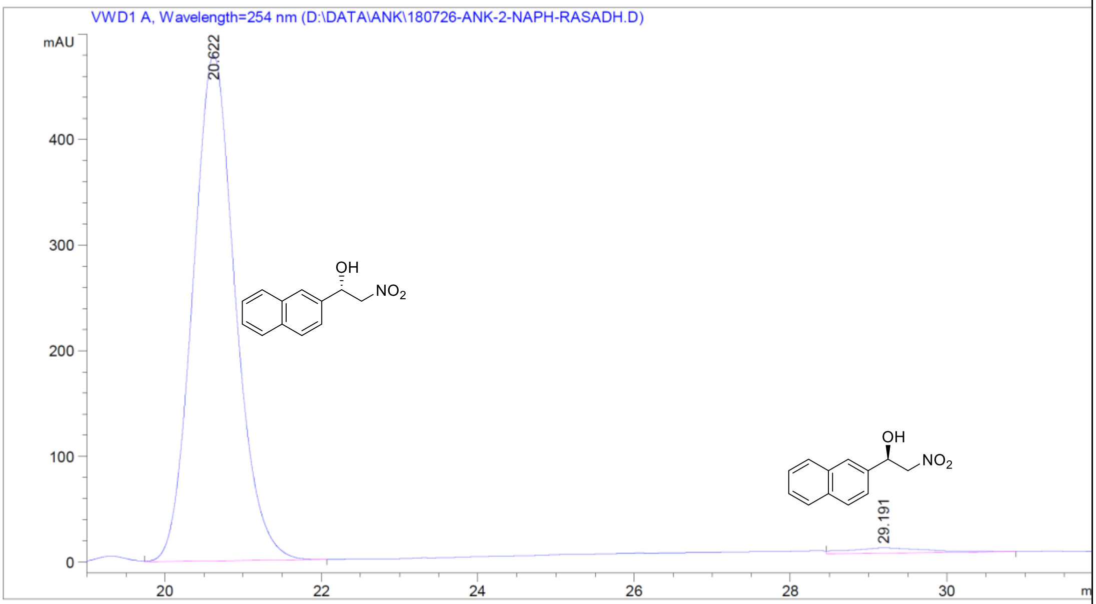
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*R*)-1-(naphthalen-2-yl)-2-nitroethan-1-ol (2u)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 254 nm UV lamp, 24 °C, t_R=20.8 min (major), t_R'=29.5 min (minor)



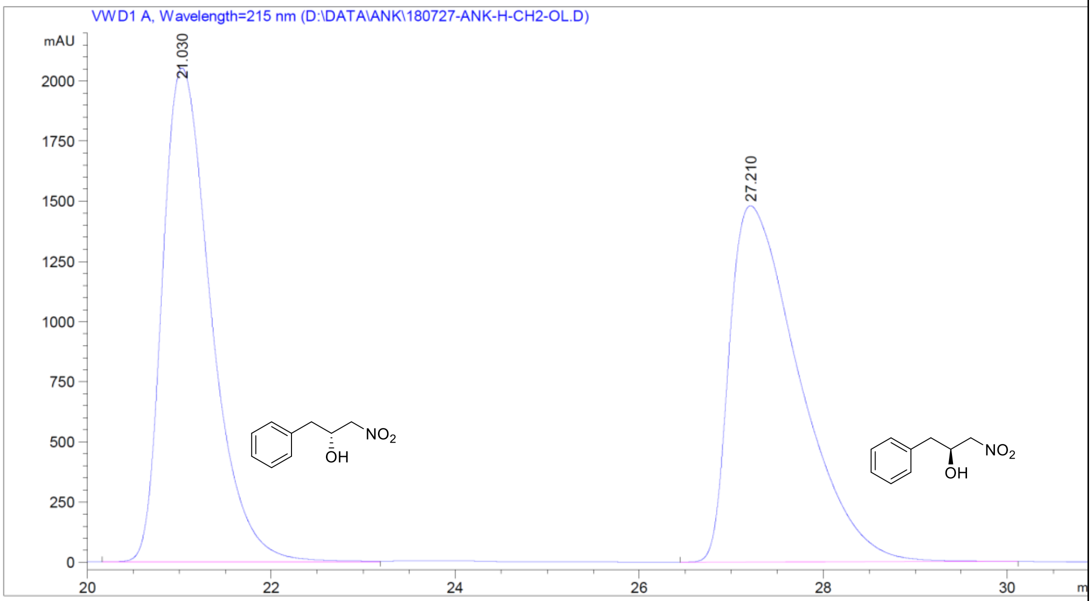
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.837	VB	0.5991	1.09844e4	281.60336	50.2624
2	29.496	BBA	0.8583	1.08697e4	196.22868	49.7376



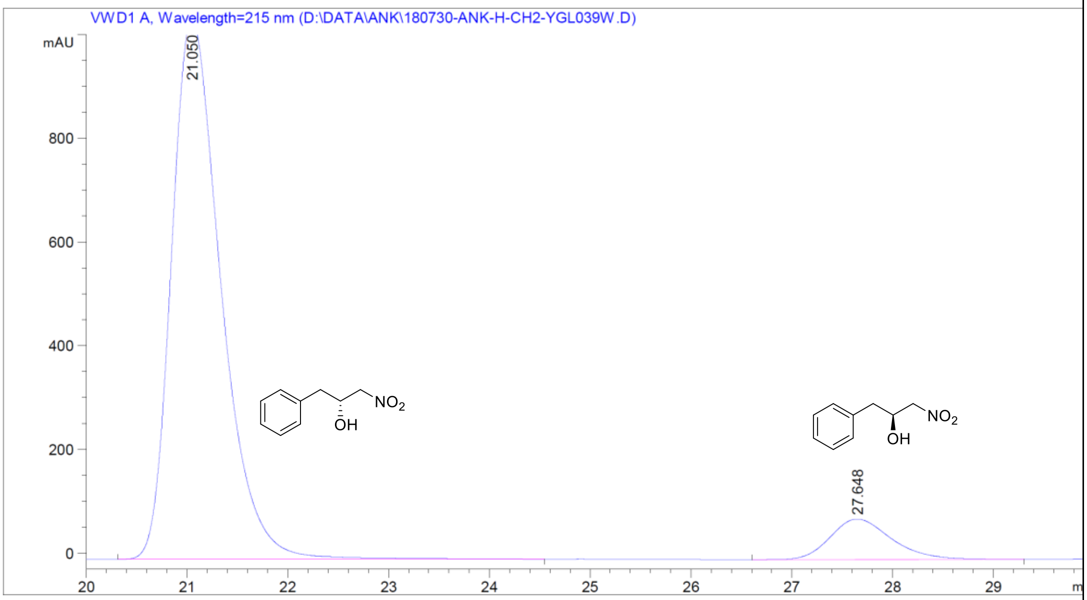
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.622	VB	0.5754	1.80165e4	478.40692	98.1764
2	29.191	VB	0.8615	334.65561	4.89560	1.8236

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(R)*-1-nitro-3-phenylpropan-2-ol (2v)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.0 min (major), t_R'=27.2 min (minor)



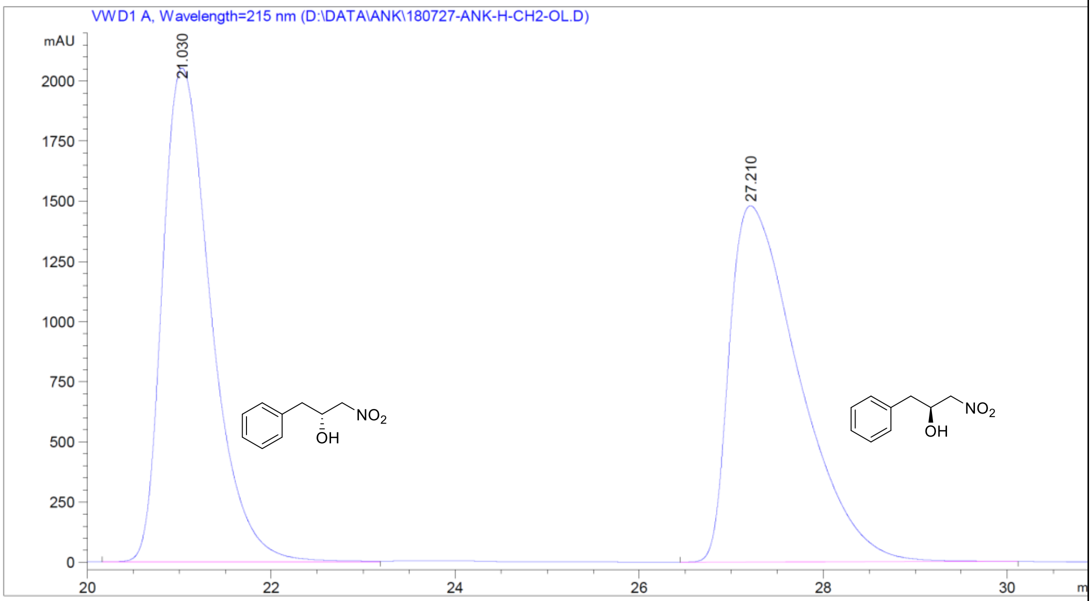
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.030	BV	0.5622	7.52421e4	2052.45850	49.1546
2	27.210	BB	0.8019	7.78303e4	1480.34192	50.8454



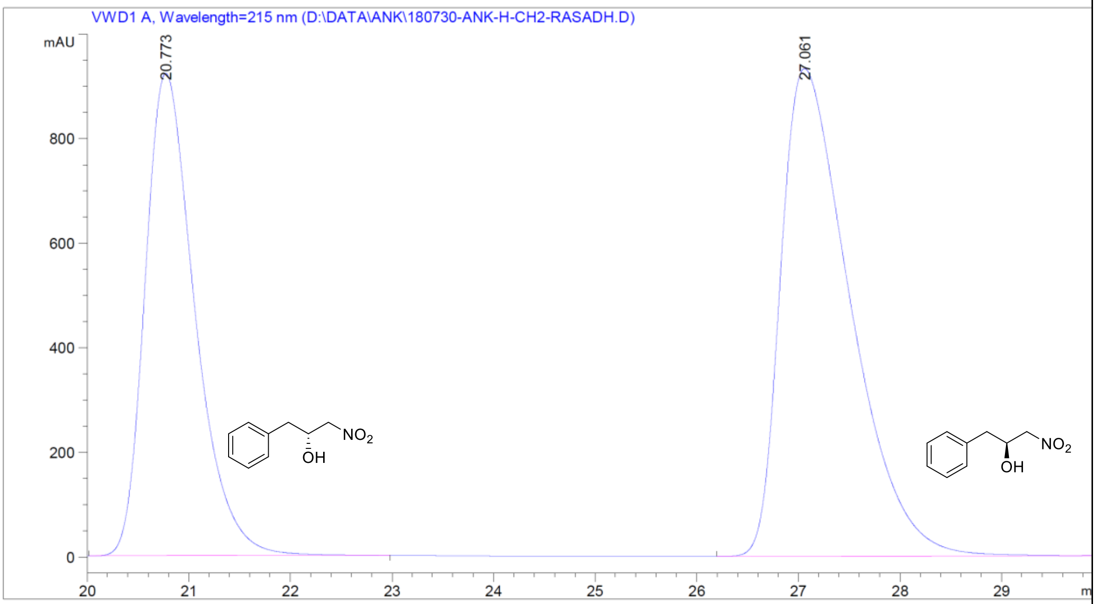
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.050	BB	0.5201	3.54198e4	1043.29993	91.4829
2	27.648	BB	0.6292	3297.60107	78.00505	8.5171

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(S)*-1-nitro-3-phenylpropan-2-ol (2v)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.0 min (minor), t_R'=27.2 min (major)



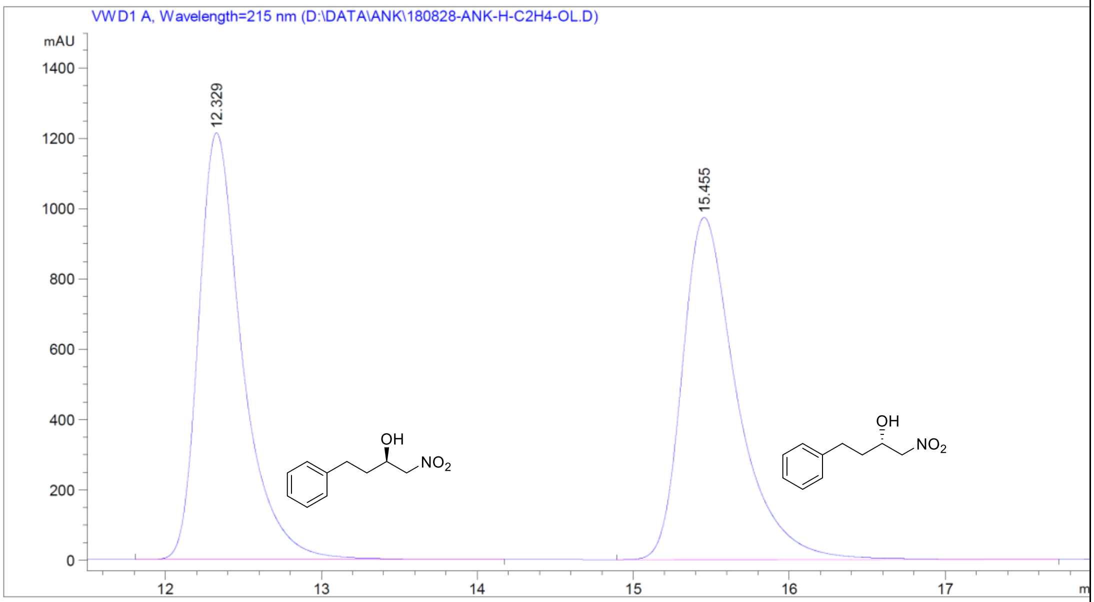
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.030	BV	0.5622	7.52421e4	2052.45850	49.1546
2	27.210	BB	0.8019	7.78303e4	1480.34192	50.8454



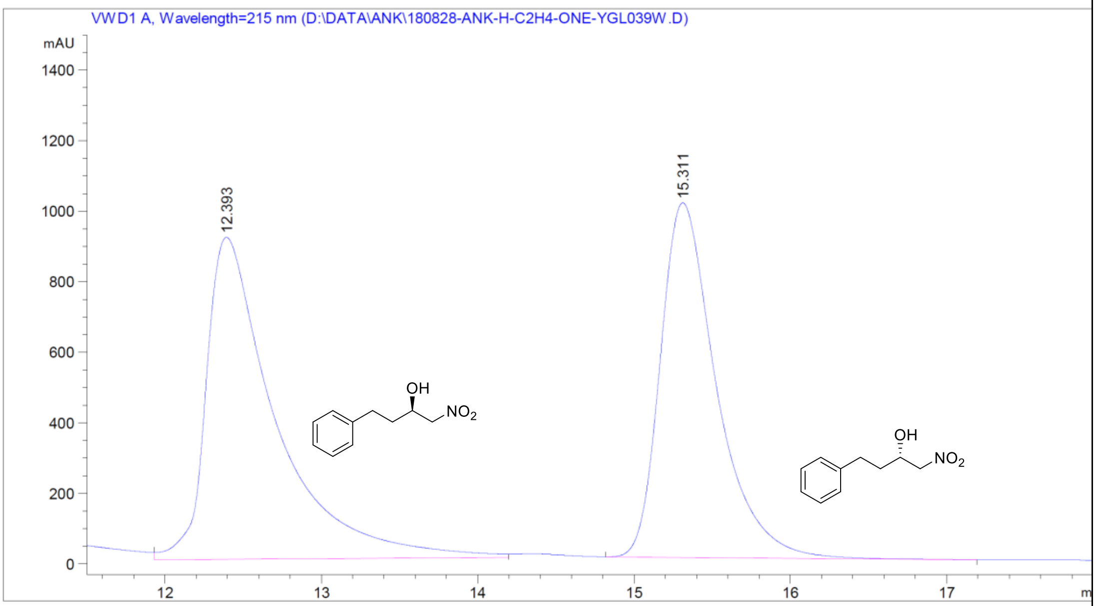
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.773	BB	0.5177	3.14625e4	923.01001	41.5238
2	27.061	BB	0.7109	4.43073e4	932.44904	58.4762

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

***(R)*-1-nitro-4-phenylbutan-2-ol (2w)**
Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.9 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.3 min (major), t_R'=15.5 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.329	BB	0.2915	2.35661e4	1214.11853	49.7255
2	15.455	BB	0.3666	2.38263e4	973.39539	50.2745

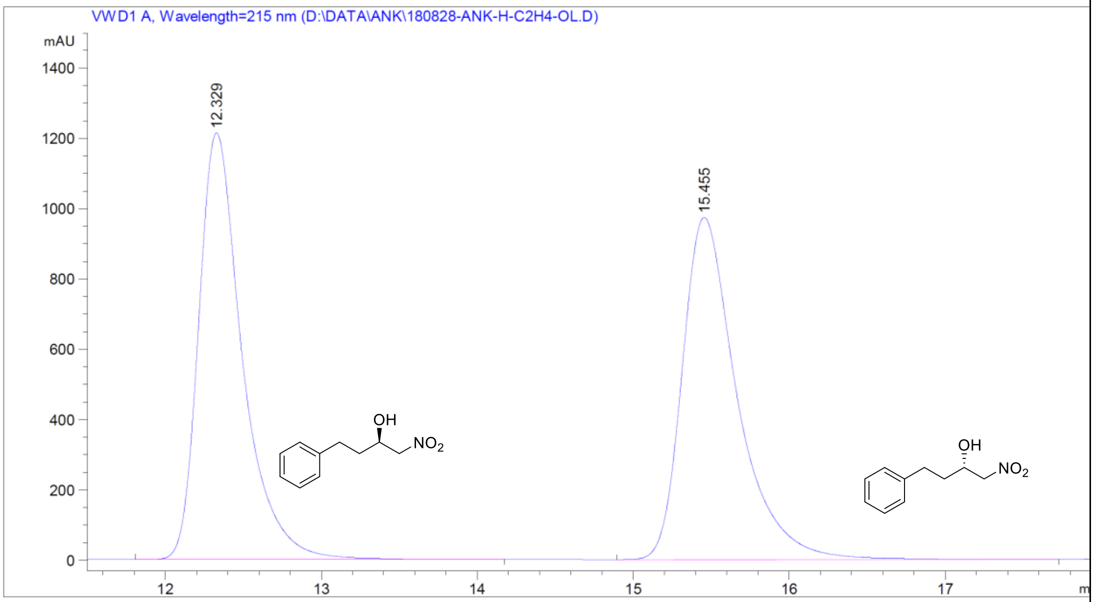


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.393	VV	0.4421	2.84408e4	913.82642	53.1908
2	15.311	BB	0.3747	2.50286e4	1006.12958	46.8092

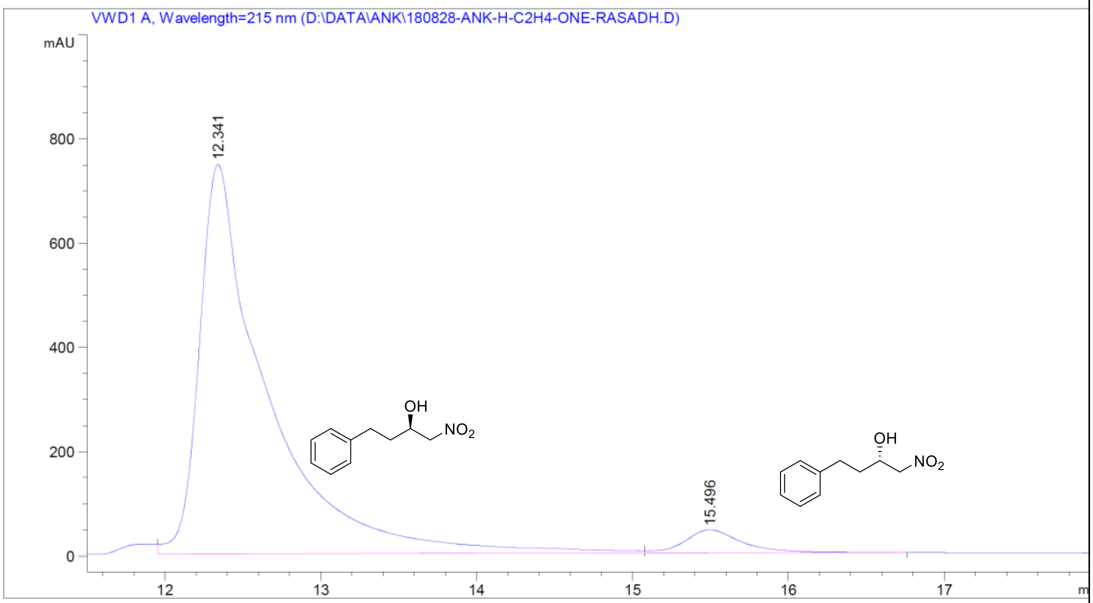
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

_(R)_-1-nitro-4-phenylbutan-2-ol (2w)

Chiracel® AD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.9 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.3 min (major), t_R'=15.5 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.329	BB	0.2915	2.35661e4	1214.11853	49.7255
2	15.455	BB	0.3666	2.38263e4	973.39539	50.2745

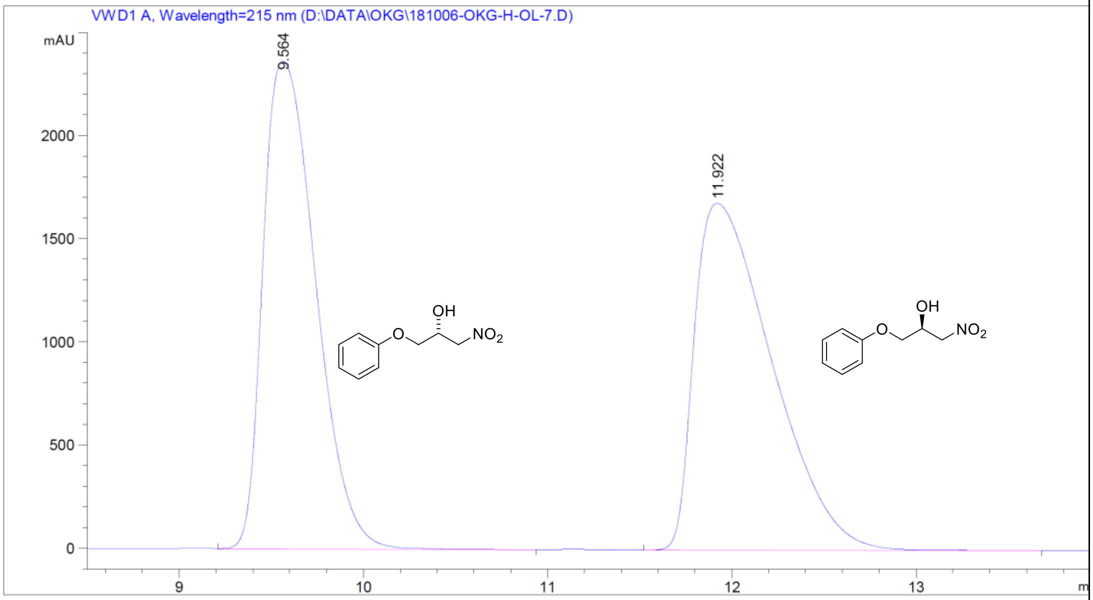


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.341	VV	0.4125	2.26708e4	747.06042	95.1529
2	15.496	VB	0.3803	1154.84412	44.56984	4.8471

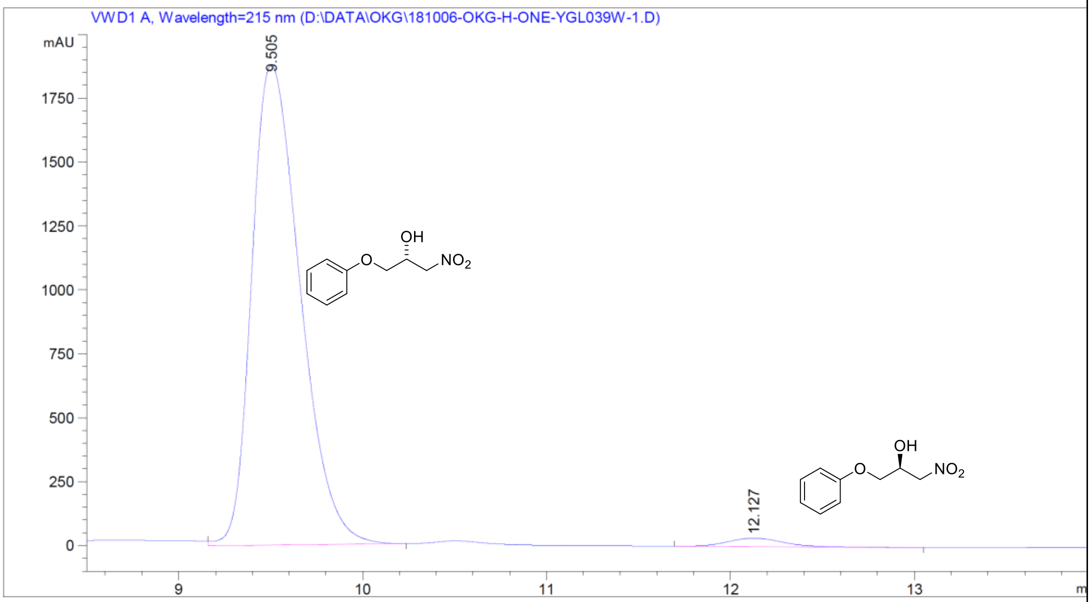
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH-catalyzed biotransformation.

(*R*)-1-nitro-3-phenoxypropan-2-ol (5a)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=9.6 min (major), t_R'=11.9 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.564	VV	0.3135	4.69228e4	2364.45605	48.8256
2	11.922	BB	0.4534	4.91801e4	1680.42651	51.1744

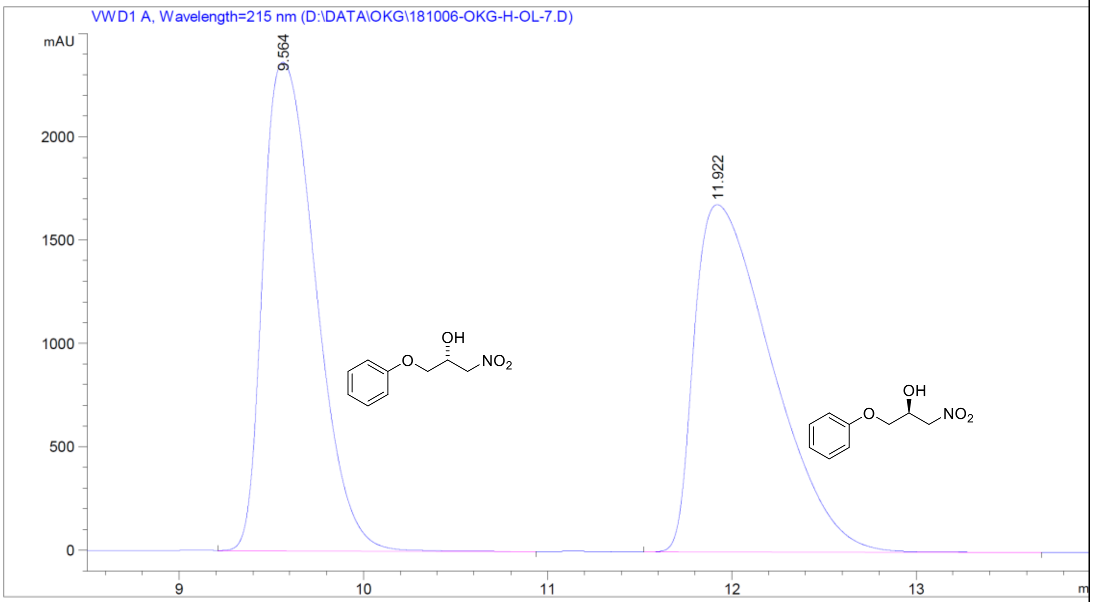


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.505	VB	0.2850	3.43097e4	1879.02429	97.9623
2	12.127	BB	0.3342	713.67523	33.27834	2.0377

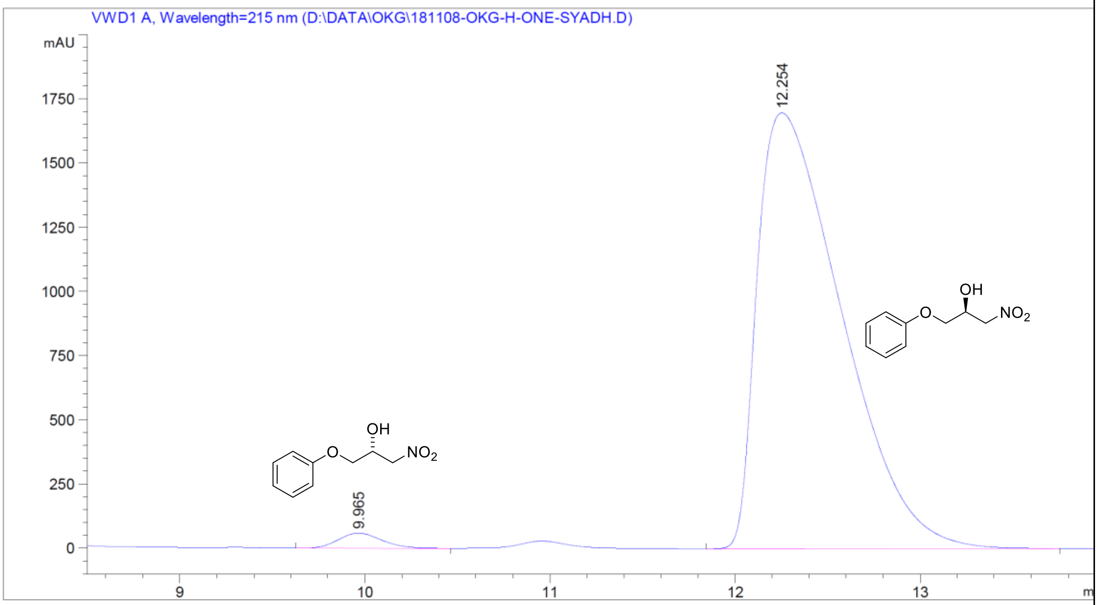
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*S*)-1-nitro-3-phenoxypropan-2-ol (5a)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=9.6 min (minor), t_R'=11.9 min (major)



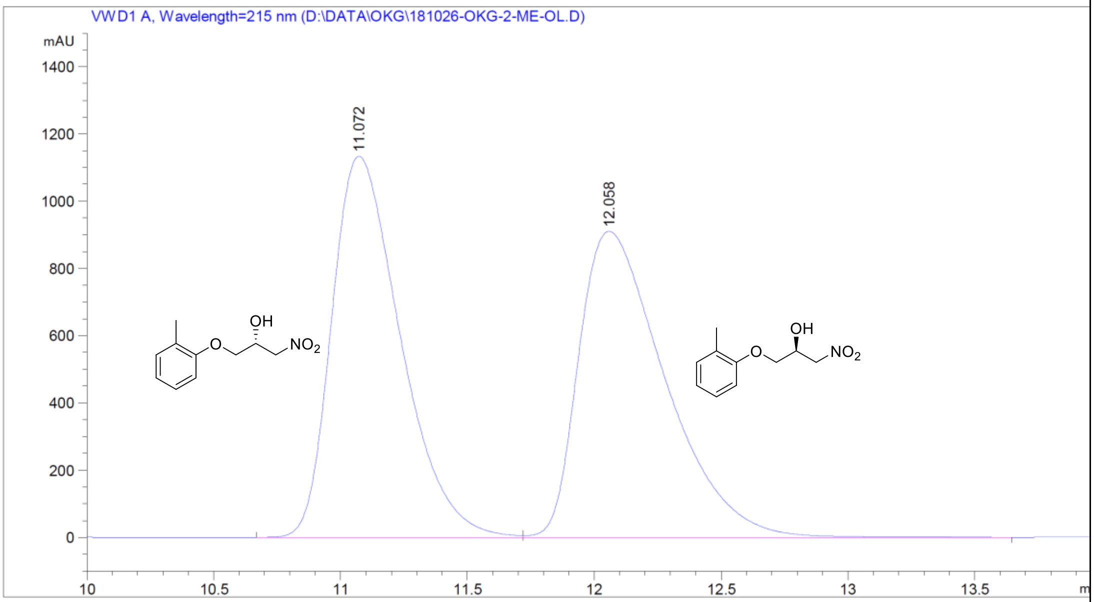
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.564	VV	0.3135	4.69228e4	2364.45605	48.8256
2	11.922	BB	0.4534	4.91801e4	1680.42651	51.1744



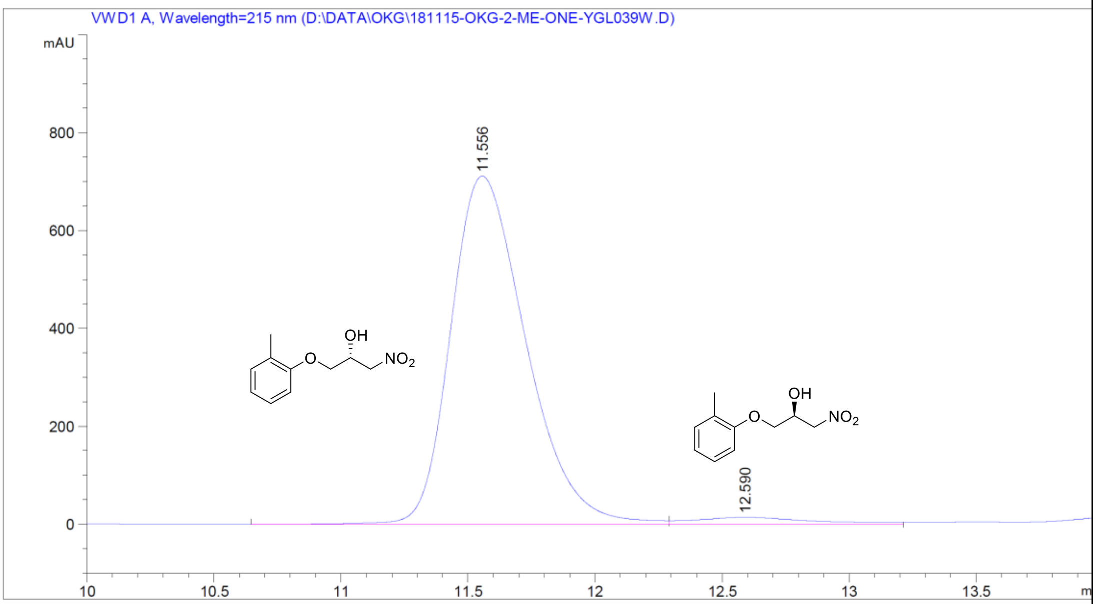
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.965	BV	0.2570	973.62451	58.84663	1.7790
2	12.254	BB	0.4955	5.37544e4	1697.19006	98.2210

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(*R*)-1-nitro-3-(o-tolyloxy)propan-2-ol (5b)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.1 min (major), t_R'=12.0 min (minor)



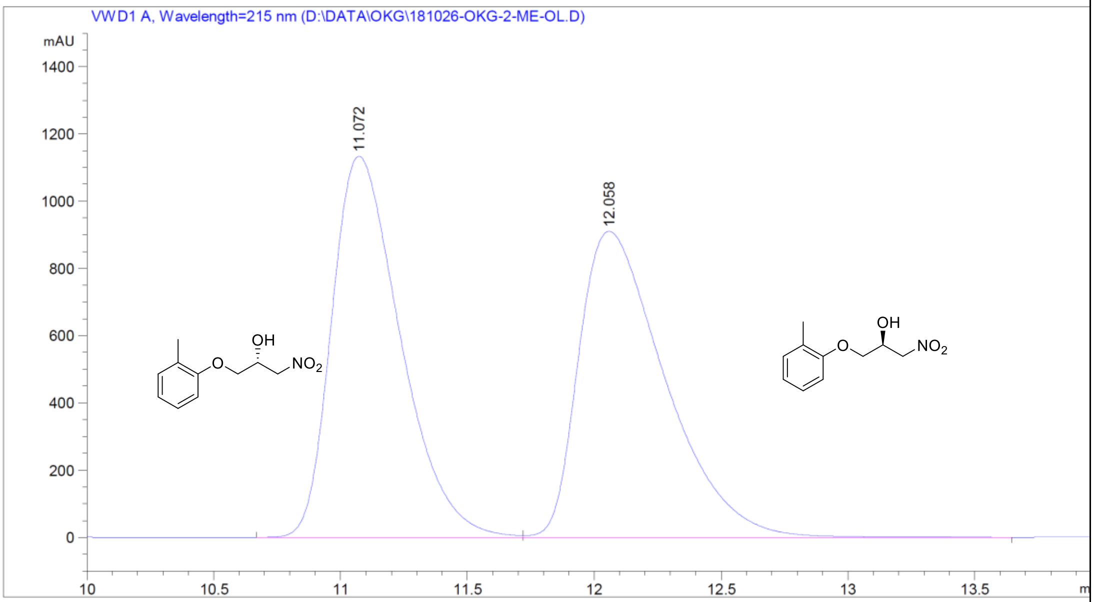
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.072	BV	0.2898	2.13445e4	1133.14941	49.7808
2	12.058	VV	0.3621	2.15324e4	909.96484	50.2192



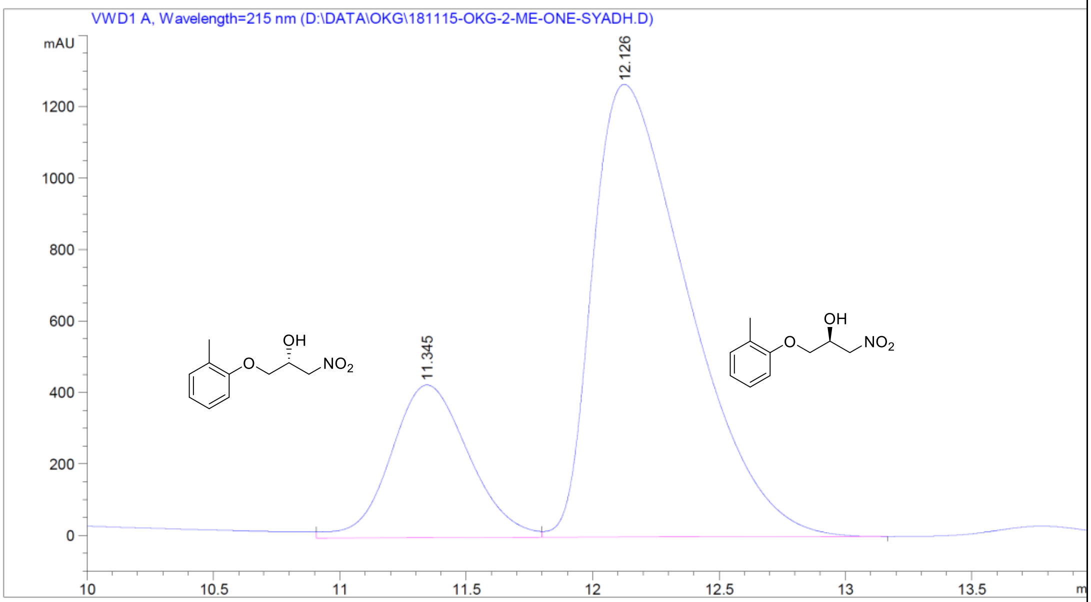
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.556	BV	0.3196	1.45970e4	710.87598	97.1445
2	12.590	VV	0.4439	429.07065	13.75502	2.8555

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(S)-1-nitro-3-(o-tolyloxy)propan-2-ol (5b)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.1 min (minor), t_R'=12.0 min (major)



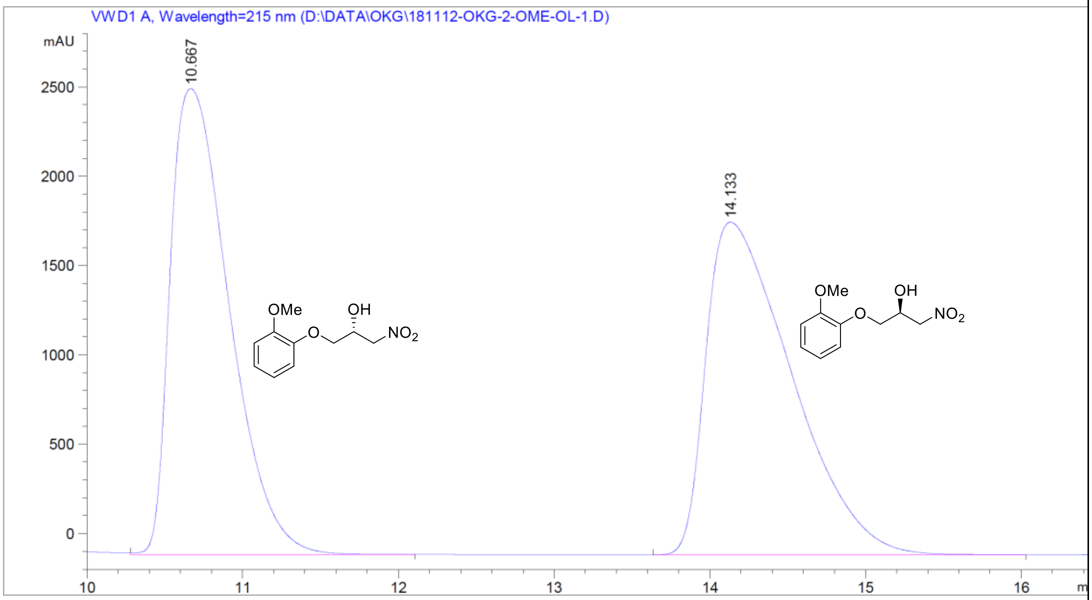
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.072	BV	0.2898	2.13445e4	1133.14941	49.7808
2	12.058	VV	0.3621	2.15324e4	909.96484	50.2192



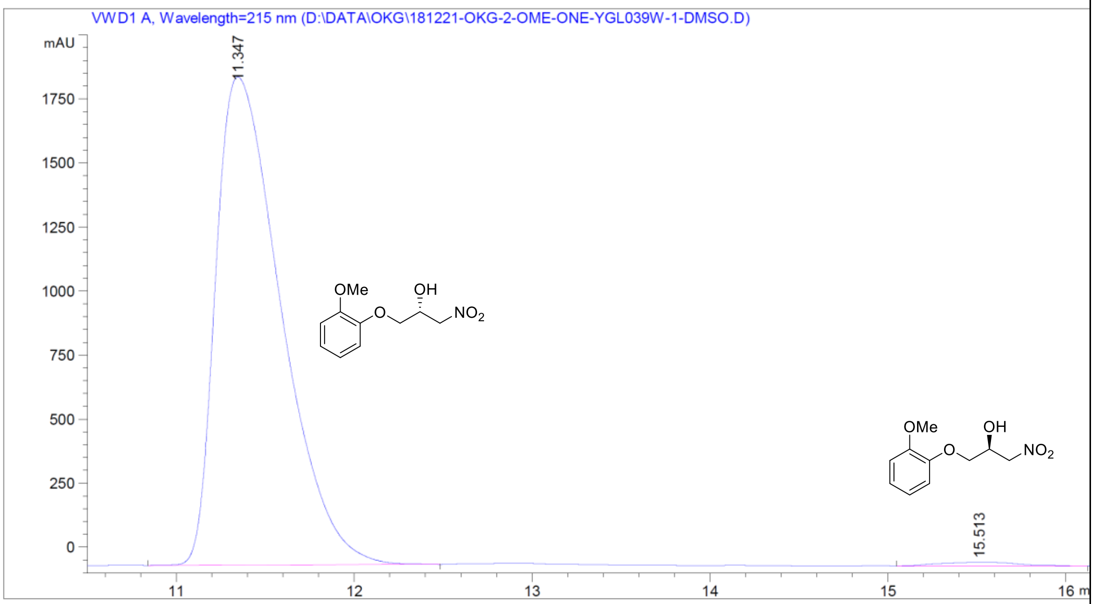
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.345	VV	0.3349	9188.84961	427.31189	21.5641
2	12.126	VB	0.4038	3.34230e4	1266.96606	78.4359

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

***(R)*-1-(2-methoxyphenoxy)-3-nitropropan-2-ol (5c)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.7 min (major), t_R'=14.1 min (minor)



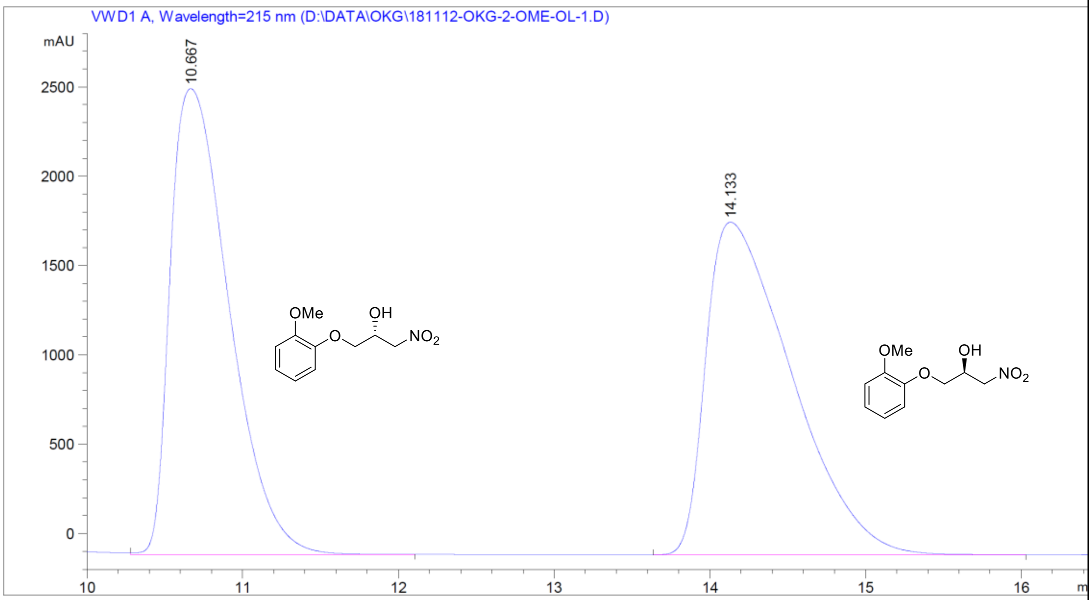
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.667	VB	0.4041	6.82455e4	2605.21729	49.0148
2	14.133	VB	0.5625	7.09890e4	1861.12354	50.9852



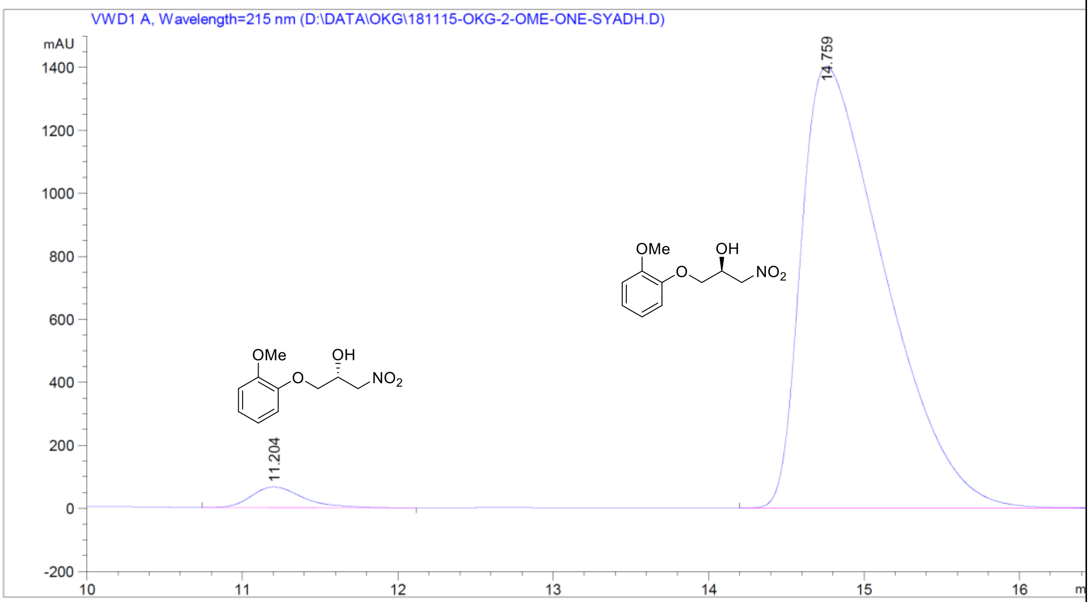
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.347	BB	0.3937	4.84626e4	1905.73657	99.0611
2	15.513	VB	0.3982	459.30707	14.28022	0.9389

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(S)*-1-(2-methoxyphenoxy)-3-nitropropan-2-ol (5c)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.7 min (minor), t_R'=14.1 min (major)



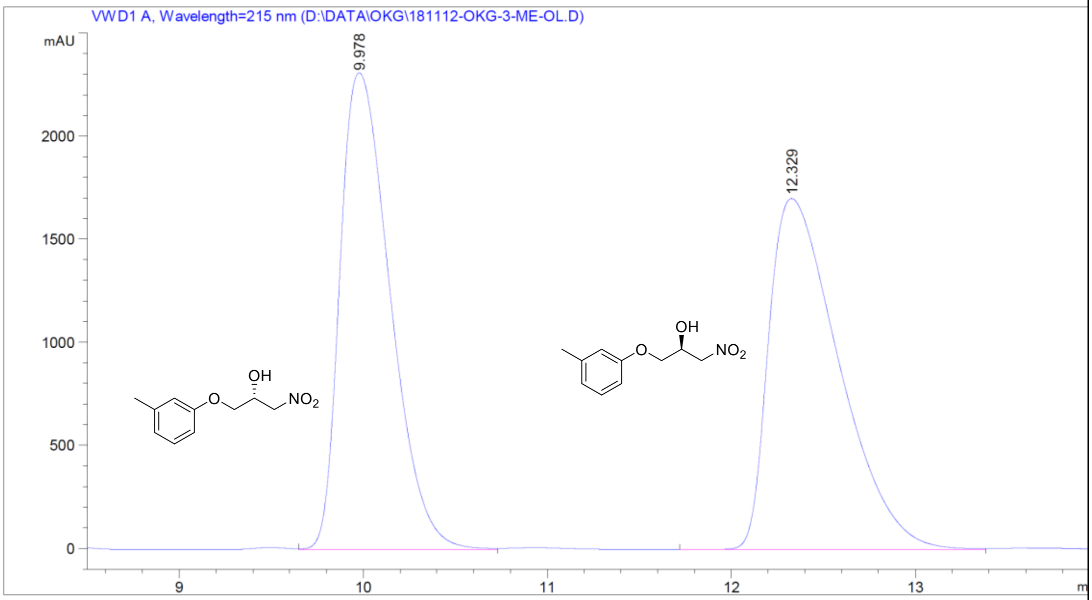
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.667	VB	0.4041	6.82455e4	2605.21729	49.0148
2	14.133	VB	0.5625	7.09890e4	1861.12354	50.9852



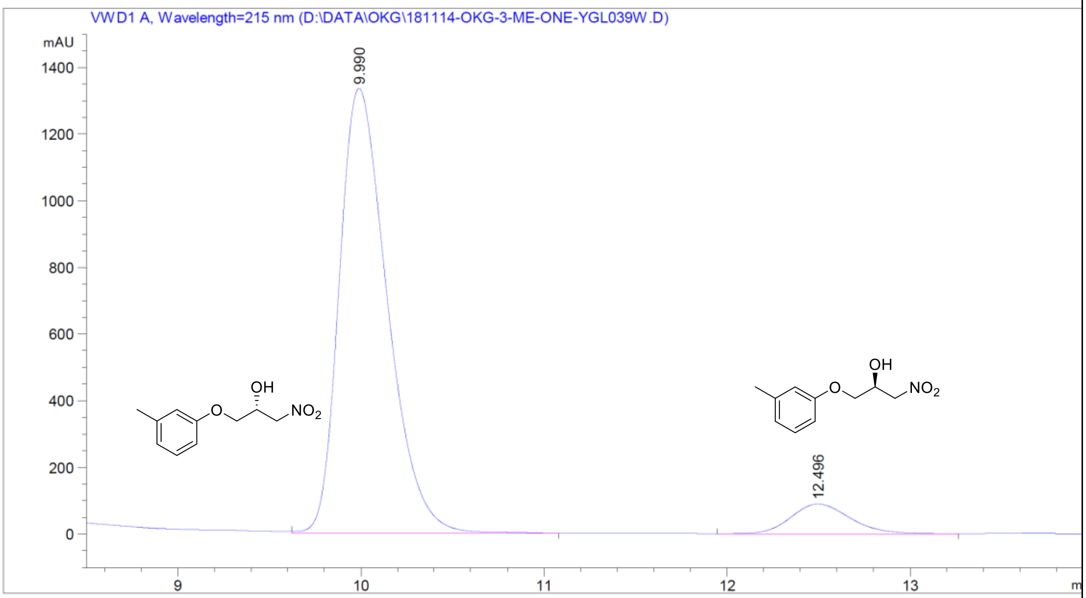
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.204	BB	0.3483	1501.03479	65.63396	2.7890
2	14.759	BB	0.5662	5.23182e4	1400.90869	97.2110

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

***(R)*-1-nitro-3-(m-tolyloxy)propan-2-ol (5d)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.0 min (major), t_R'=12.3 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.978	VV	0.2944	4.36561e4	2310.81665	49.1861
2	12.329	BV	0.4092	4.51009e4	1701.78027	50.8139

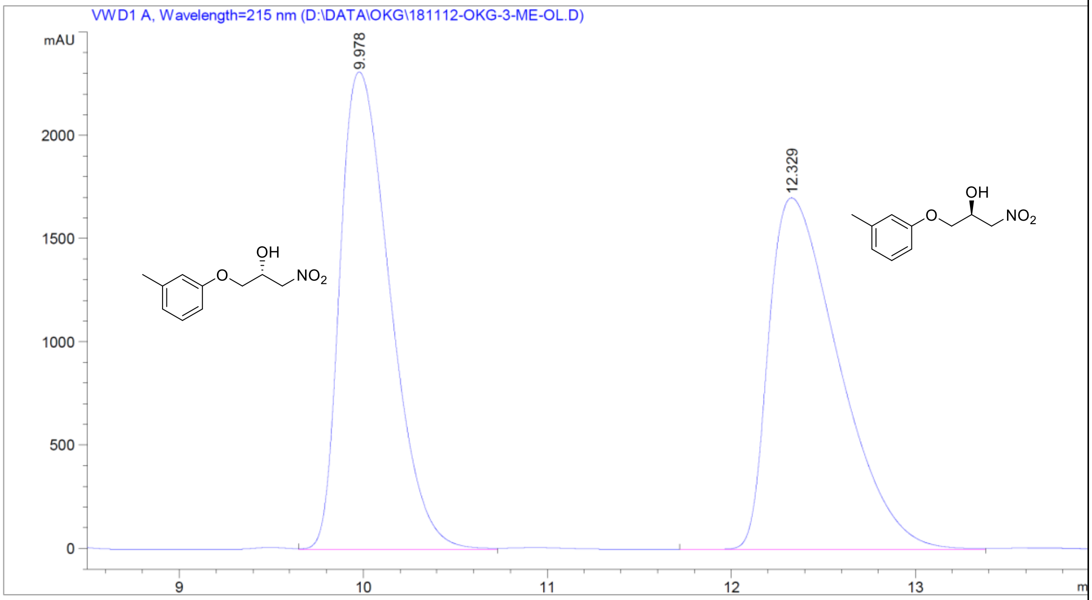


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.990	VB	0.2808	2.43380e4	1334.38684	92.4480
2	12.496	BV	0.3493	1988.16150	88.77943	7.5520

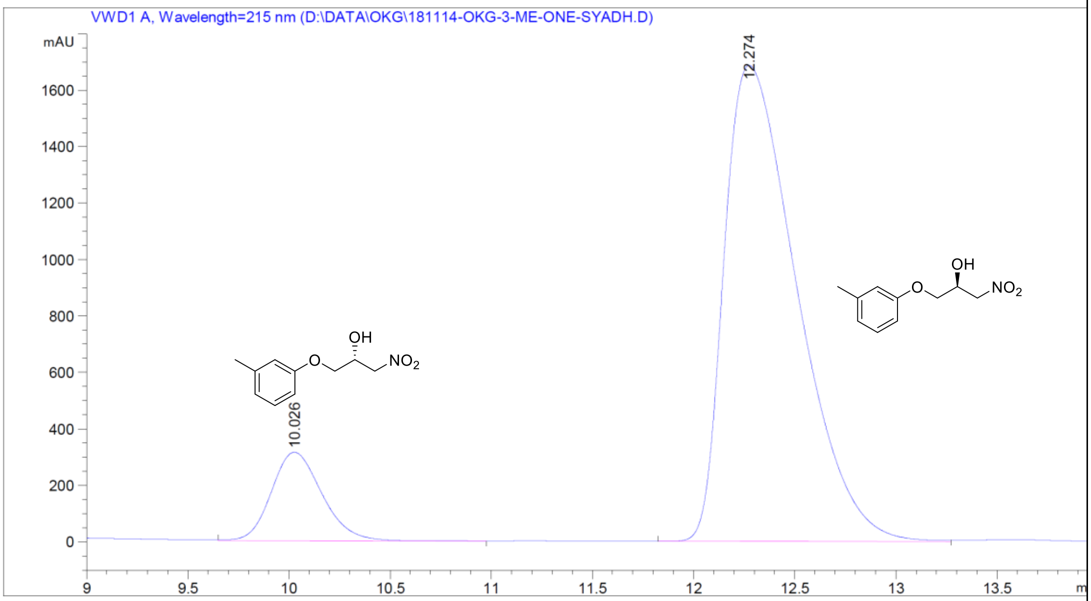
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*S*)-1-nitro-3-(m-tolyloxy)propan-2-ol (5d)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.0 min (minor), t_R'=12.3 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.978	VV	0.2944	4.36561e4	2310.81665	49.1861
2	12.329	BV	0.4092	4.51009e4	1701.78027	50.8139

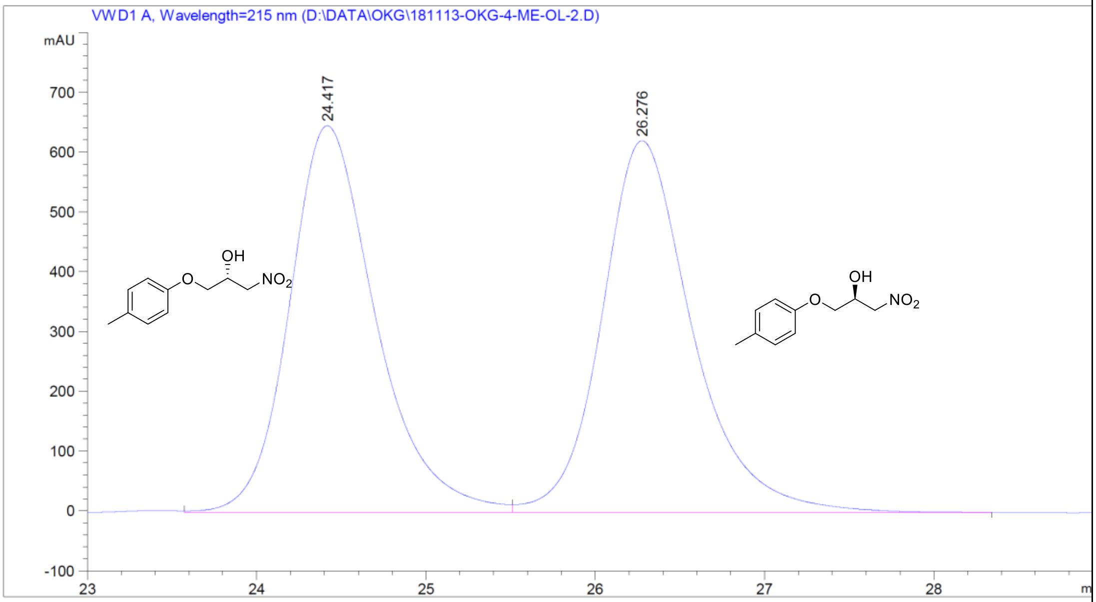


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.026	VB	0.2705	5494.53418	314.16583	11.5437
2	12.274	BV	0.3881	4.21030e4	1687.37036	88.4563

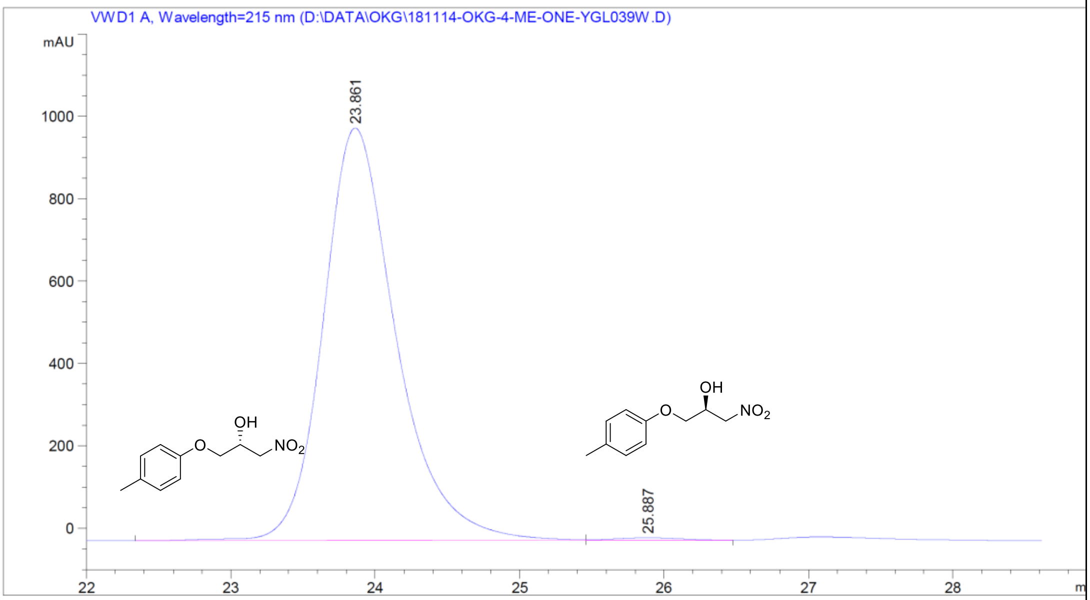
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(*R*)-1-nitro-3-(p-tolyloxy)propan-2-ol (5e)

Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 92:8, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.4 min (major), t_R'=26.3 min (minor)



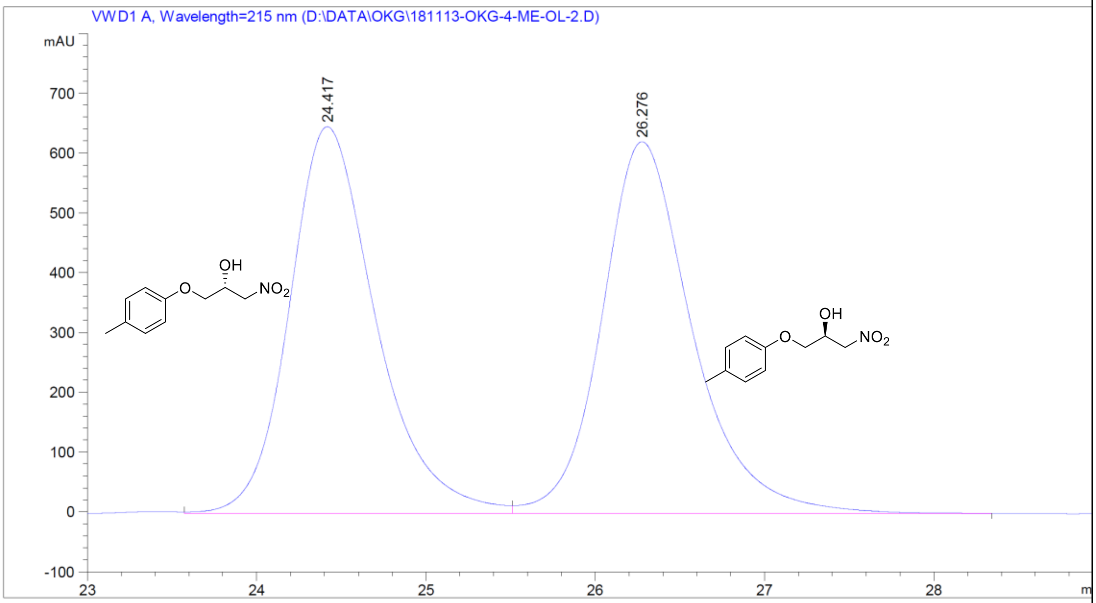
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.417	VV	0.5338	2.29941e4	646.75470	49.7175
2	26.276	VV	0.5614	2.32555e4	621.74335	50.2825



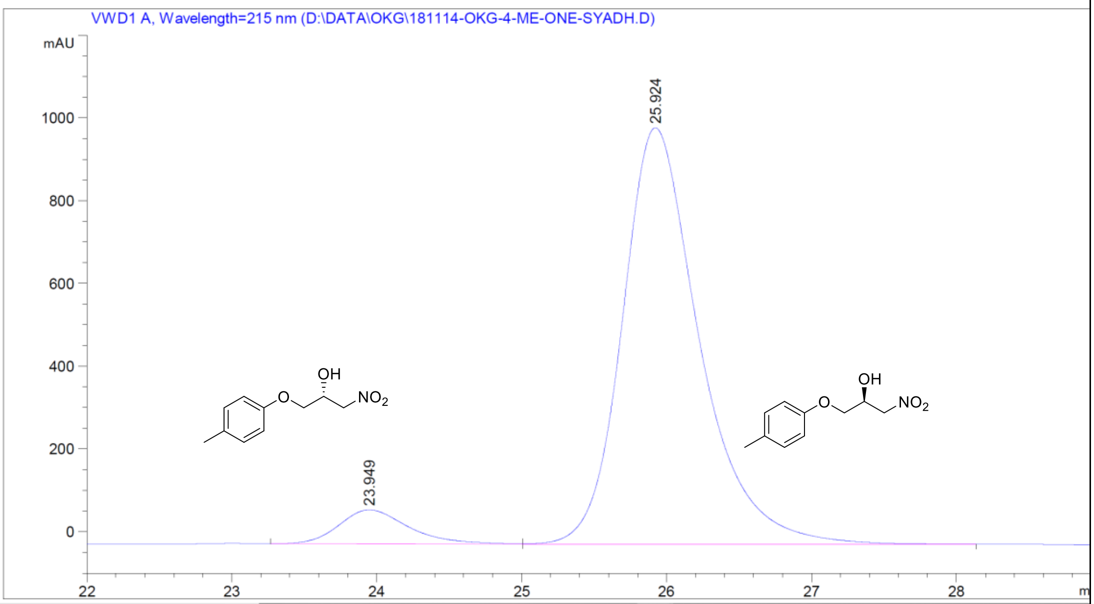
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.861	BV	0.5295	3.51996e4	1001.52600	99.4772
2	25.887	VB	0.3771	184.98007	5.84713	0.5228

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*S*)-1-nitro-3-(p-tolyloxy)propan-2-ol (5e)
Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 92:8, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.4 min (minor), $t_R{'}$=26.3 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.417	VV	0.5338	2.29941e4	646.75470	49.7175
2	26.276	VV	0.5614	2.32555e4	621.74335	50.2825

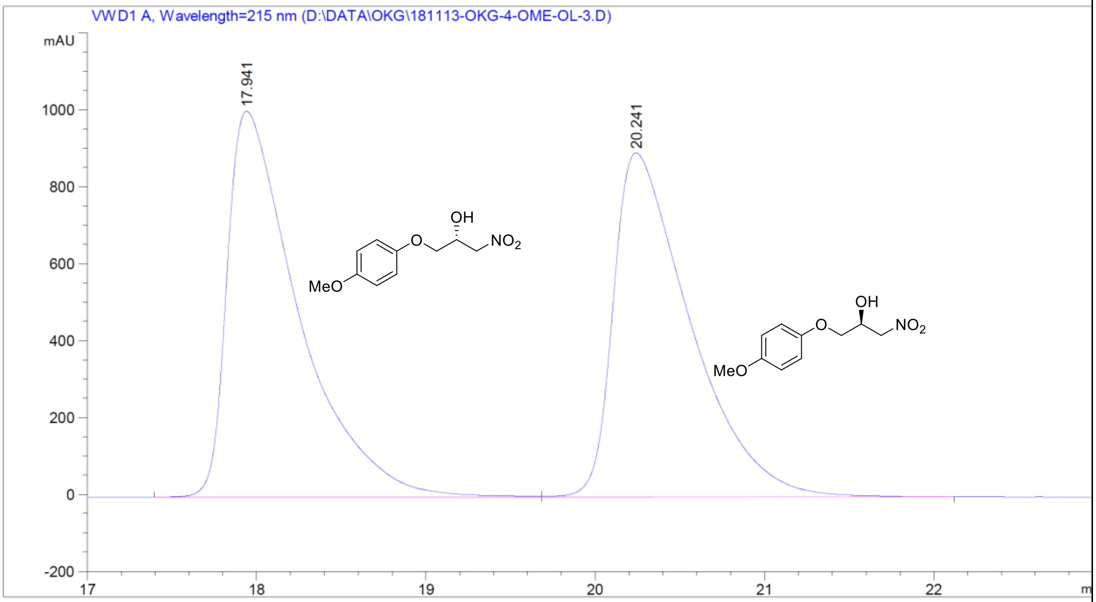


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.949	BV	0.5027	2721.72266	81.90096	6.8282
2	25.924	VB	0.5549	3.71384e4	1005.64050	93.1718

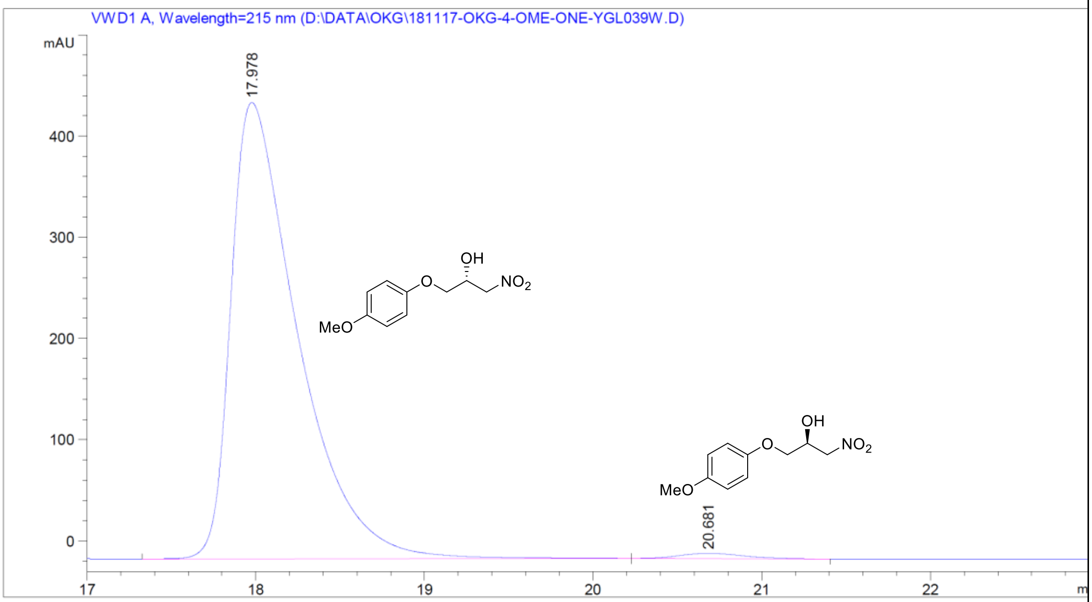
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(R)-1-(4-methoxyphenoxy)-3-nitropropan-2-ol (5f)

Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=17.9 min (major), t_R'=20.2 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.941	VV	0.4347	2.94267e4	1003.30011	50.9828
2	20.241	VB	0.4704	2.82922e4	894.67535	49.0172

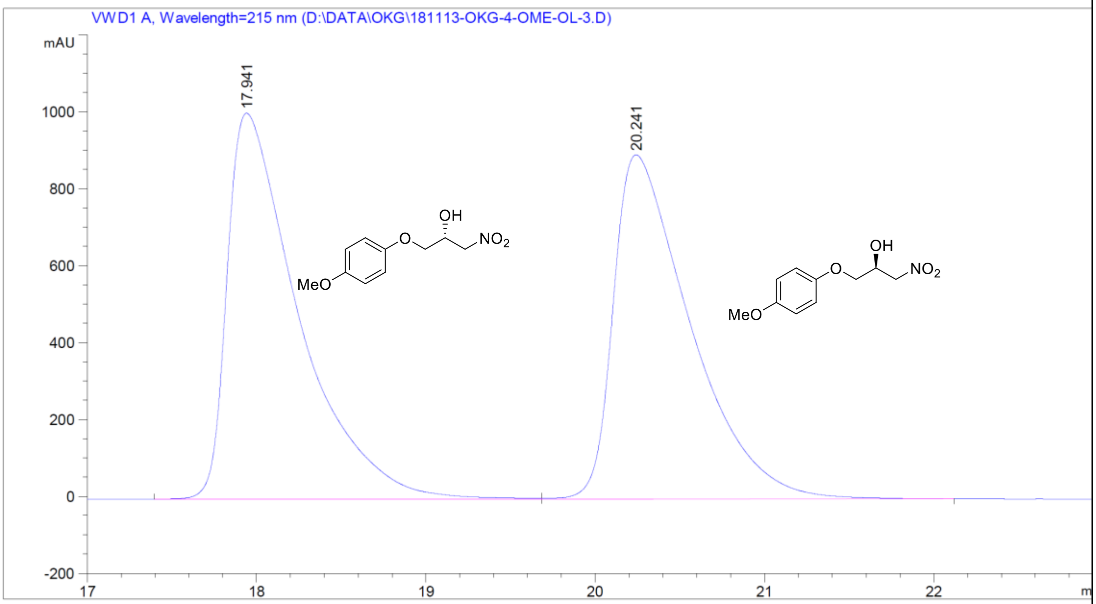


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.978	BB	0.4088	1.24192e4	450.88504	98.8723
2	20.681	BB	0.3386	141.64224	5.21936	1.1277

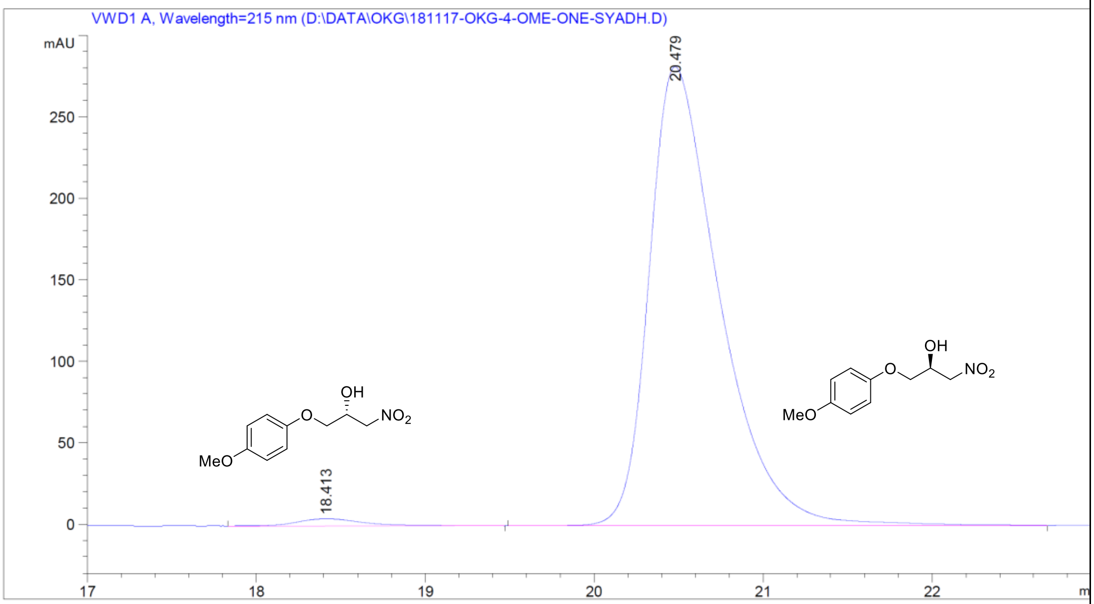
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(S)-1-(4-methoxyphenoxy)-3-nitropropan-2-ol (5f)

Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=17.9 min (minor), t_R'=20.2 min (major)



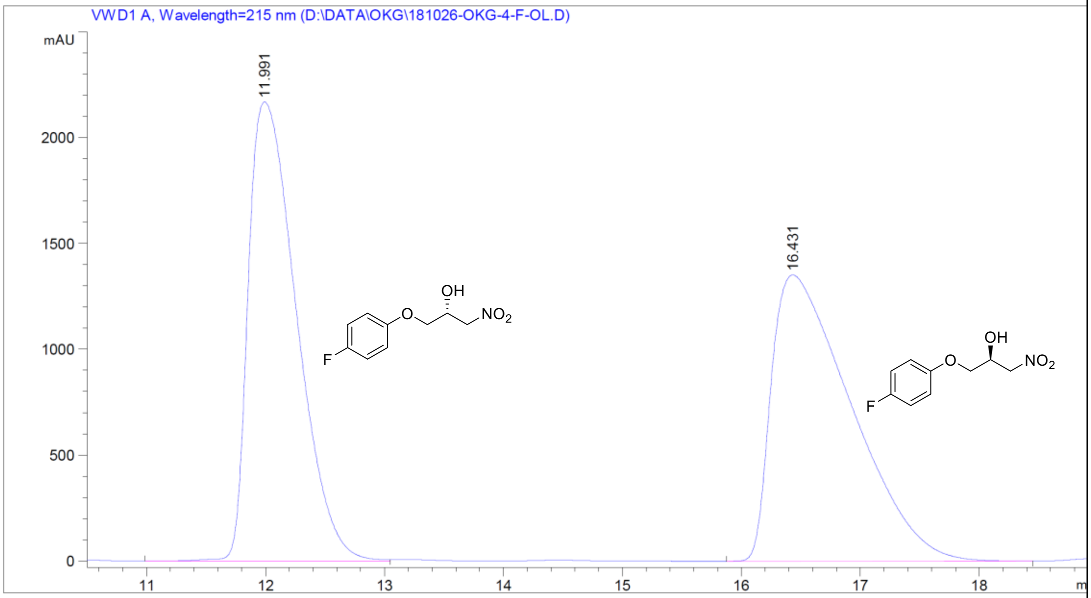
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.941	VV	0.4347	2.94267e4	1003.30011	50.9828
2	20.241	VB	0.4704	2.82922e4	894.67535	49.0172



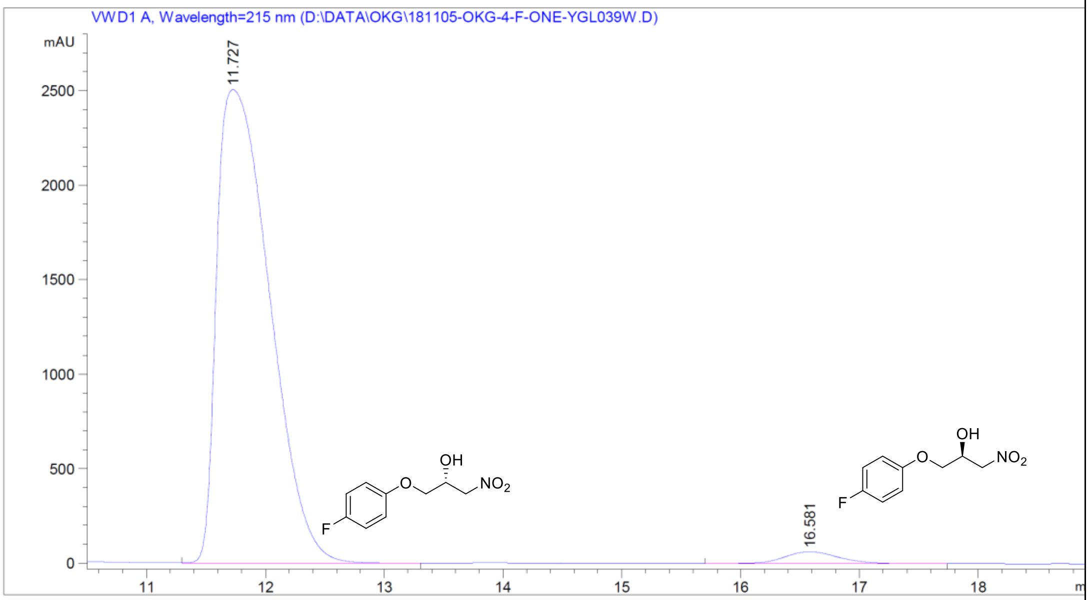
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.413	BB	0.3601	121.00271	4.38984	1.4614
2	20.479	BB	0.4346	8158.71240	281.55539	98.5386

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(*R*)-1-(4-fluorophenoxy)-3-nitropropan-2-ol (5g)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.0 min (major), t_R'=16.4 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.991	BV	0.4379	6.09688e4	2169.43750	49.1833
2	16.431	BB	0.7194	6.29936e4	1352.54553	50.8167

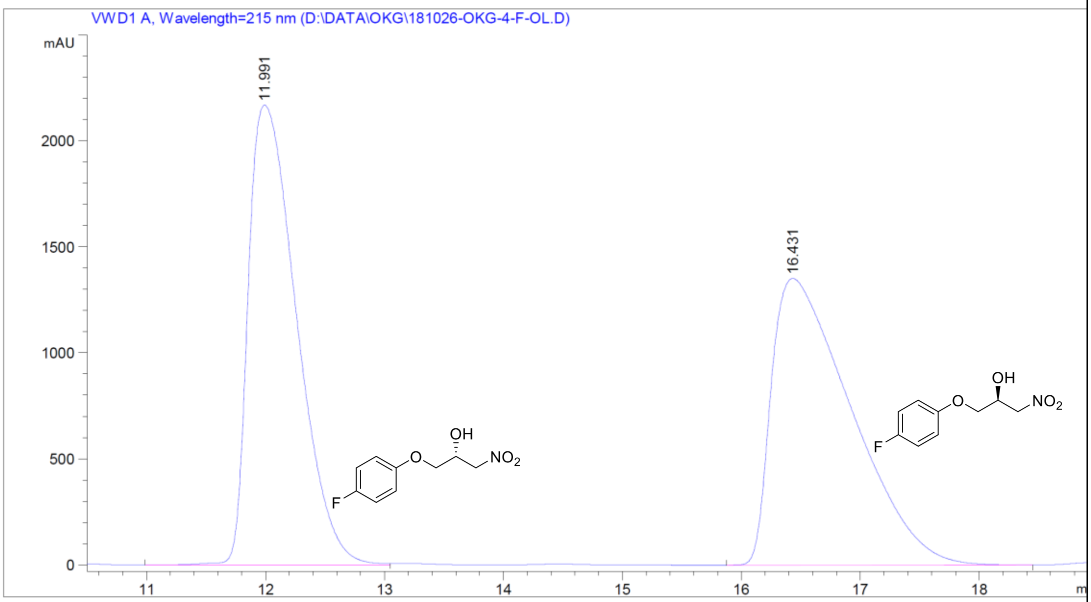


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.727	VB	0.4890	7.72955e4	2504.86719	97.4549
2	16.581	BB	0.5033	2018.60217	61.92169	2.5451

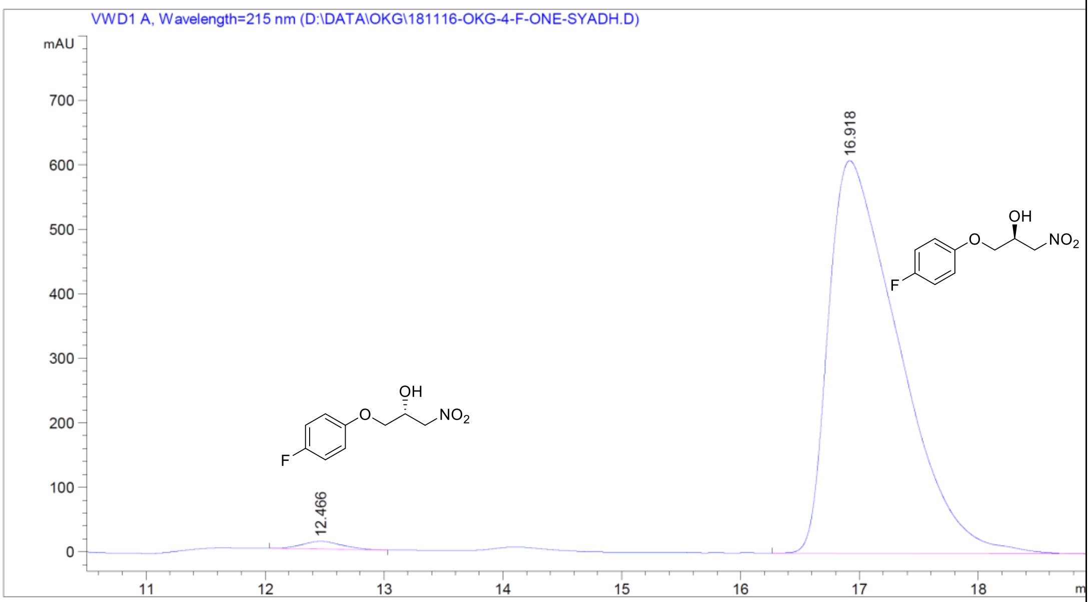
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(S)-1-(4-fluorophenoxy)-3-nitropropan-2-ol (5g)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.0 min (minor), t_R'=16.4 min (major)



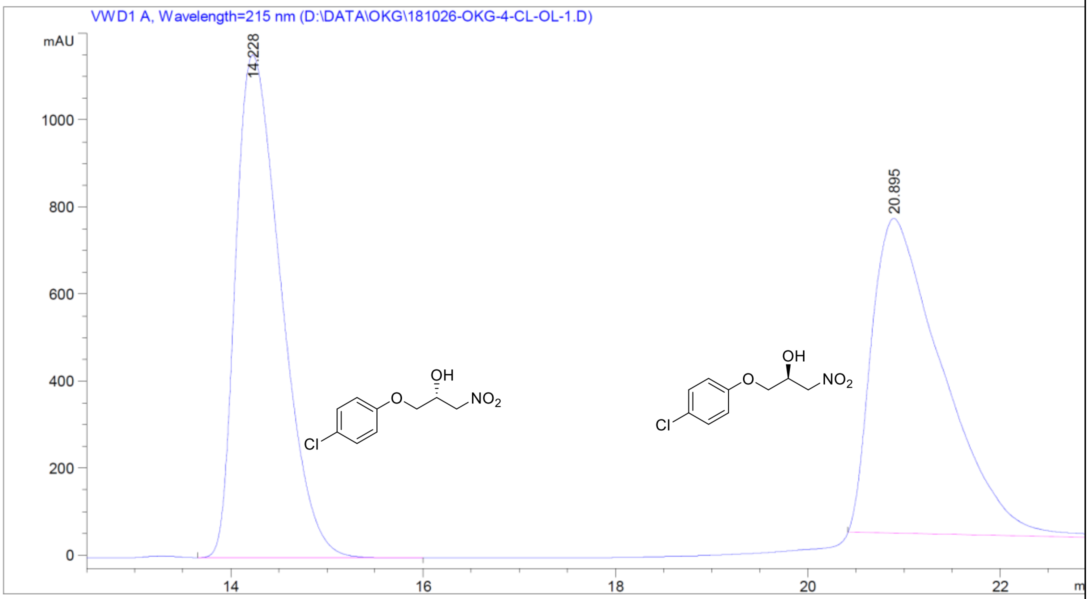
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.991	BV	0.4379	6.09688e4	2169.43750	49.1833
2	16.431	BB	0.7194	6.29936e4	1352.54553	50.8167



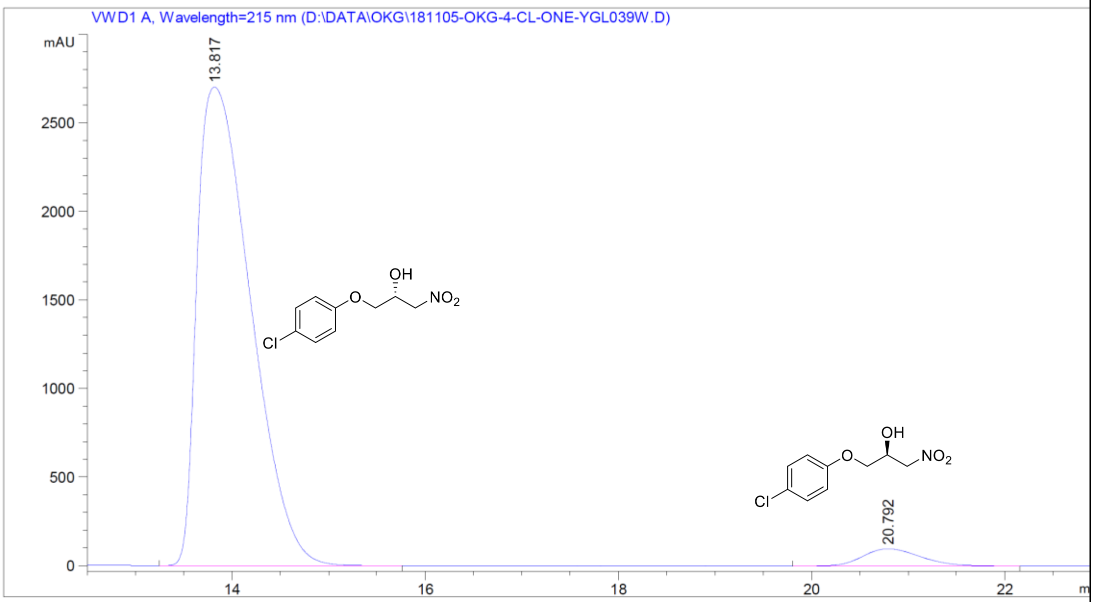
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.466	BB	0.3427	277.13306	11.92029	1.0949
2	16.918	BB	0.6016	2.50340e4	608.94000	98.9051

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(*R*)-1-(4-chlorophenoxy)-3-nitropropan-2-ol (5h)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (major), t_R'=20.9 min (minor)



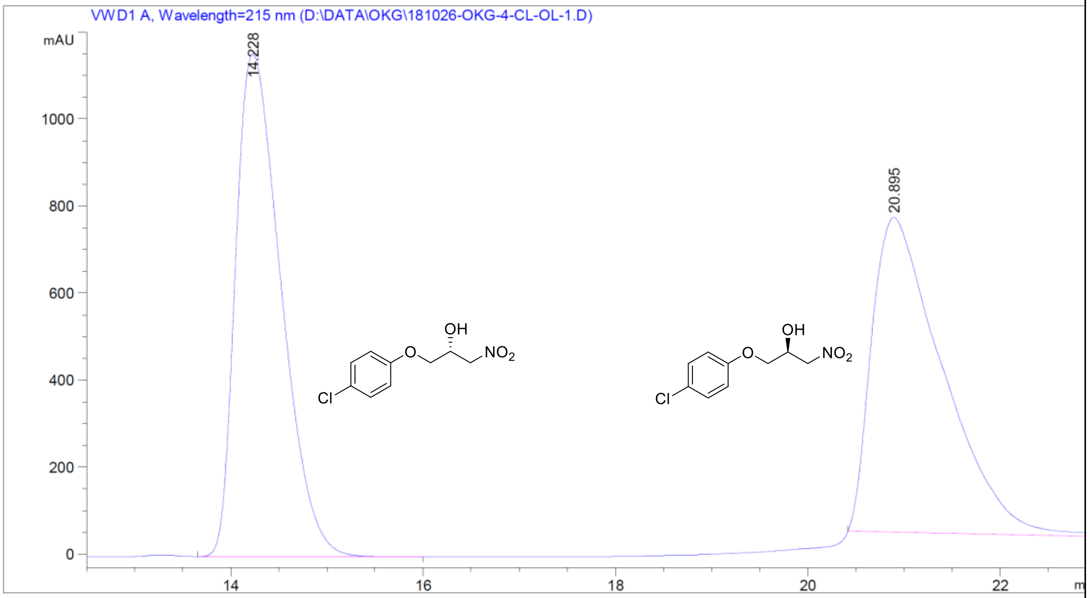
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.228	VB	0.5133	3.78776e4	1155.97607	50.2692
2	20.895	BBA	0.7142	3.74719e4	723.56659	49.7308



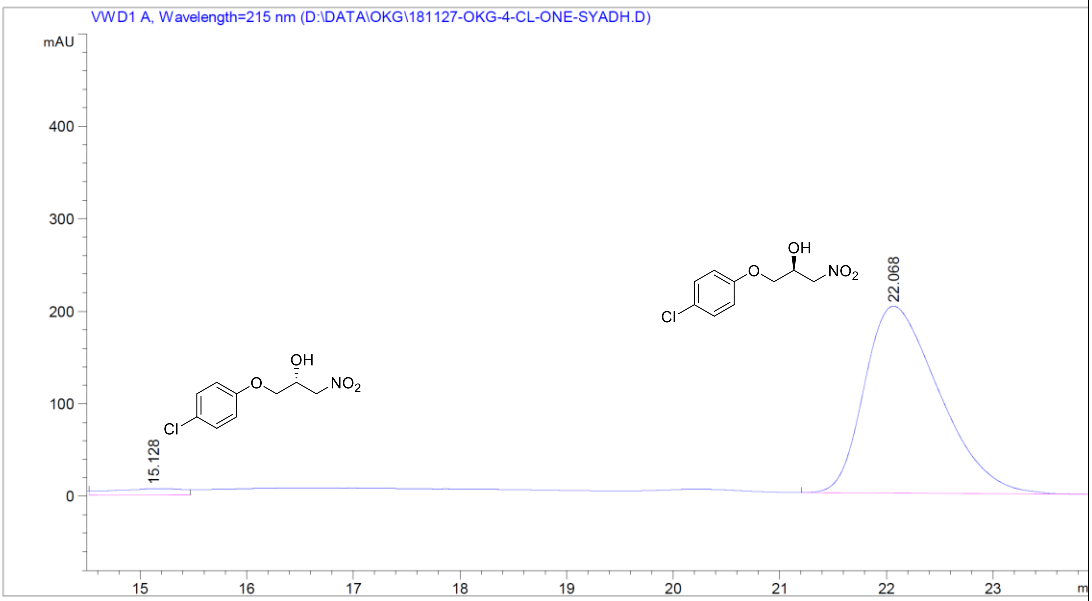
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.817	BB	0.6002	1.03743e5	2700.58716	96.2625
2	20.792	BB	0.6490	4027.90625	96.90102	3.7375

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(*S*)-1-(4-chlorophenoxy)-3-nitropropan-2-ol (5h)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (minor), t_R'=20.9 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.228	VB	0.5133	3.78776e4	1155.97607	50.2692
2	20.895	BBA	0.7142	3.74719e4	723.56659	49.7308

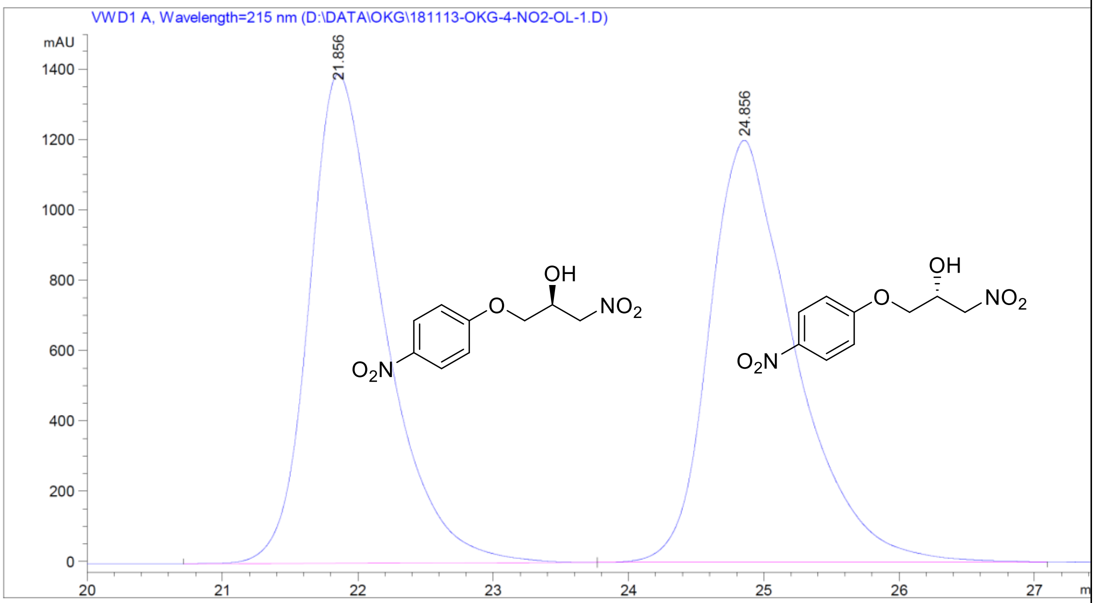


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.128	VV	0.5836	322.23334	6.91605	3.1603
2	22.068	BB	0.7543	9874.06348	201.98811	96.8397

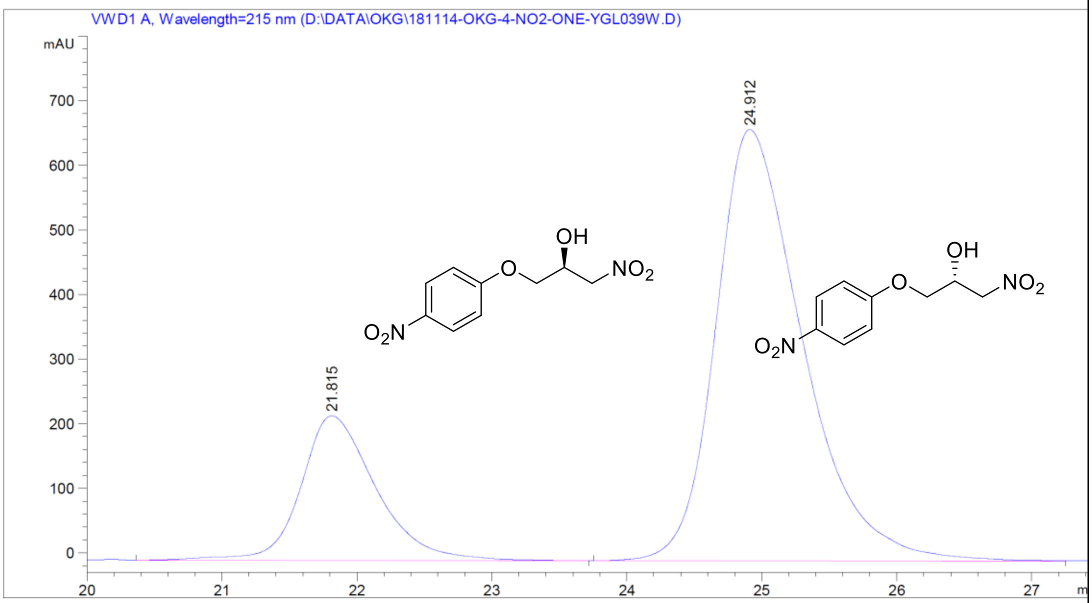
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

(R)-1-nitro-3-(4-nitrophenoxy)propan-2-ol (5i)

Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.8 min (minor), t_R'=24.8 min (major)



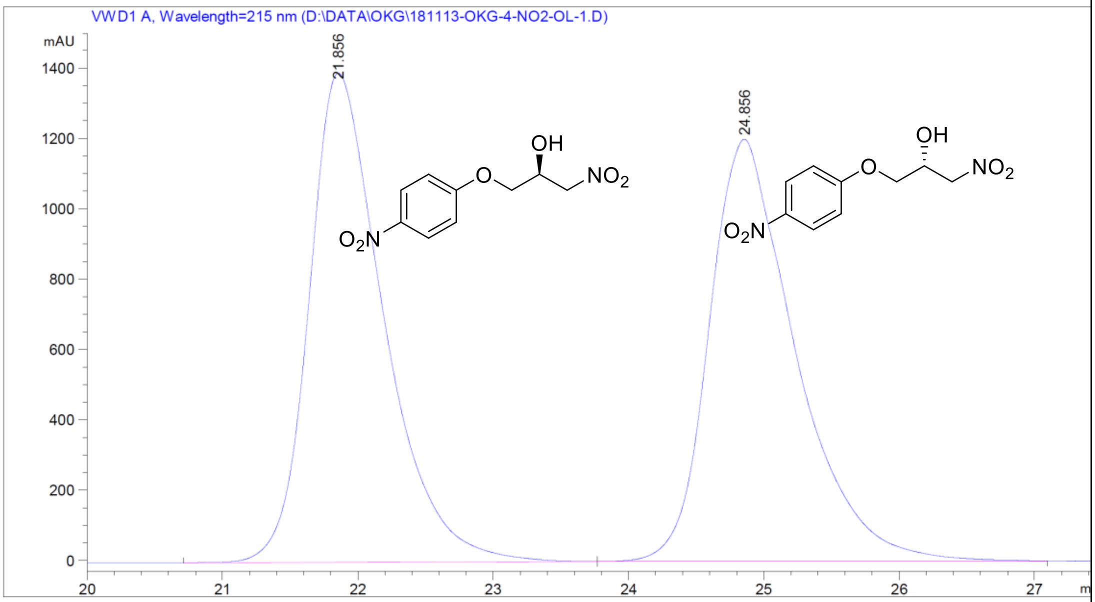
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.856	BB	0.5751	5.33469e4	1392.03748	50.0170
2	24.856	BV	0.6345	5.33107e4	1201.77563	49.9830



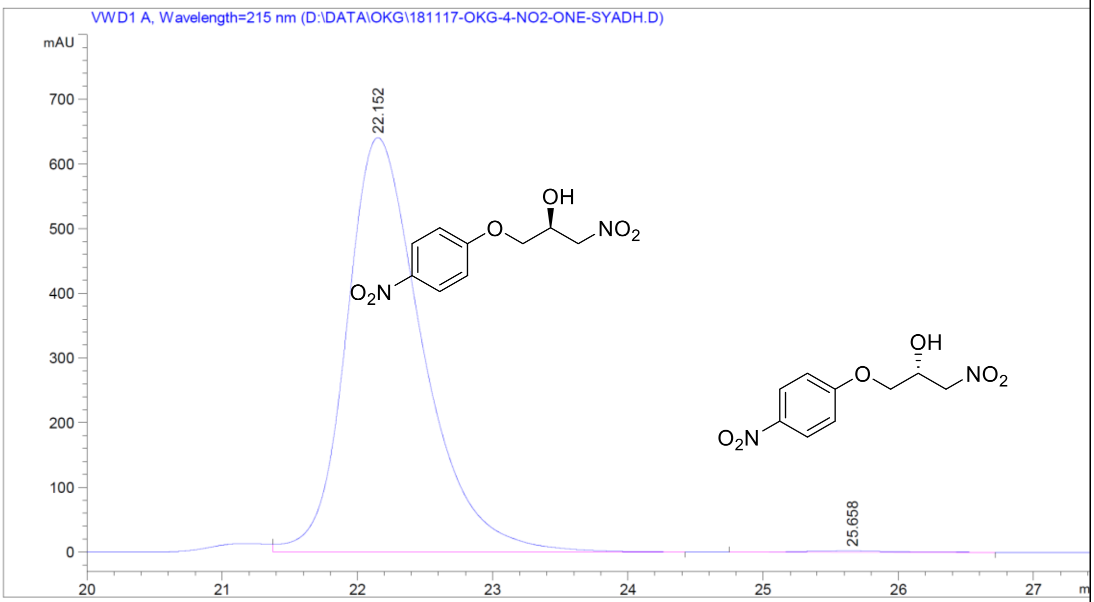
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.815	BB	0.5796	8706.20703	223.93513	22.5408
2	24.912	BV	0.6798	2.99179e4	667.61121	77.4592

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

(S)-1-nitro-3-(4-nitrophenoxy)propan-2-ol (5i)
Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.8 min (major), t_R'=24.8 min (minor)



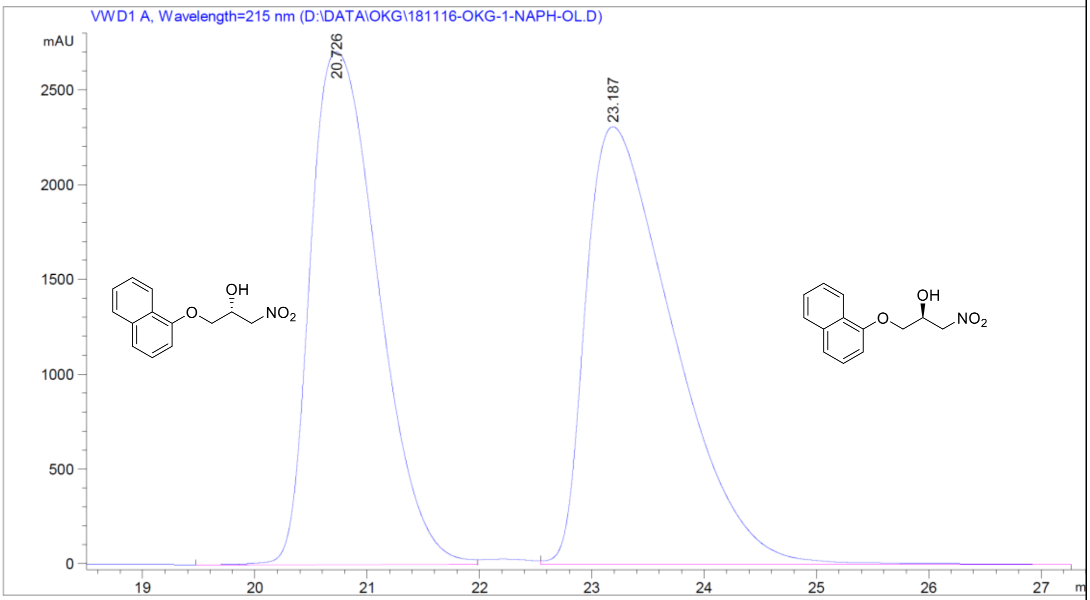
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.856	BB	0.5751	5.33469e4	1392.03748	50.0170
2	24.856	BV	0.6345	5.33107e4	1201.77563	49.9830



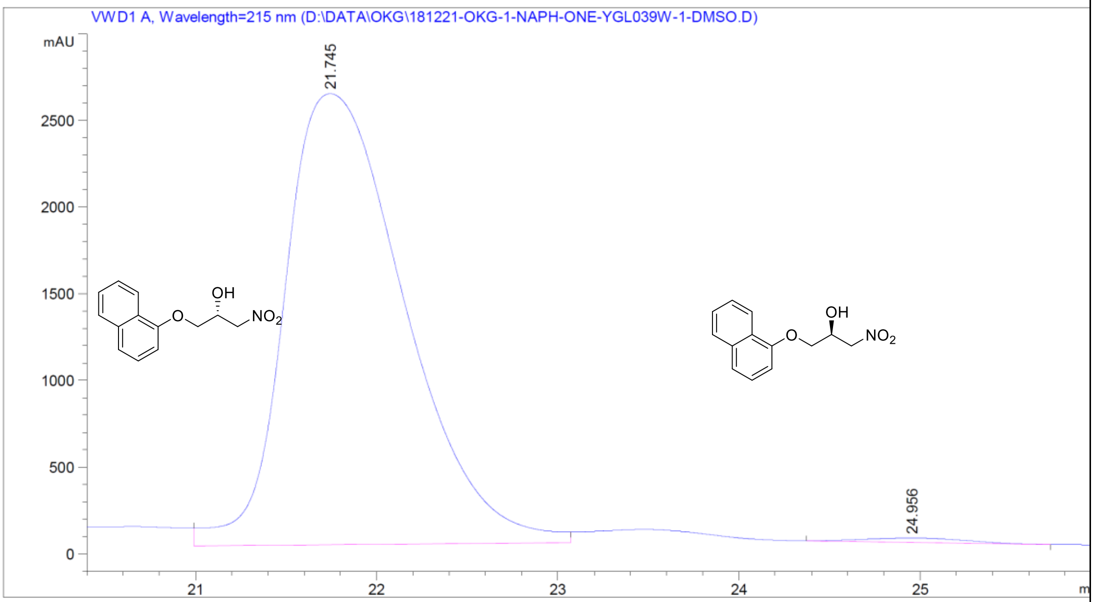
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.152	VV	0.5940	2.50987e4	640.76178	99.6014
2	25.658	BB	0.5519	100.45337	2.14285	0.3986

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

***(R)*-1-(naphthalen-1-yloxy)-3-nitropropan-2-ol (5j)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=20.7 min (major), t_R'=23.2 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.726	BV	0.5722	1.13360e5	2706.28735	47.4350
2	23.187	VBA	0.7922	1.25620e5	2310.82715	52.5650

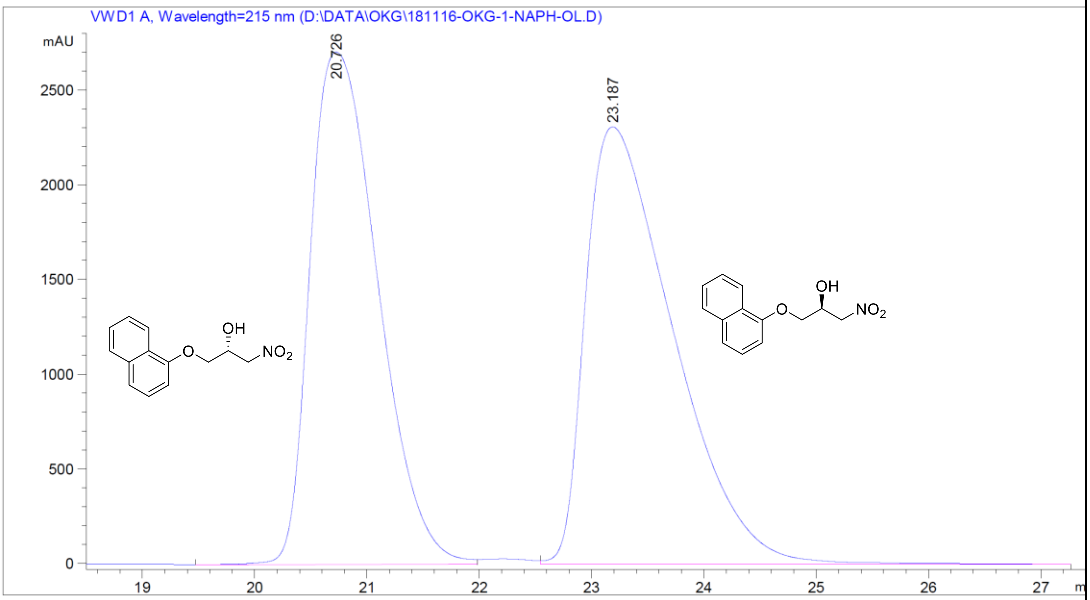


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.745	VV	0.5438	1.19980e5	2602.73779	99.1693
2	24.956	BB	0.5155	1004.98682	25.76683	0.8307

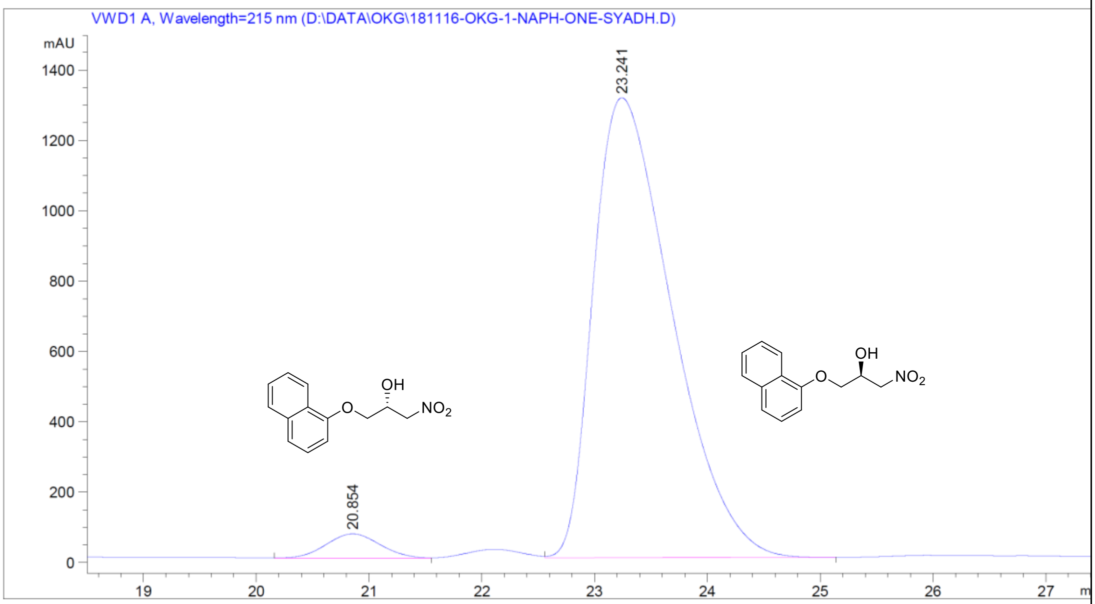
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(S)*-1-(naphthalen-1-yloxy)-3-nitropropan-2-ol (5j)**

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=20.7 min (minor), t_R'=23.2 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.726	BV	0.5722	1.13360e5	2706.28735	47.4350
2	23.187	VBA	0.7922	1.25620e5	2310.82715	52.5650



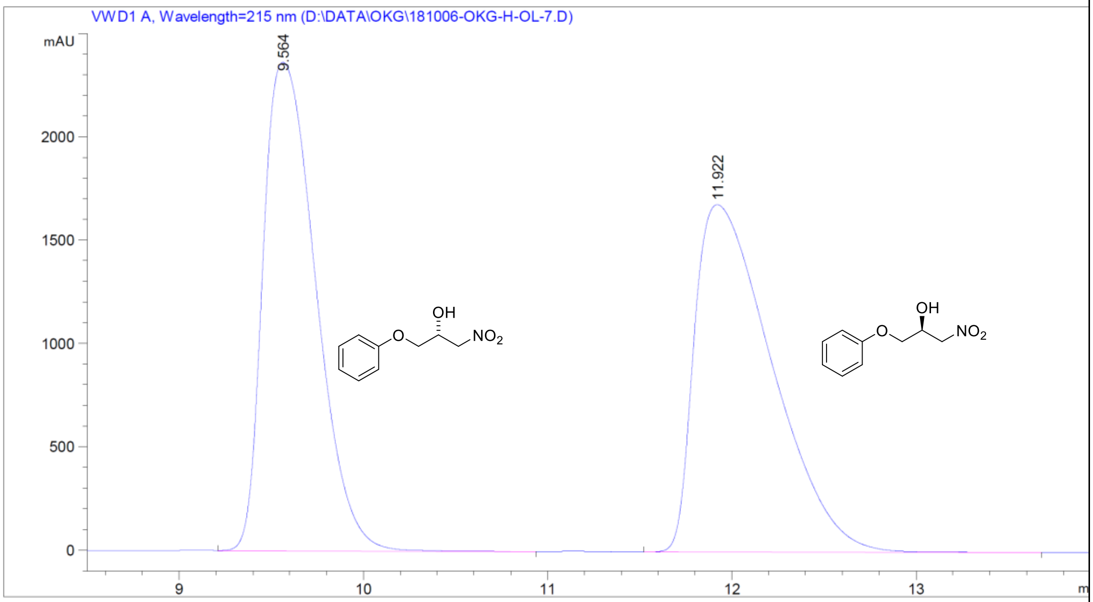
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.854	BB	0.5045	2236.38696	68.21342	3.4092
2	23.241	VB	0.7480	6.33623e4	1308.43591	96.5908

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

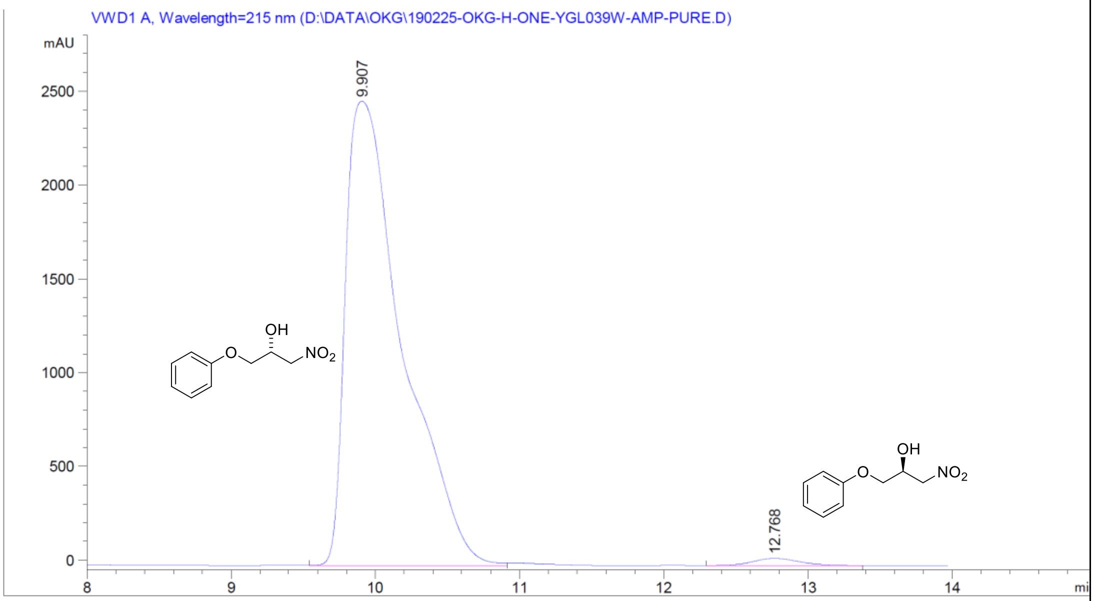
HPLC spectra of the products from CFE catalyzed preparative scale reactions

(*R*)-1-nitro-3-phenoxypropan-2-ol (5a)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=9.6 min (major), t_R'=11.9 min (minor)



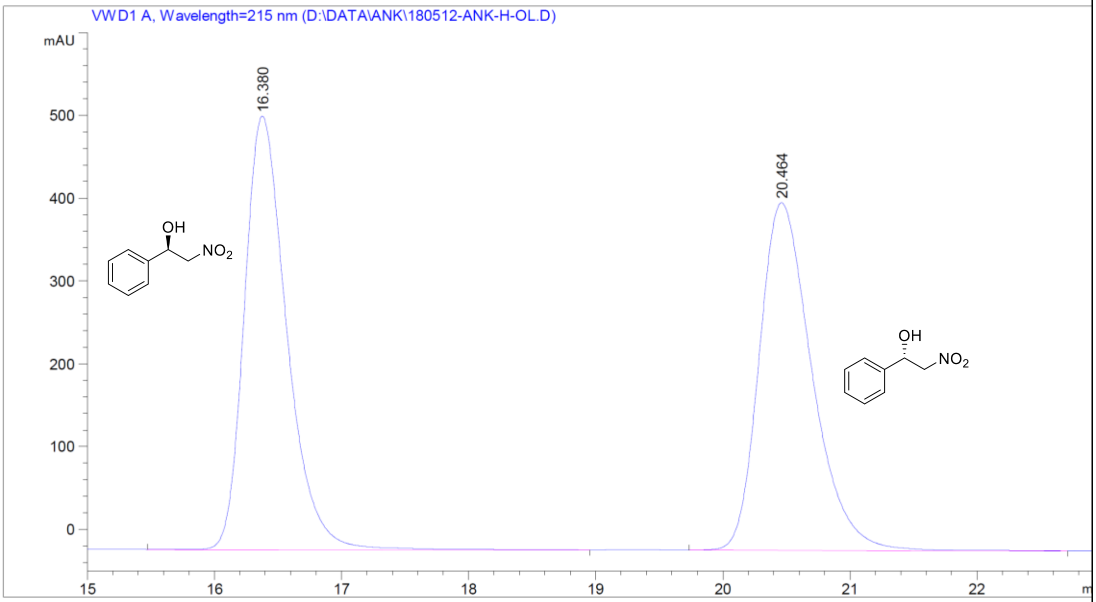
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.564	VV	0.3135	4.69228e4	2364.45605	48.8256
2	11.922	BB	0.4534	4.91801e4	1680.42651	51.1744



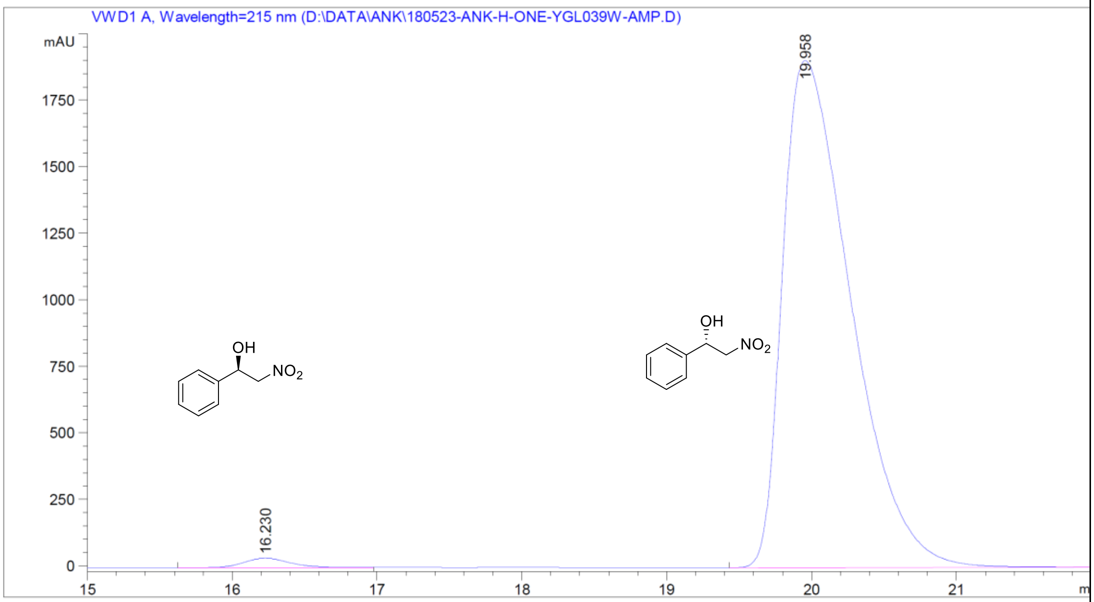
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.907	VV	0.4060	6.78745e4	2474.37183	98.7173
2	12.768	VV	0.3526	881.92596	38.59317	1.2827

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w-catalyzed biotransformation.

***(S)*-2-nitro-1-phenylethanol (2a)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.4 min (minor), t_R'=20.5 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.380	VB	0.3549	1.21474e4	523.11871	50.1021
2	20.464	BB	0.4403	1.20979e4	419.70804	49.8979

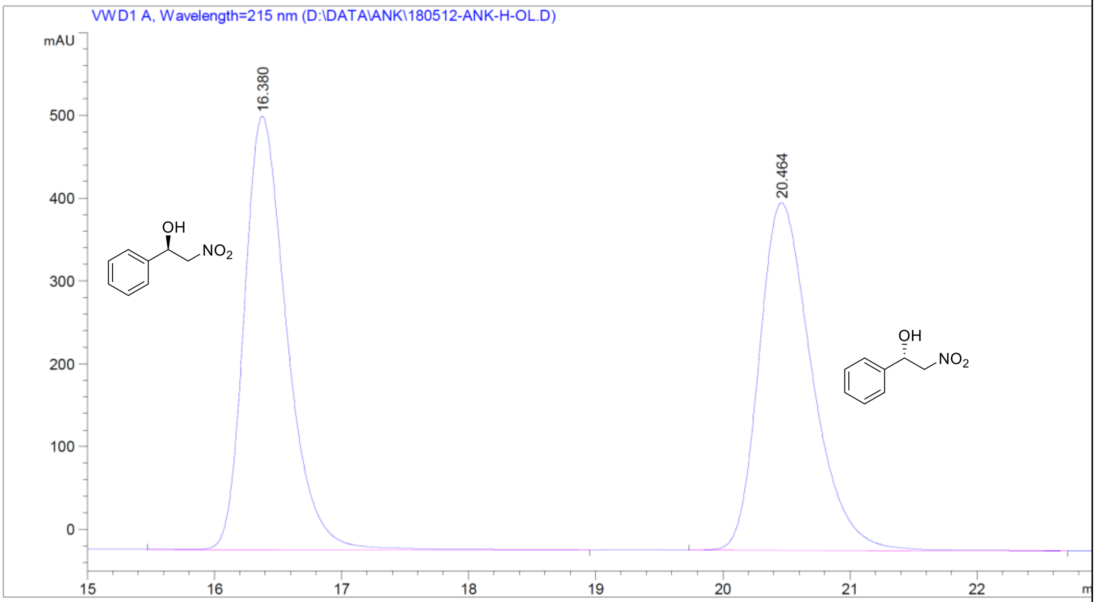


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.230	BV	0.3458	812.39240	35.65673	1.2893
2	19.958	BB	0.5088	6.21970e4	1905.45288	98.7107

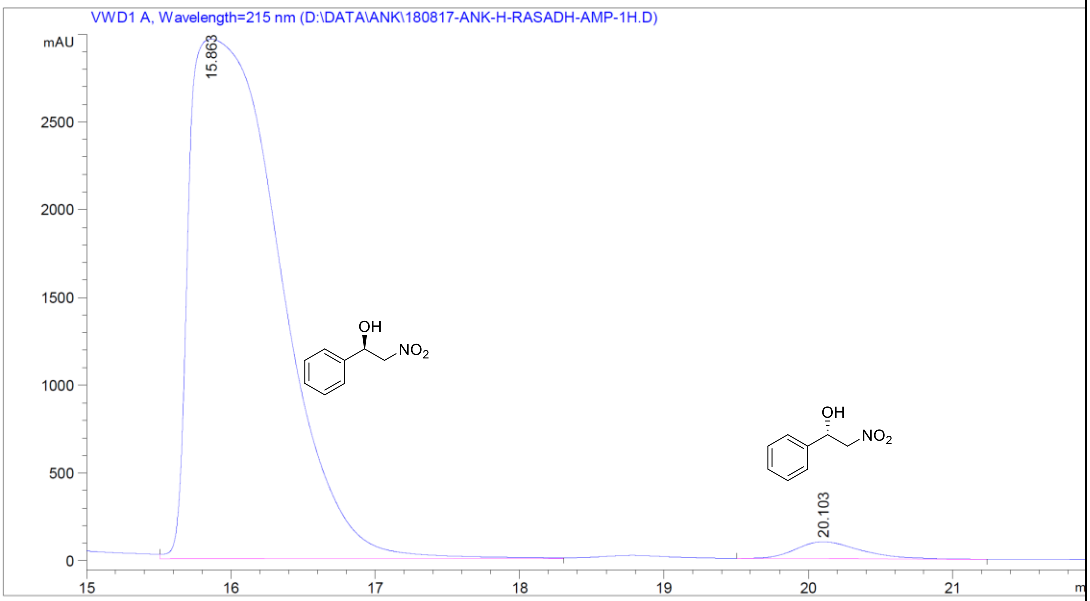
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

***(R)*-2-nitro-1-phenylethanol (2a)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.4 min (minor), t_R'=20.5 min (major)



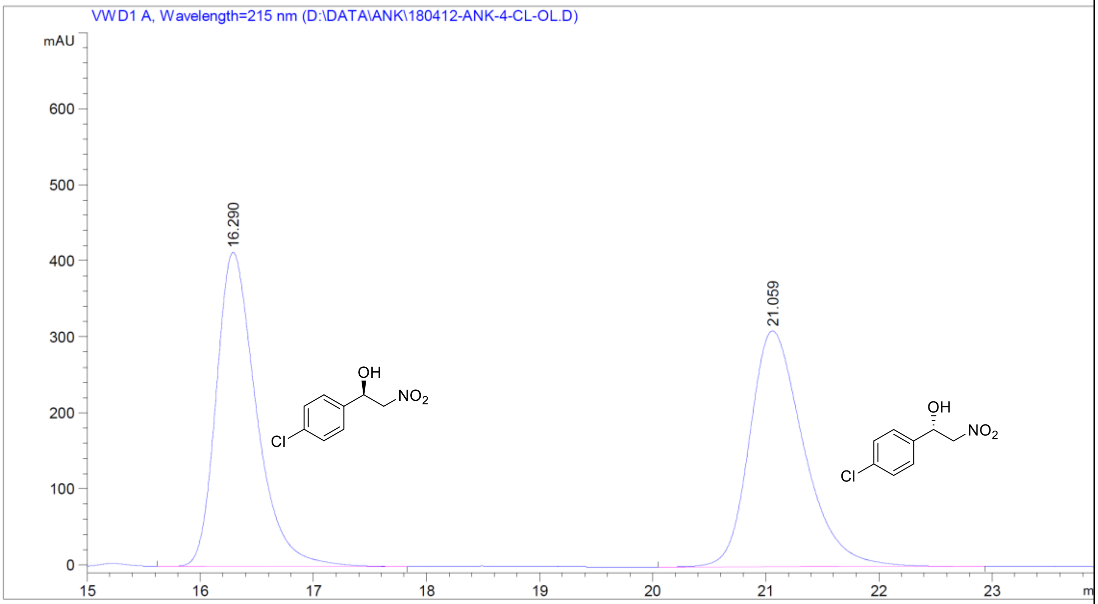
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.380	VB	0.3549	1.21474e4	523.11871	50.1021
2	20.464	BB	0.4403	1.20979e4	419.70804	49.8979



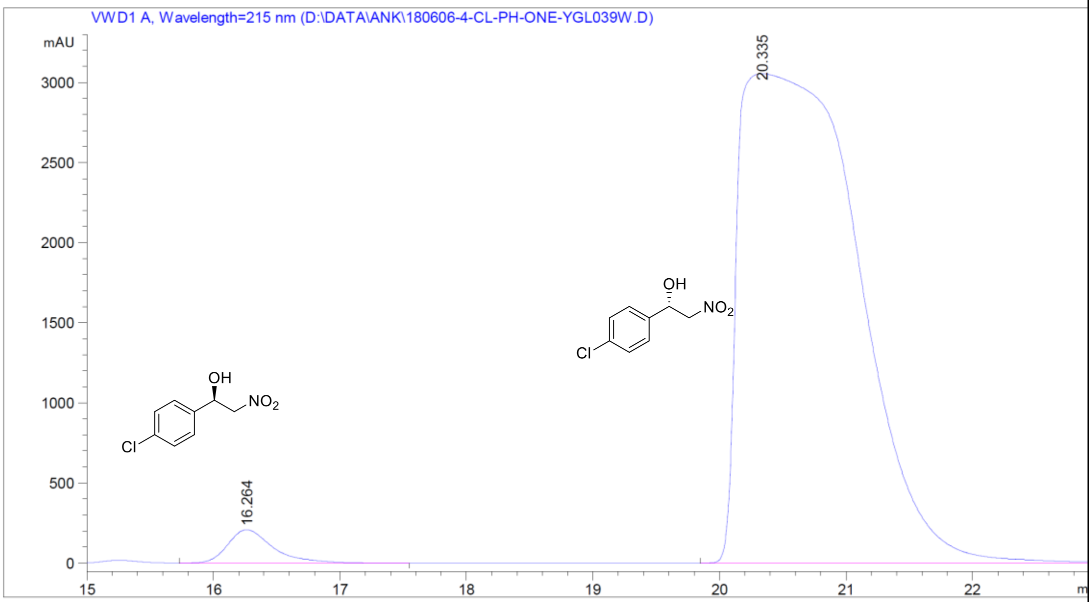
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.863	VV	0.5122	1.29025e5	2958.94434	97.7362
2	20.103	BB	0.4632	2988.55664	95.98825	2.2638

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH (CFE) catalyzed biotransformation.

***(S)*-1-(4-chlorophenyl)-2-nitroethan-1-ol (2i)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.3 min (minor), t_R'=21.0 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.290	BB	0.3745	1.01797e4	413.15271	49.6323
2	21.059	BB	0.5072	1.03306e4	310.44525	50.3677

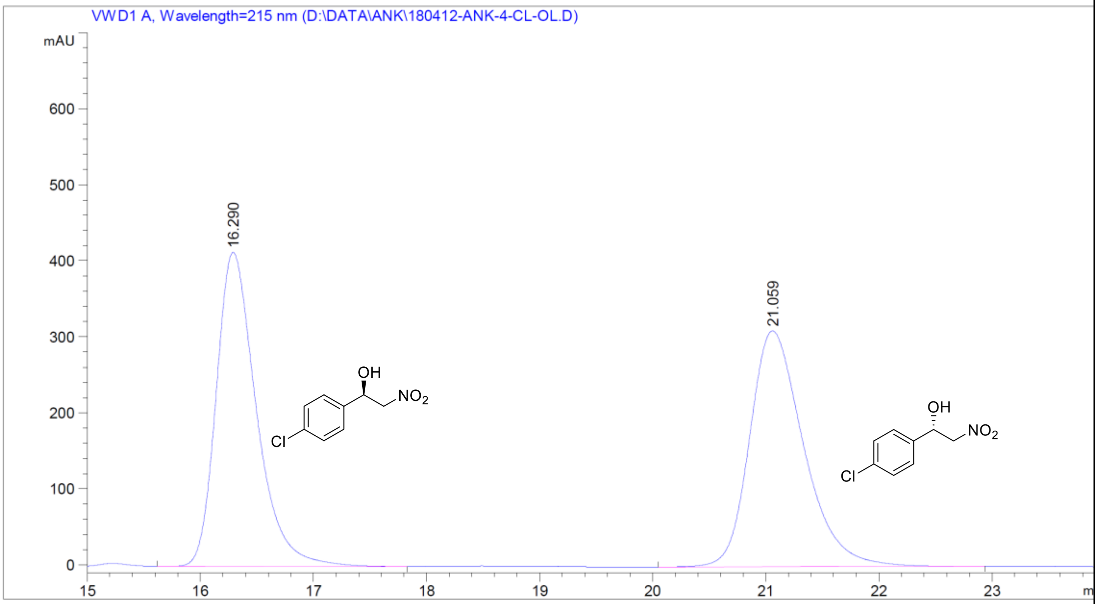


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.264	VB	0.3753	5195.66699	208.07703	2.5290
2	20.335	BB	0.8872	2.00244e5	3053.04053	97.4710

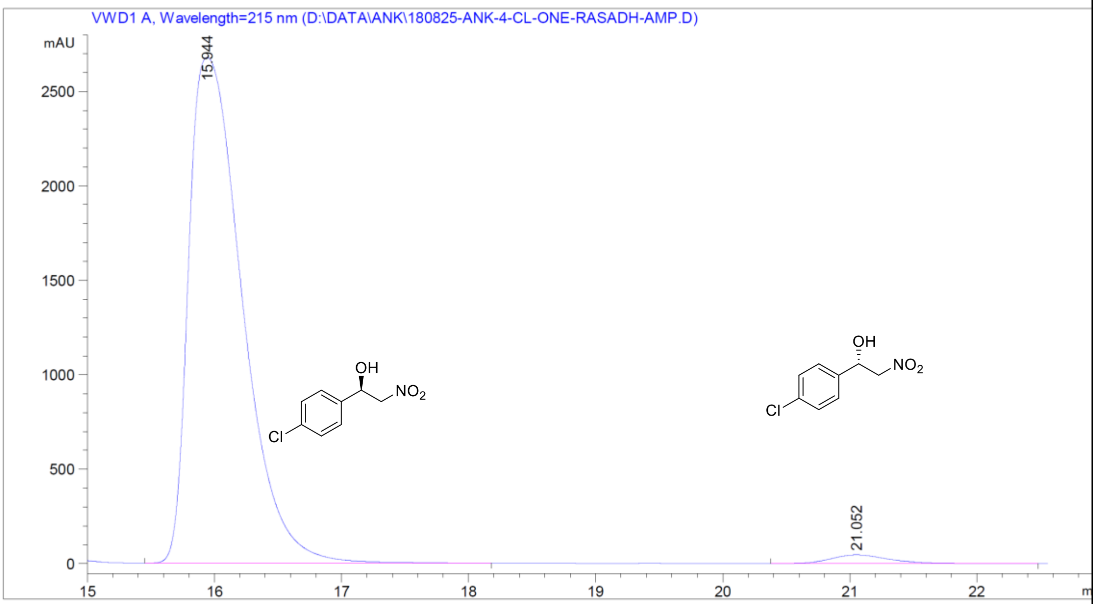
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*R*)-1-(4-chlorophenyl)-2-nitroethan-1-ol (2i)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=16.3 min (minor), t_R'=21.0 min (major)



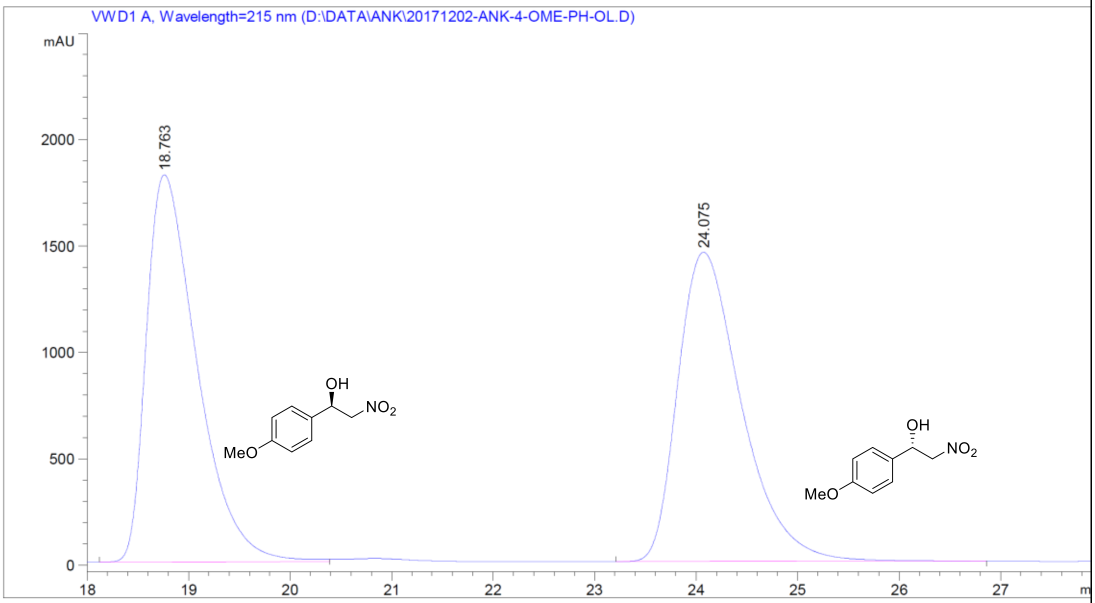
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.290	BB	0.3745	1.01797e4	413.15271	49.6323
2	21.059	BB	0.5072	1.03306e4	310.44525	50.3677



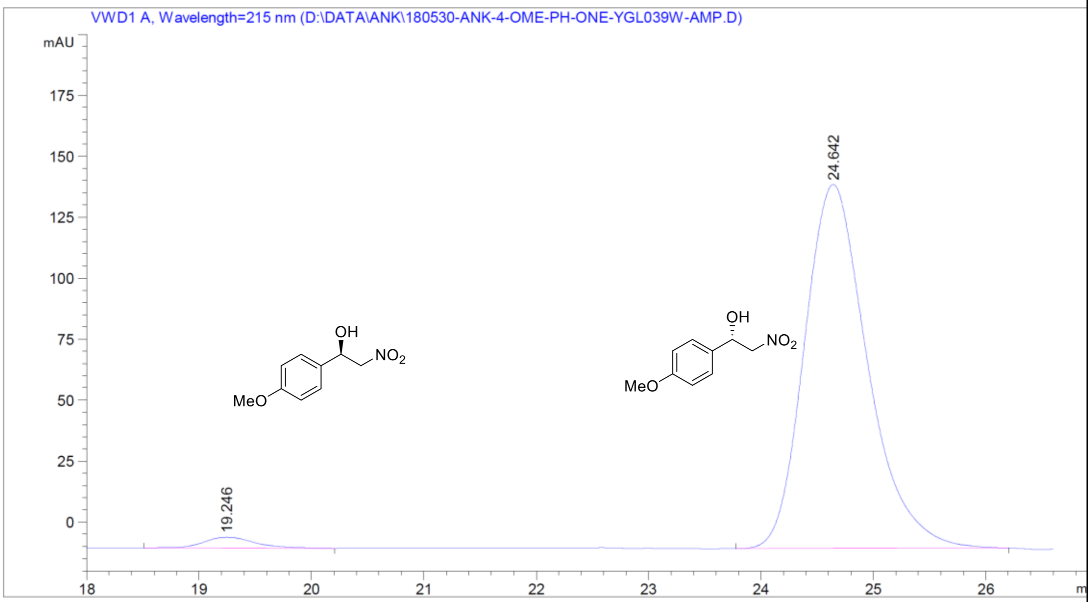
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.944	VB	0.4544	7.81059e4	2677.31860	98.1346
2	21.052	BB	0.4837	1484.70032	45.86351	1.8654

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH (CFE) catalyzed biotransformation.

***(S)*-1-(4-methoxyphenyl)-2-nitroethan-1-ol (2k)**
Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=18.8 min (minor), t_R'=24.1 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.763	BV	0.5293	6.30614e4	1819.79443	49.9132
2	24.075	BB	0.6718	6.32808e4	1453.74915	50.0868

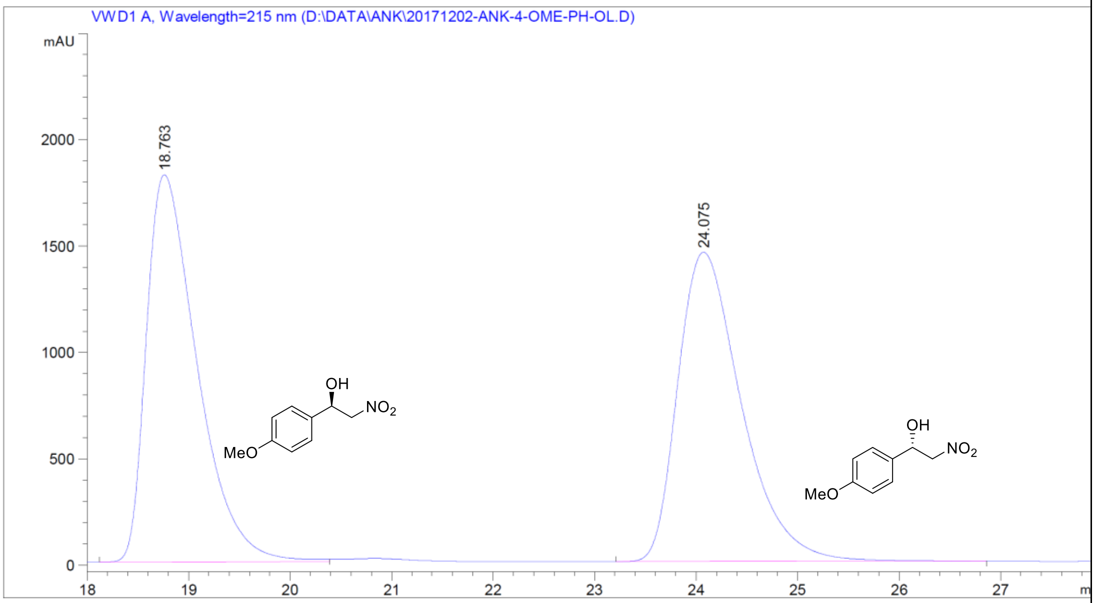


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.246	BB	0.4856	140.37476	4.47934	2.3554
2	24.642	BB	0.5981	5819.22217	149.19283	97.6446

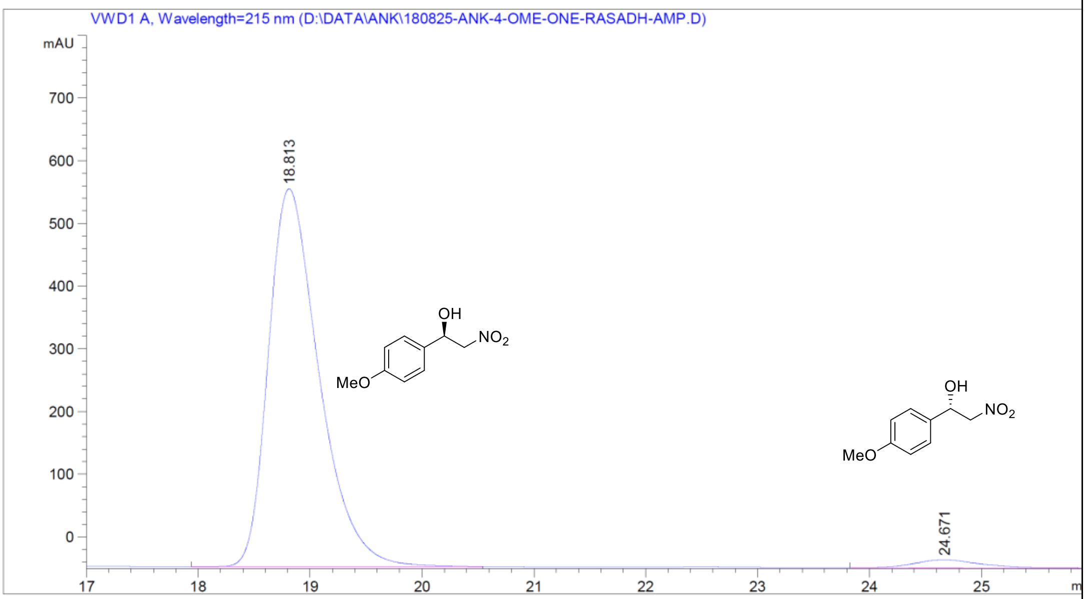
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*R*)-1-(4-methoxyphenyl)-2-nitroethan-1-ol (2k)

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=18.8 min (minor), t_R'=24.1 min (major)



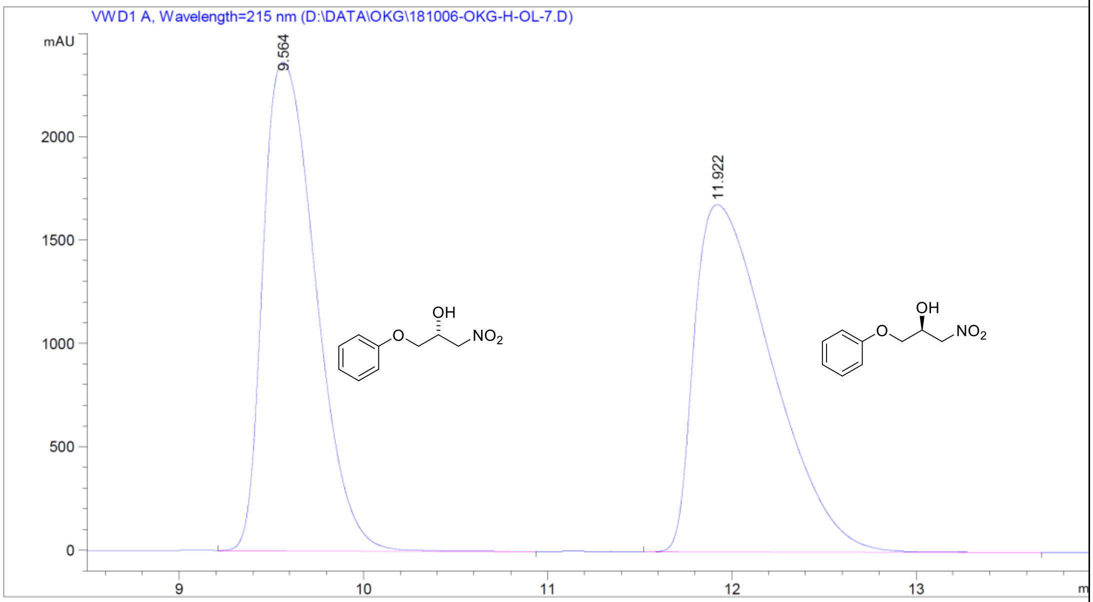
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.763	BV	0.5293	6.30614e4	1819.79443	49.9132
2	24.075	BB	0.6718	6.32808e4	1453.74915	50.0868



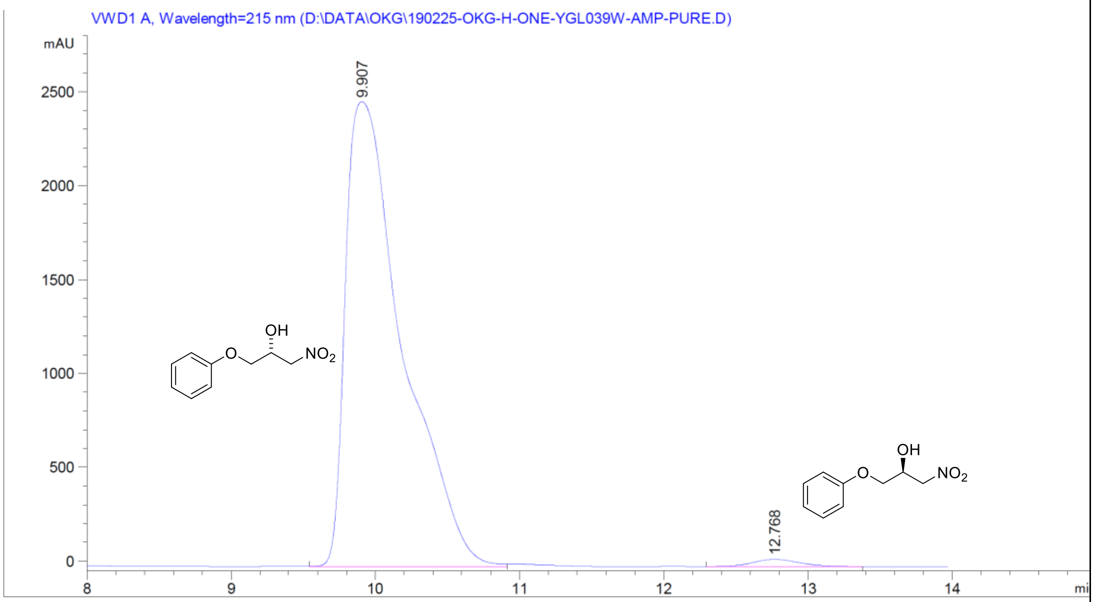
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.813	BB	0.4799	1.89438e4	602.44208	97.3623
2	24.671	BBA	0.5039	513.22235	12.60906	2.6377

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of RasADH (CFE) catalyzed biotransformation.

(R)-1-nitro-3-phenoxypropan-2-ol (5a)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=9.6 min (major), t_R'=11.9 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.564	VV	0.3135	4.69228e4	2364.45605	48.8256
2	11.922	BB	0.4534	4.91801e4	1680.42651	51.1744

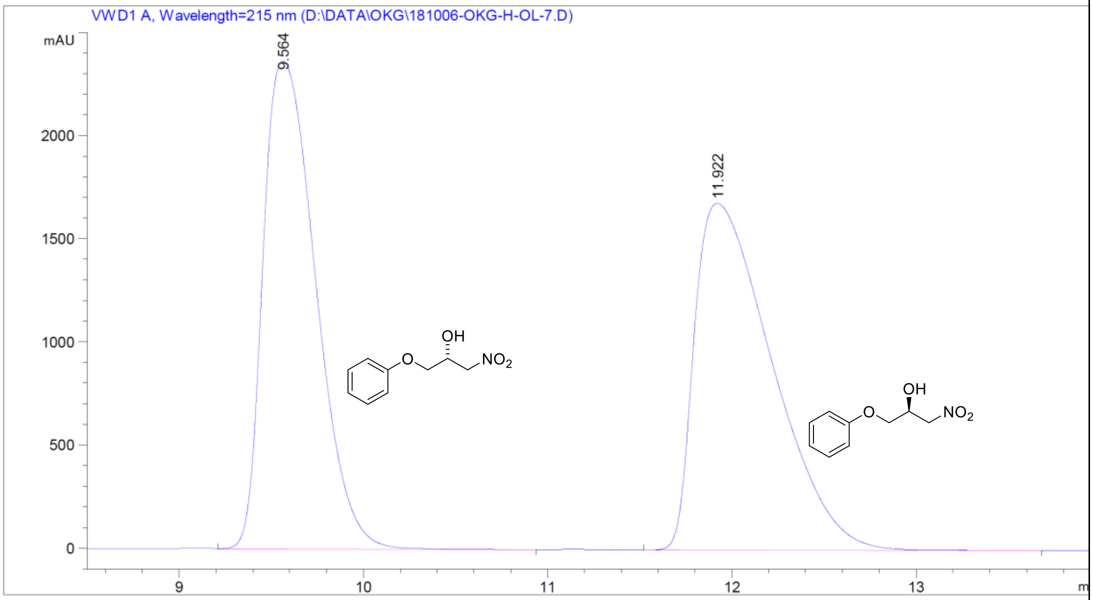


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.907	VV	0.4060	6.78745e4	2474.37183	98.7173
2	12.768	VV	0.3526	881.92596	38.59317	1.2827

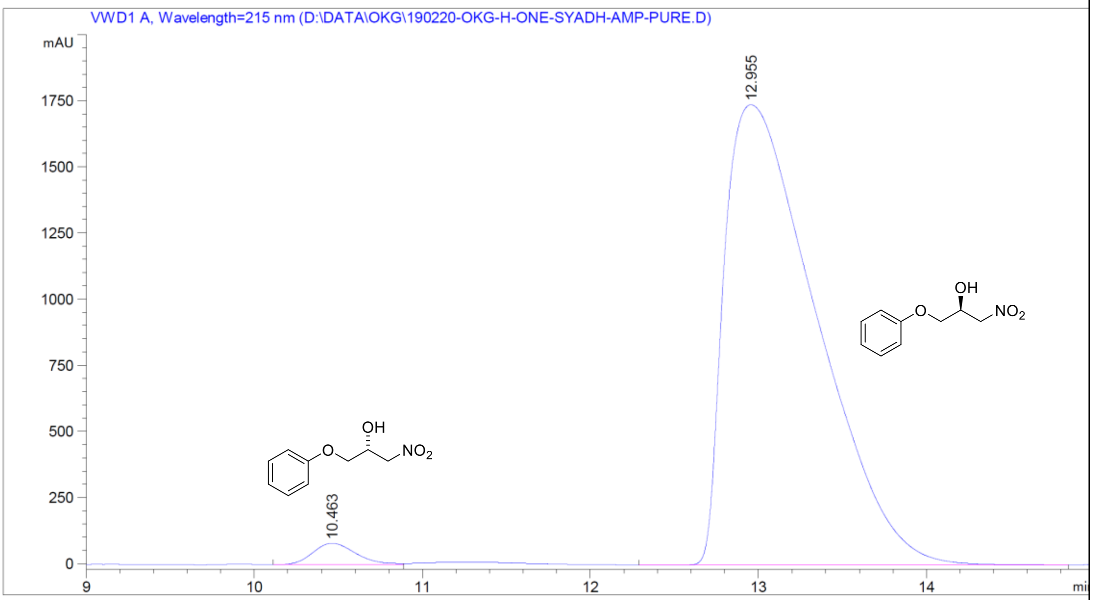
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*S*)-1-nitro-3-phenoxypropan-2-ol (5a)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=9.6 min (minor), t_R'=11.9 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.564	VV	0.3135	4.69228e4	2364.45605	48.8256
2	11.922	BB	0.4534	4.91801e4	1680.42651	51.1744

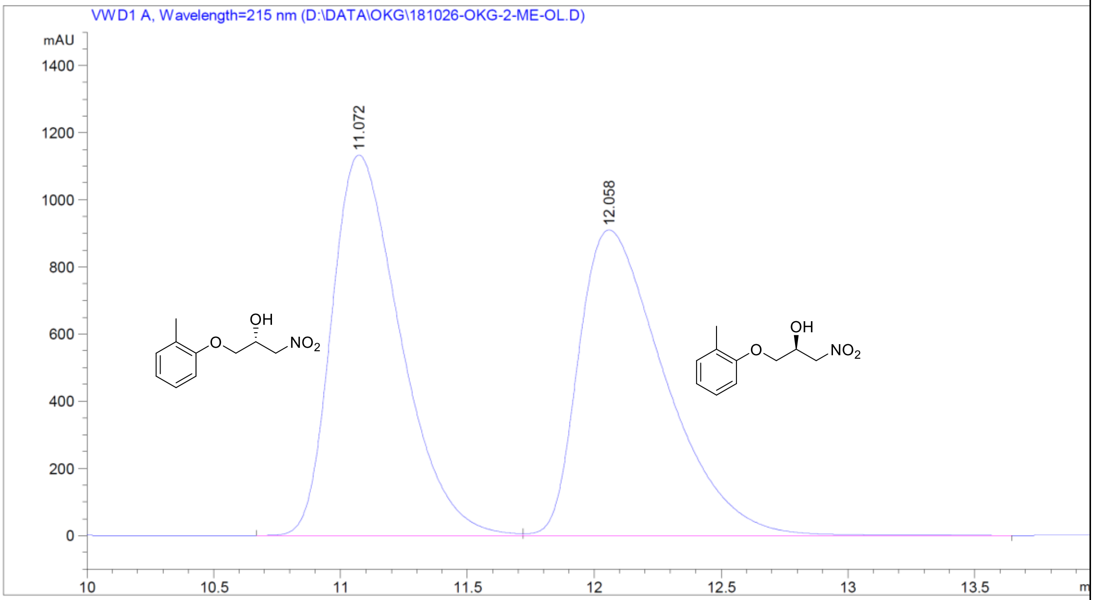


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.463	VV	0.2782	1461.47461	81.48500	2.1647
2	12.955	BB	0.5685	6.60525e4	1739.56079	97.8353

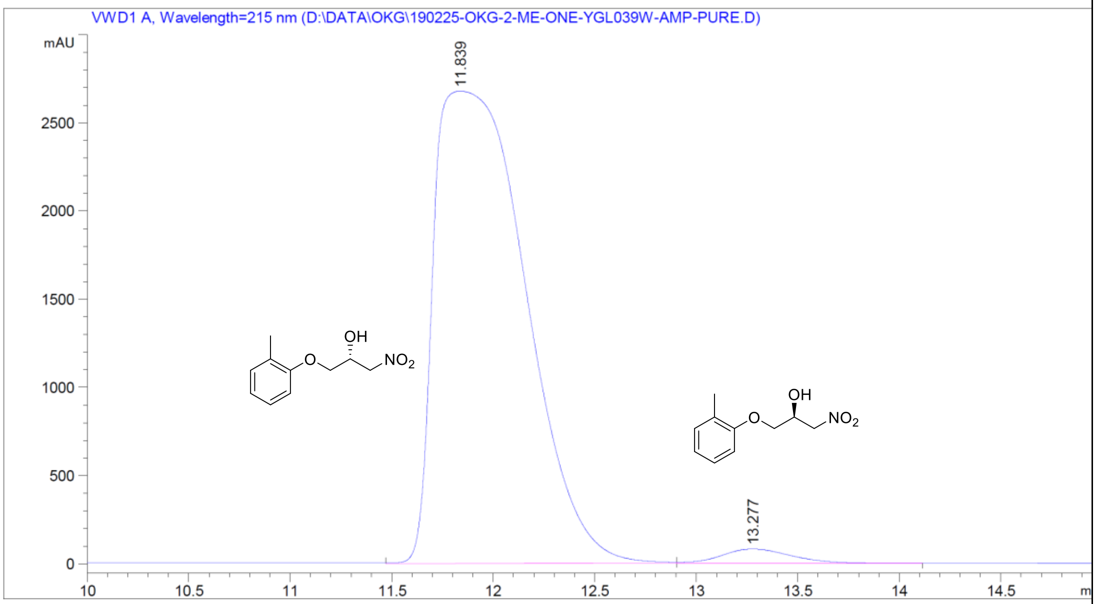
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(*R*)-1-nitro-3-(o-tolyloxy)propan-2-ol (5b)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.1 min (major), t_R'=12.0 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.072	BV	0.2898	2.13445e4	1133.14941	49.7808
2	12.058	VV	0.3621	2.15324e4	909.96484	50.2192

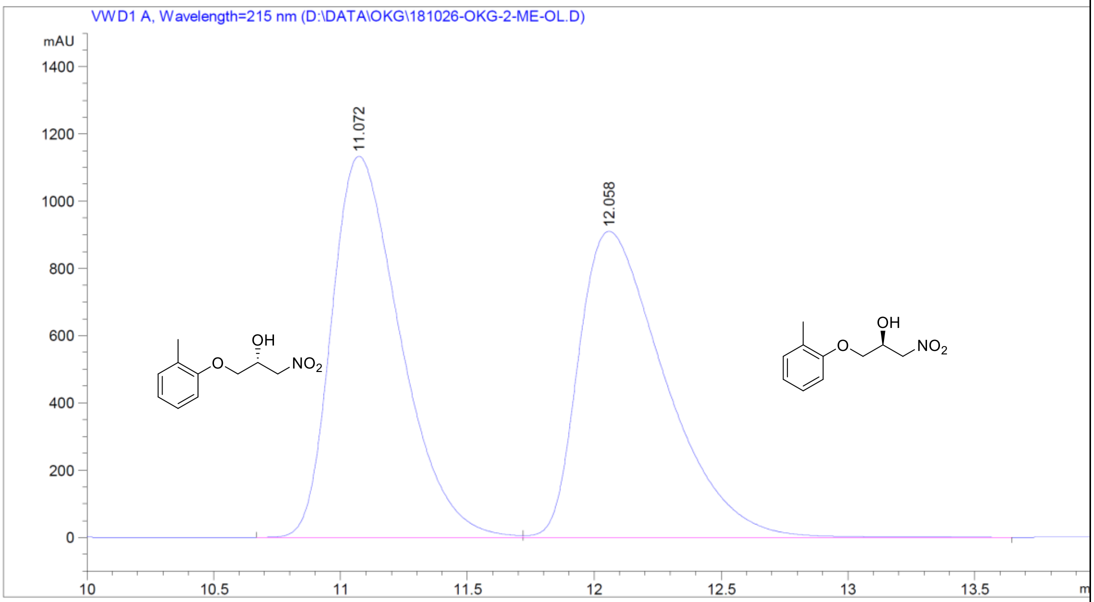


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.839	VV	0.4158	8.39355e4	2677.16504	97.7043
2	13.277	VB	0.3683	1972.18311	82.07229	2.2957

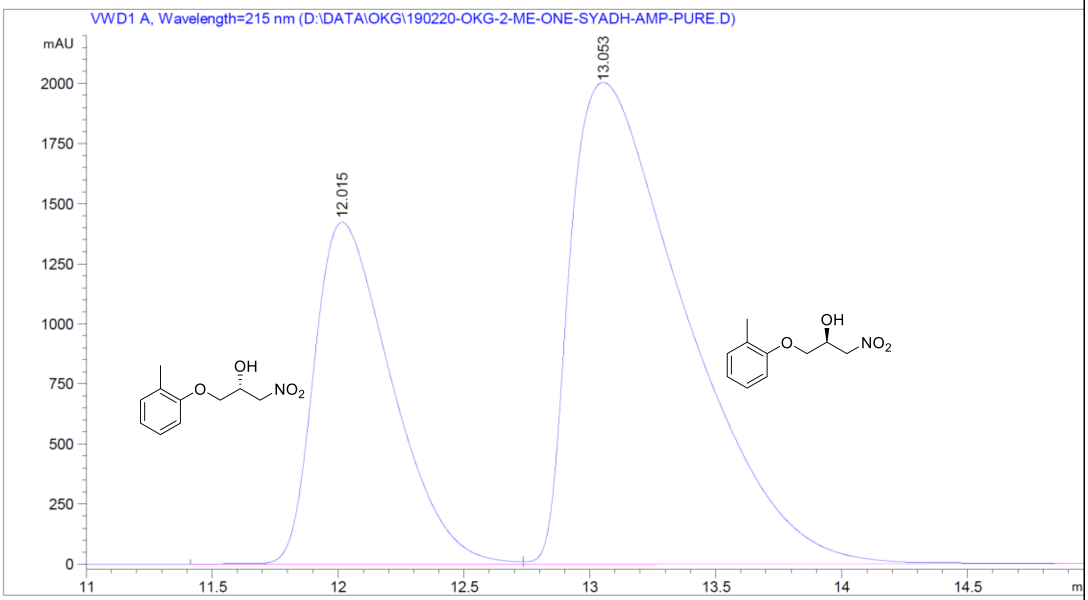
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*S*)-1-nitro-3-(o-tolyloxy)propan-2-ol (5b)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 85:15, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=11.1 min (minor), t_R'=12.0 min (major)



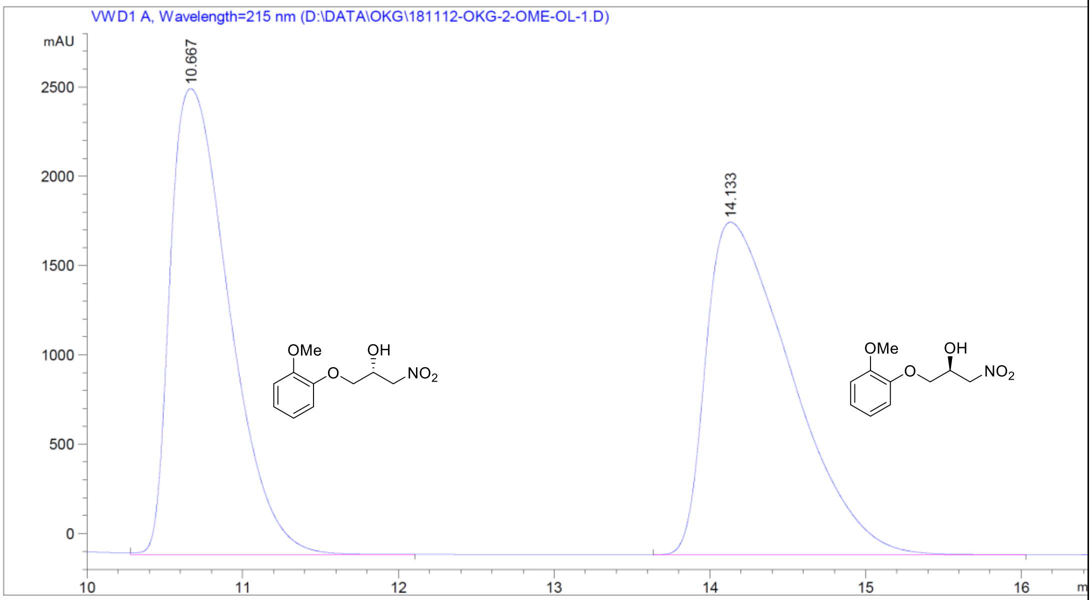
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.072	BV	0.2898	2.13445e4	1133.14941	49.7808
2	12.058	VV	0.3621	2.15324e4	909.96484	50.2192



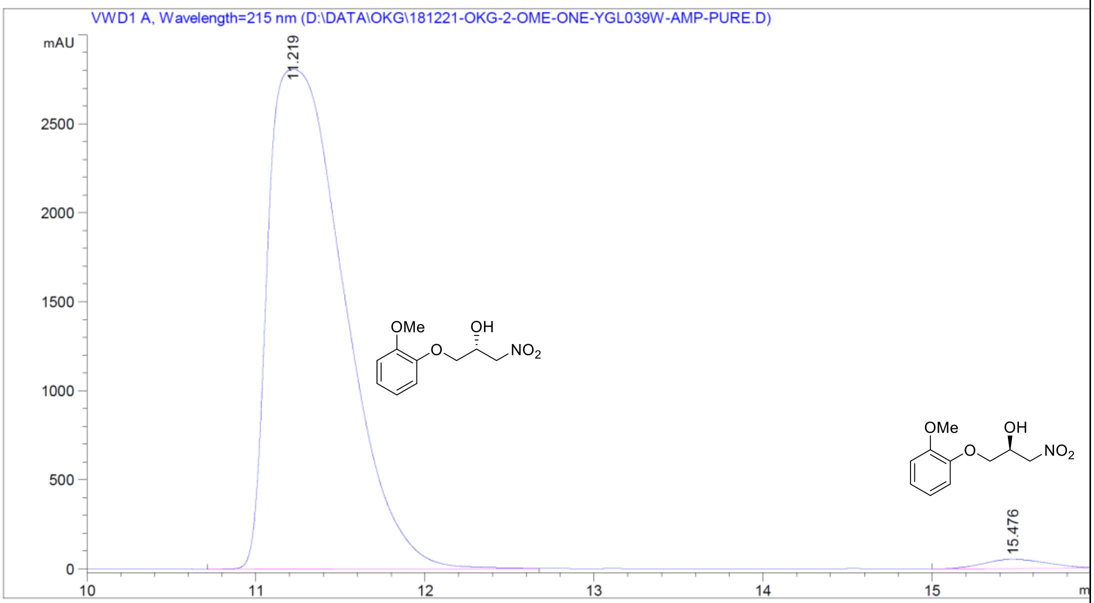
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.015	BV	0.3292	3.03804e4	1422.16760	32.1995
2	13.053	VB	0.4660	6.39701e4	2003.63330	67.8005

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

***(R)*-1-(2-methoxyphenoxy)-3-nitropropan-2-ol (5c)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.7 min (major), t_R'=14.1 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.667	VB	0.4041	6.82455e4	2605.21729	49.0148
2	14.133	VB	0.5625	7.09890e4	1861.12354	50.9852

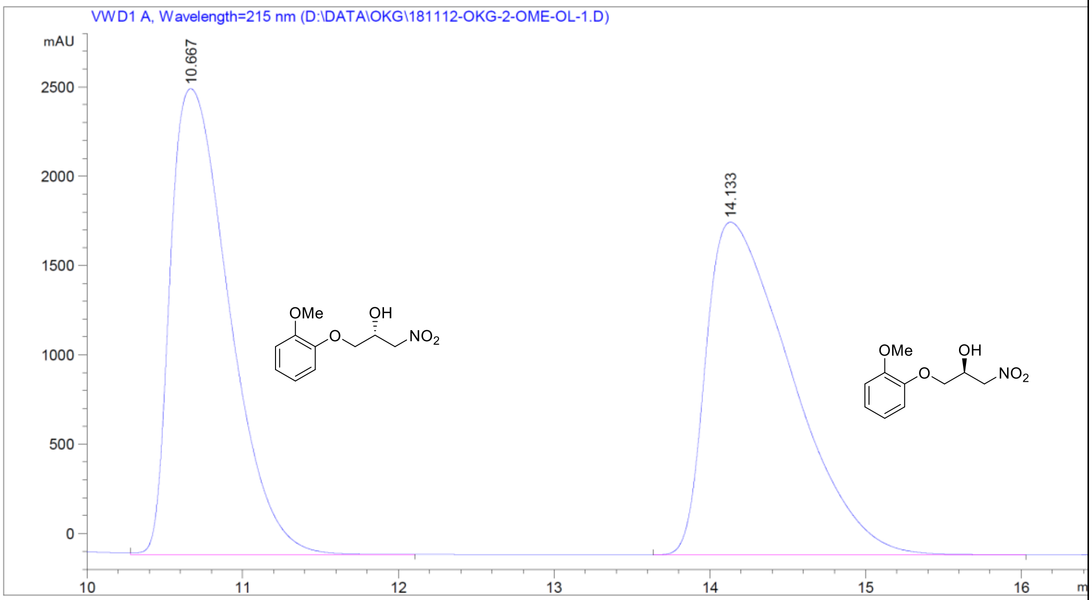


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.219	BV	0.3674	8.78191e4	2807.68970	98.4737
2	15.476	BBA	0.3834	1361.18689	52.07686	1.5263

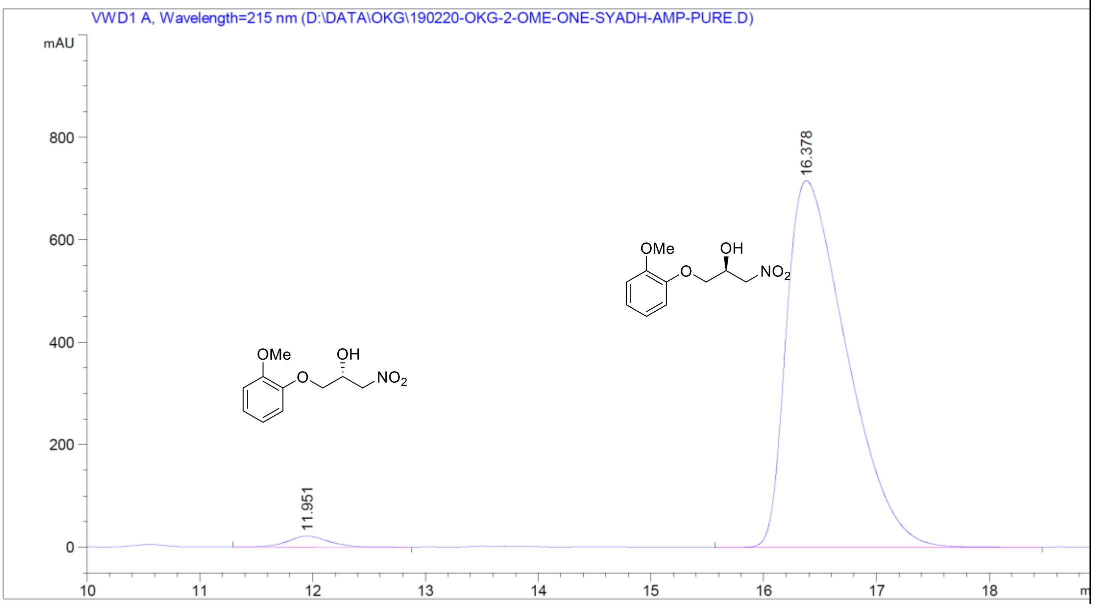
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*S*)-1-(2-methoxyphenoxy)-3-nitropropan-2-ol (5c)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.7 min (minor), t_R'=14.1 min (major)



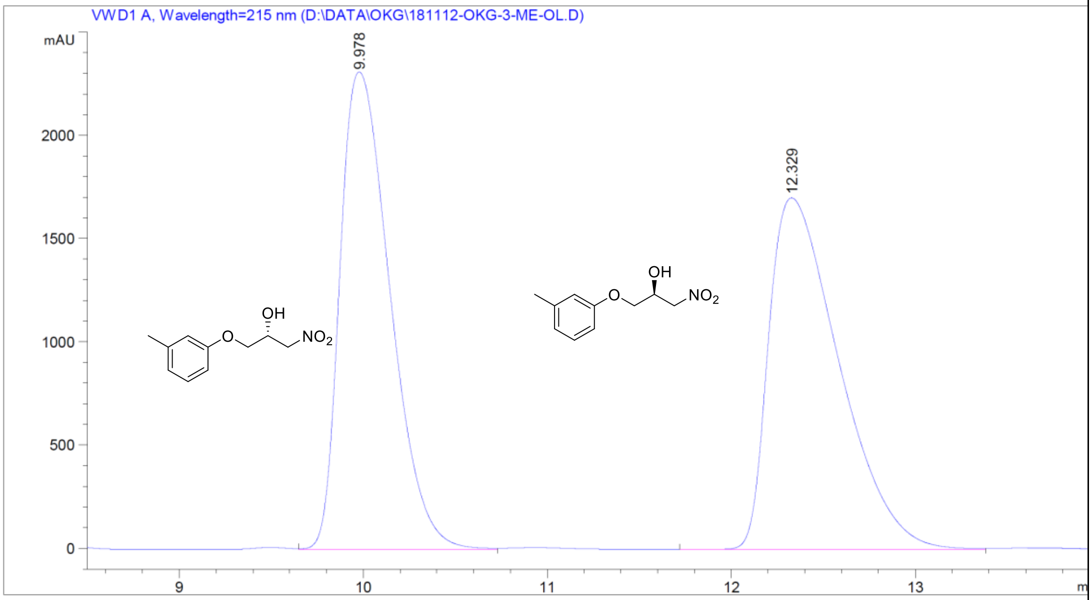
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.667	VB	0.4041	6.82455e4	2605.21729	49.0148
2	14.133	VB	0.5625	7.09890e4	1861.12354	50.9852



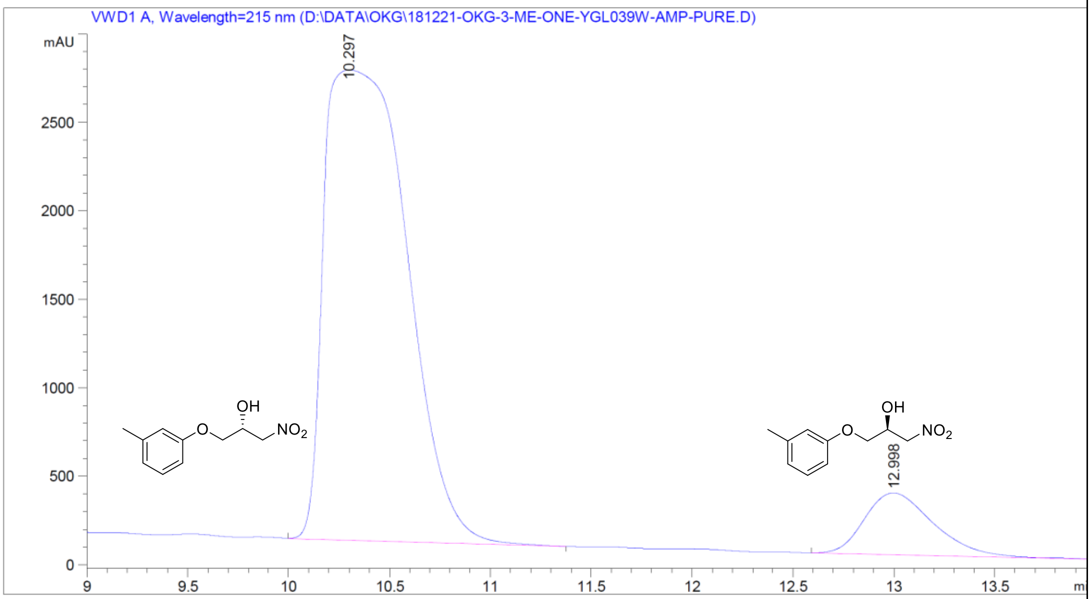
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.951	BB	0.3791	553.36261	21.73283	2.0360
2	16.378	BB	0.5677	2.66257e4	716.27216	97.9640

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

***(R)*-1-nitro-3-(m-tolyloxy)propan-2-ol (5d)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.0 min (major), t_R'=12.3 min (minor)



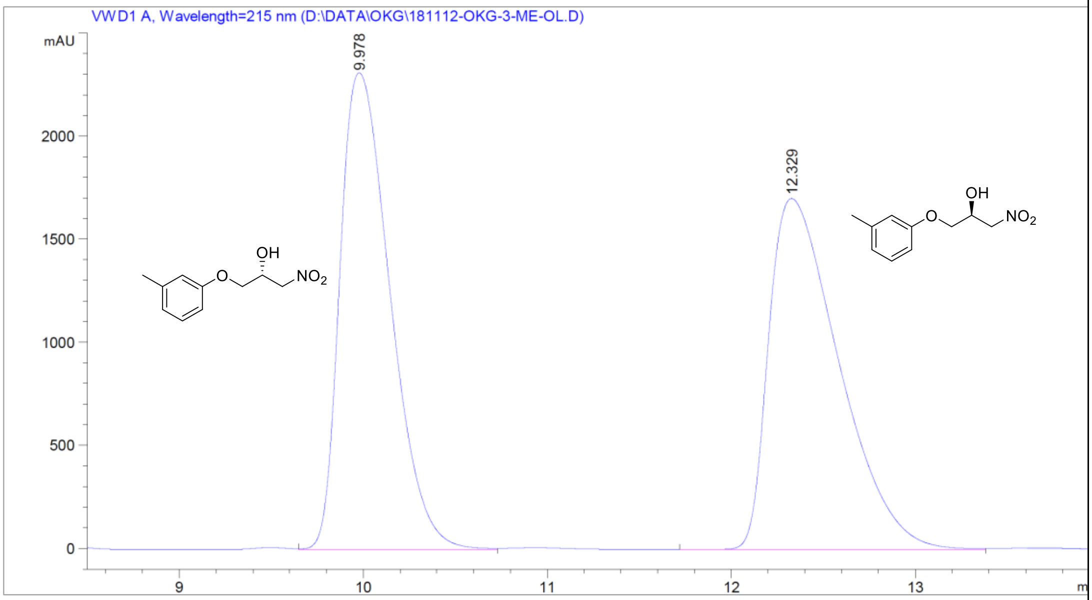
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.978	VV	0.2944	4.36561e4	2310.81665	49.1861
2	12.329	BV	0.4092	4.51009e4	1701.78027	50.8139



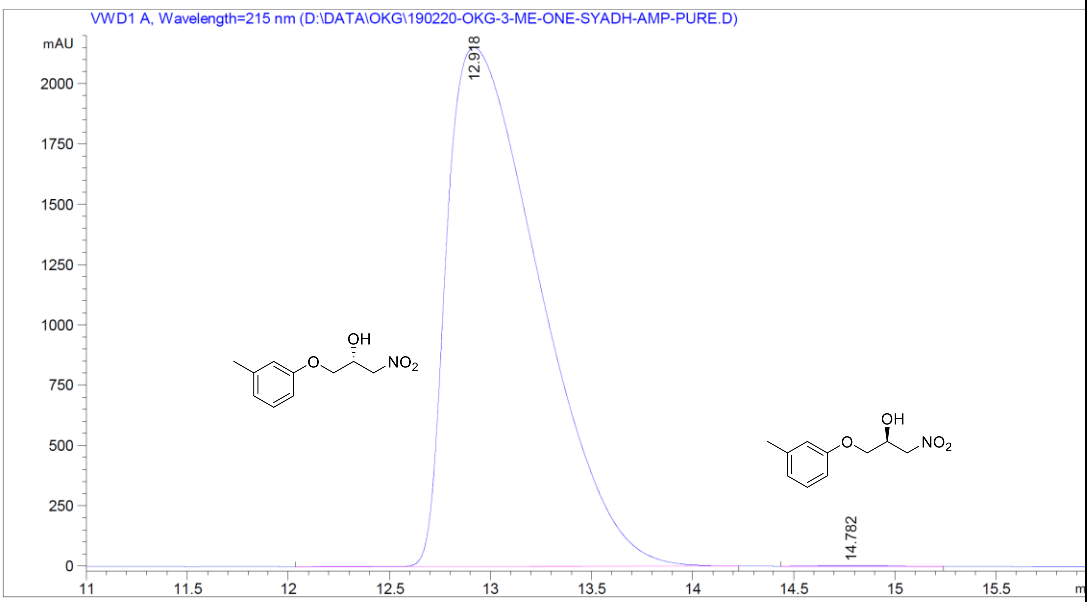
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.297	VB	0.3423	7.61408e4	2657.52075	90.1500
2	12.998	VB	0.3669	8319.32617	349.32050	9.8500

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

***(S)*-1-nitro-3-(m-tolyloxy)propan-2-ol (5d)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.8 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=10.0 min (minor), t_R'=12.3 min (major)



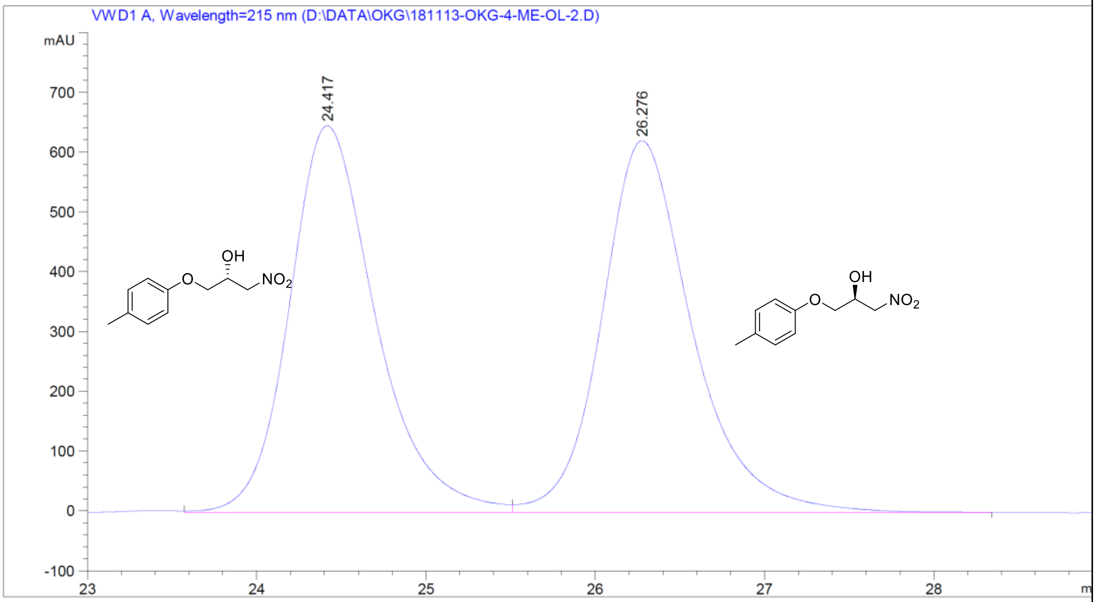
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.978	VV	0.2944	4.36561e4	2310.81665	49.1861
2	12.329	BV	0.4092	4.51009e4	1701.78027	50.8139



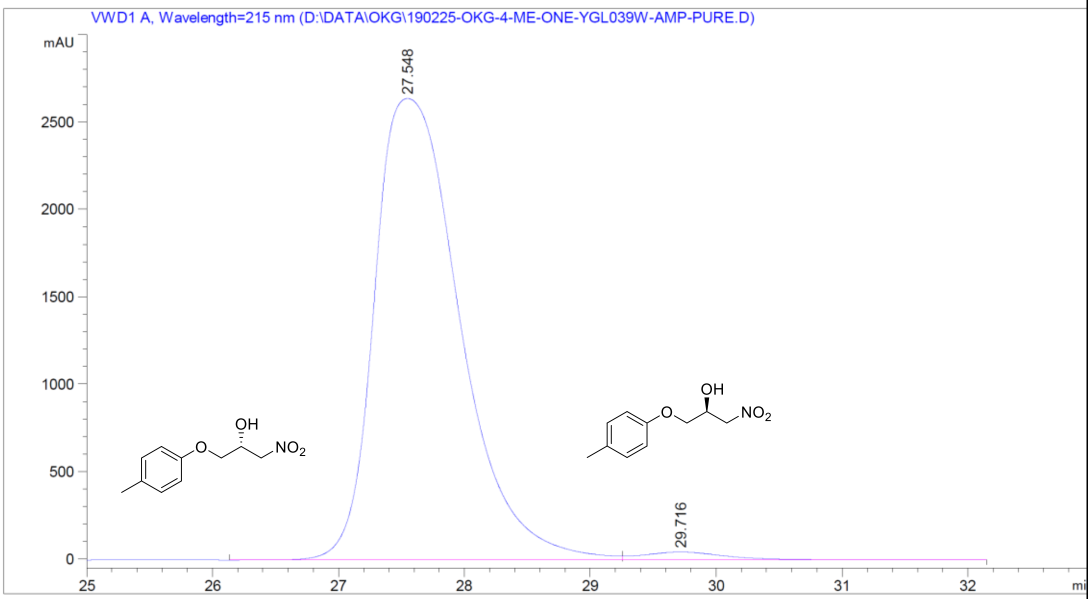
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.918	BB	0.4886	6.84516e4	2151.73120	99.8461
2	14.782	BB	0.2795	105.53273	4.45310	0.1539

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(*R*)-1-nitro-3-(p-tolyloxy)propan-2-ol (5e)
Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 92:8, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.4 min (major), t_R'=26.3 min (minor)



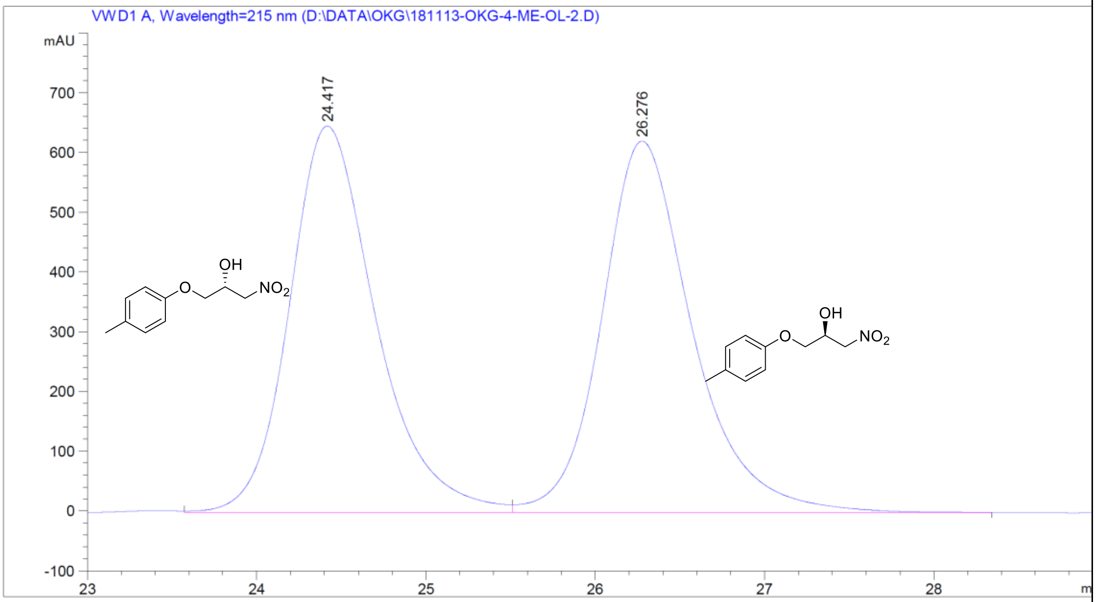
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.417	VV	0.5338	2.29941e4	646.75470	49.7175
2	26.276	VV	0.5614	2.32555e4	621.74335	50.2825



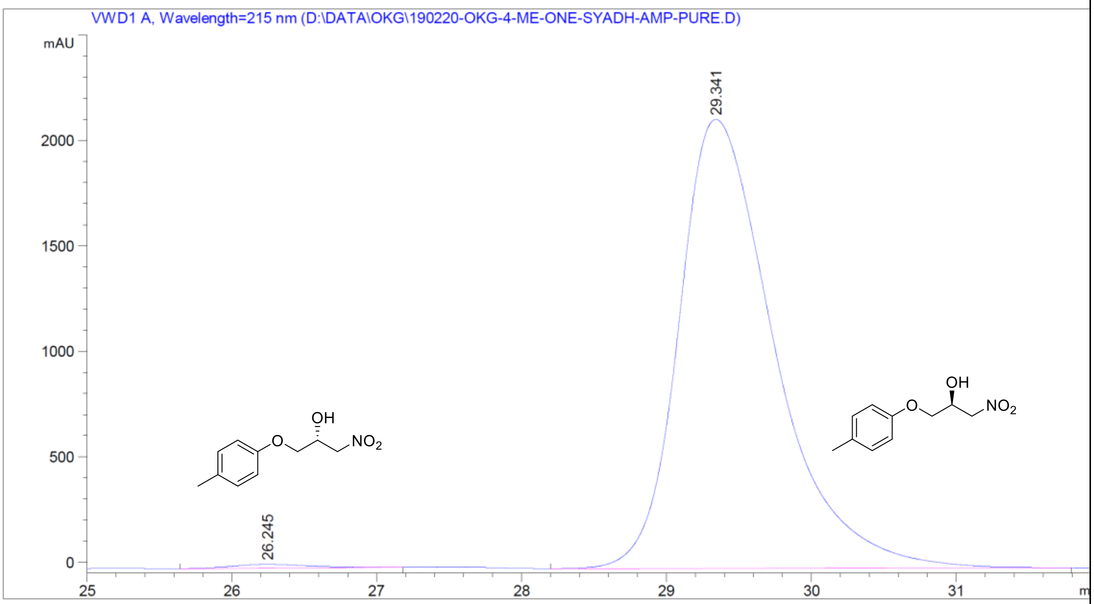
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	27.548	BV	0.7305	1.24288e5	2638.64380	98.3433
2	29.716	VBA	0.6734	2093.71777	45.54100	1.6567

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(*S*)-1-nitro-3-(p-tolyloxy)propan-2-ol (5e)
Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 92:8, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=24.4 min (minor), t_R'=26.3 min (major)



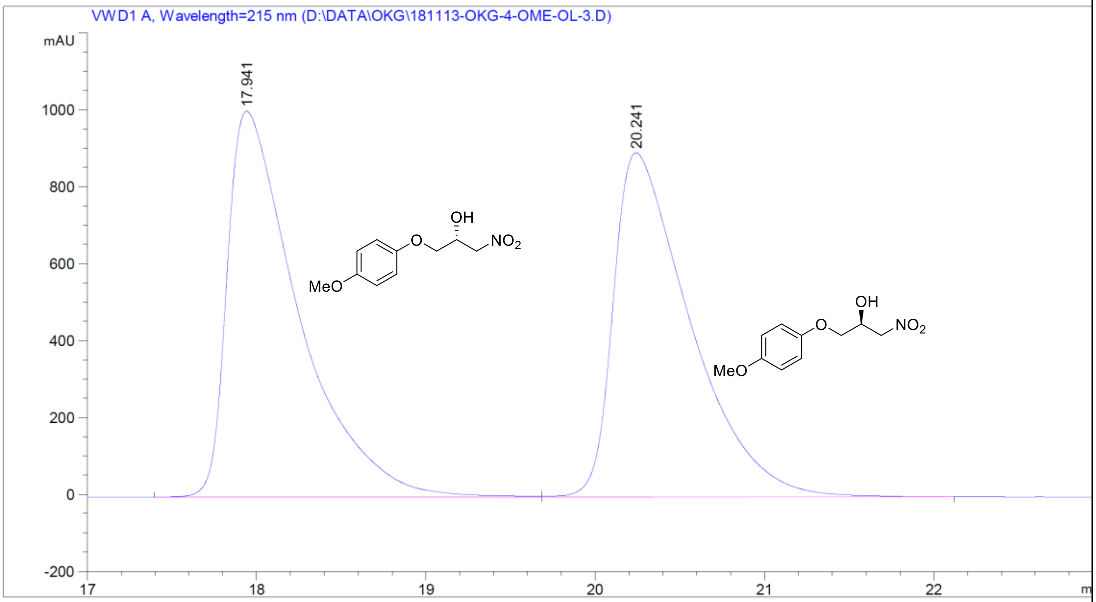
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.417	VV	0.5338	2.29941e4	646.75470	49.7175
2	26.276	VV	0.5614	2.32555e4	621.74335	50.2825



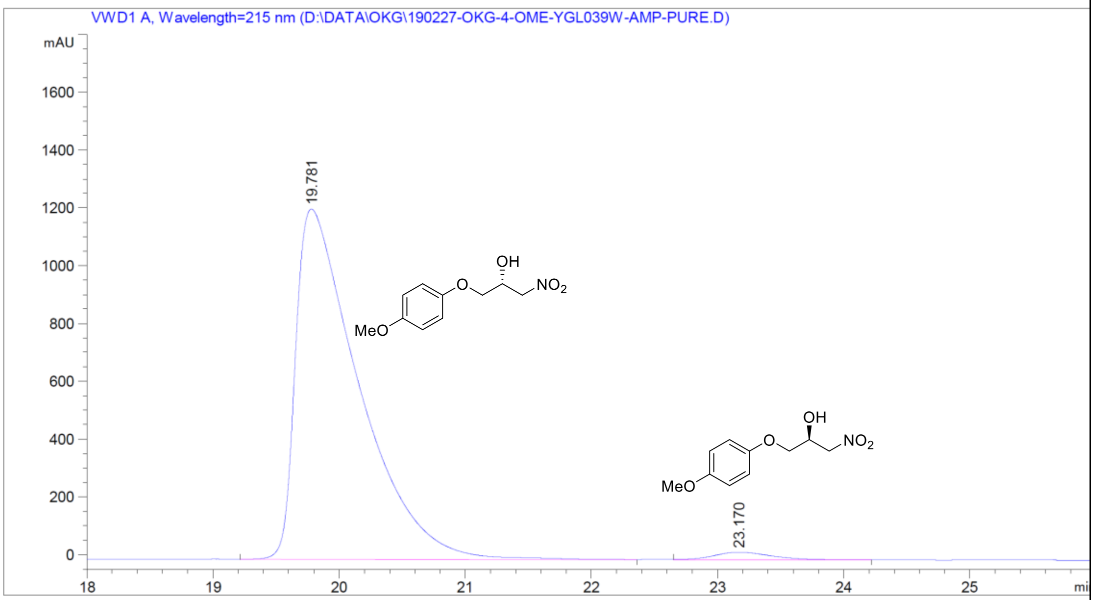
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	26.245	BB	0.4968	690.50452	18.70135	0.7037
2	29.341	BB	0.6720	9.74399e4	2129.02905	99.2963

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(R)-1-(4-methoxyphenoxy)-3-nitropropan-2-ol (5f)
Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=17.9 min (major), t_R'=20.2 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.941	VV	0.4347	2.94267e4	1003.30011	50.9828
2	20.241	VB	0.4704	2.82922e4	894.67535	49.0172

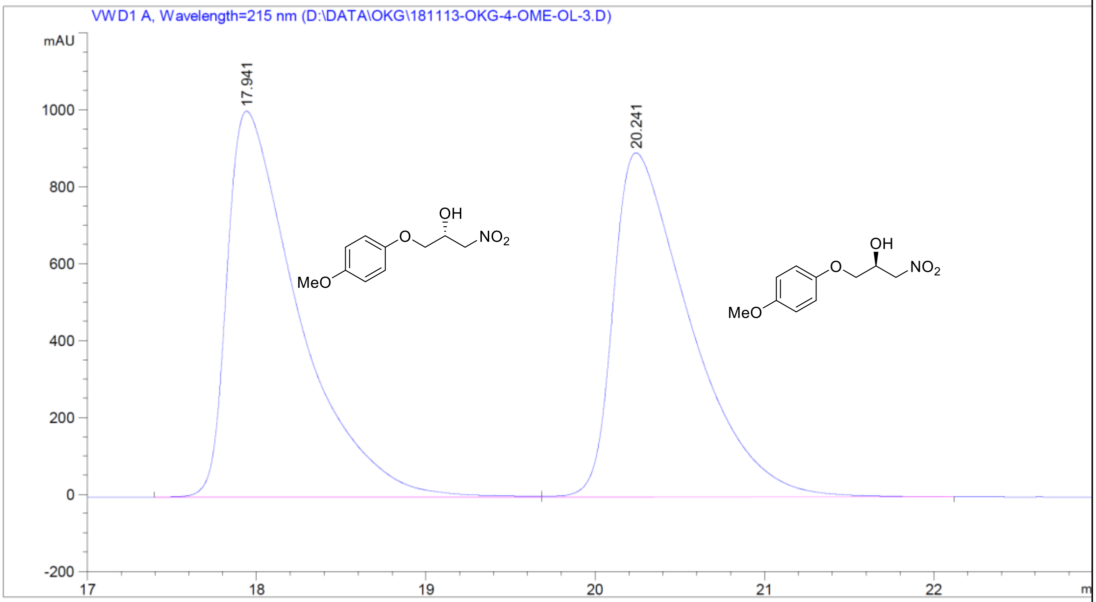


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.781	BB	0.5067	4.22299e4	1211.50317	98.1272
2	23.170	VB	0.4733	805.99695	26.02413	1.8728

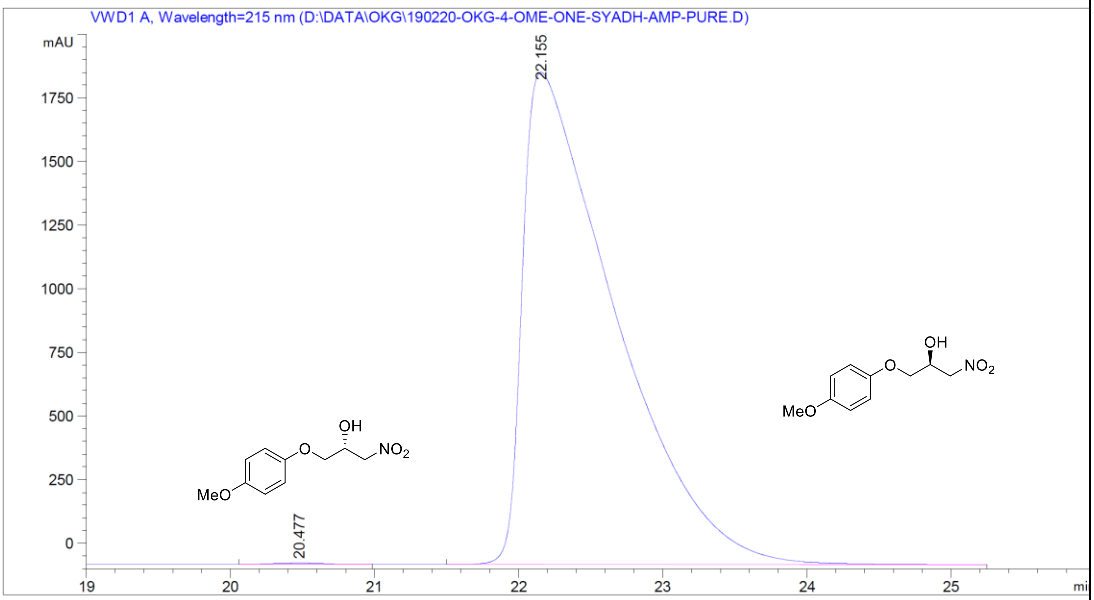
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(S)-1-(4-methoxyphenoxy)-3-nitropropan-2-ol (5f)

Chiracel® IB, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=17.9 min (minor), t_R'=20.2 min (major)



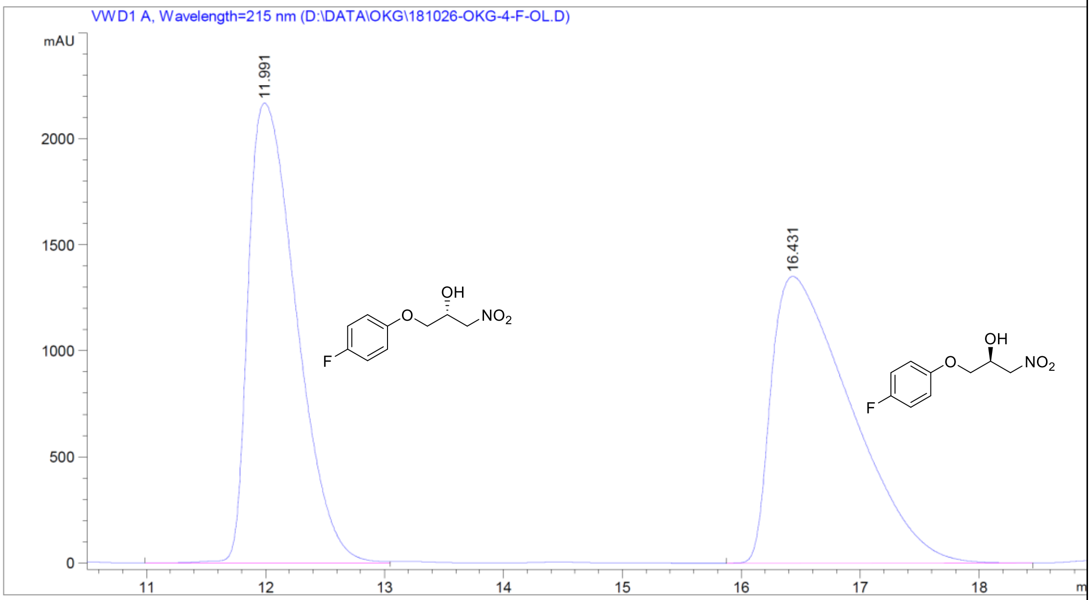
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	17.941	VV	0.4347	2.94267e4	1003.30011	50.9828
2	20.241	VB	0.4704	2.82922e4	894.67535	49.0172



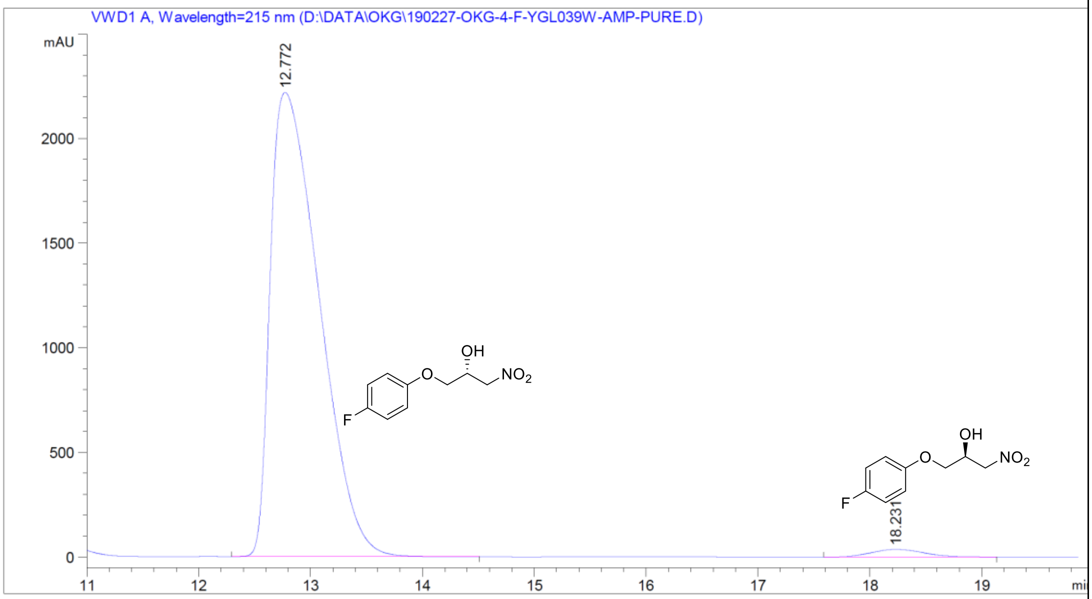
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.477	BB	0.2924	127.55696	5.14161	0.1482
2	22.155	BBA	0.6084	8.59265e4	1933.85559	99.8518

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(*R*)-1-(4-fluorophenoxy)-3-nitropropan-2-ol (5g)
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.0 min (major), t_R'=16.4 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.991	BV	0.4379	6.09688e4	2169.43750	49.1833
2	16.431	BB	0.7194	6.29936e4	1352.54553	50.8167

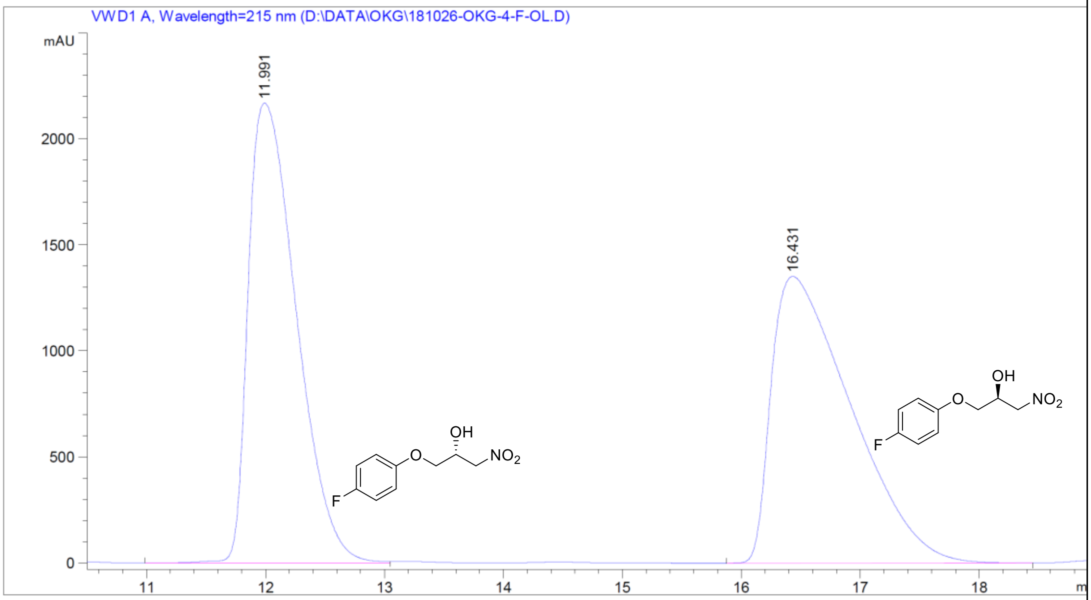


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.772	VV	0.4826	6.72584e4	2219.24390	98.1831
2	18.231	BV	0.5272	1244.65564	37.12327	1.8169

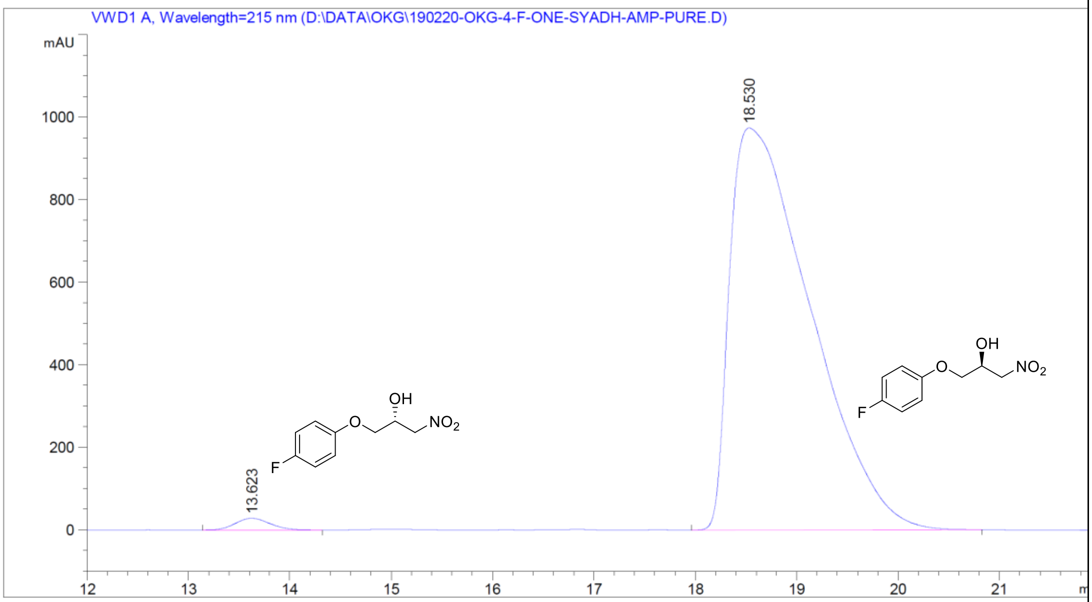
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(S)-1-(4-fluorophenoxy)-3-nitropropan-2-ol (5g)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=12.0 min (minor), t_R'=16.4 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.991	BV	0.4379	6.09688e4	2169.43750	49.1833
2	16.431	BB	0.7194	6.29936e4	1352.54553	50.8167

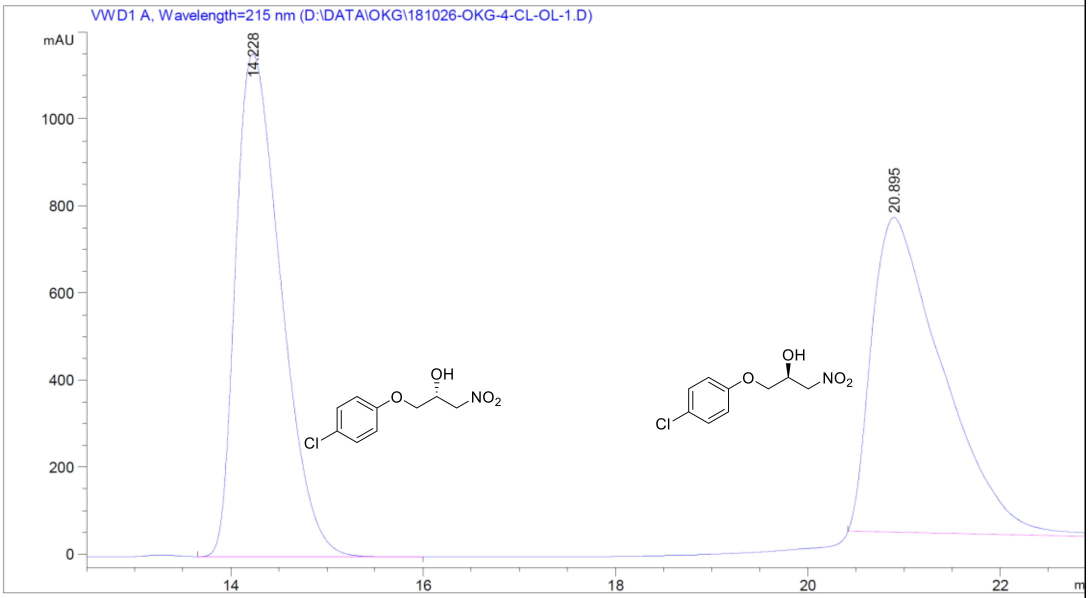


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.623	BB	0.3588	674.90784	28.44190	1.2325
2	18.530	BB	0.8211	5.40828e4	974.31848	98.7675

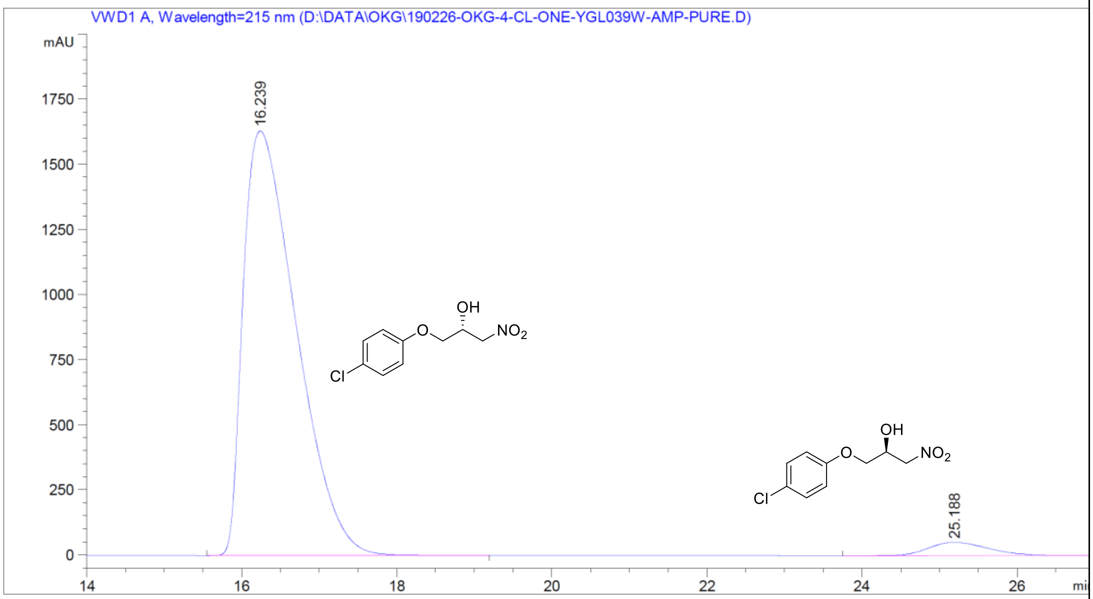
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(*R*)-1-(4-chlorophenoxy)-3-nitropropan-2-ol (5h)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (major), t_R'=20.9 min (minor)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.228	VB	0.5133	3.78776e4	1155.97607	50.2692
2	20.895	BBA	0.7142	3.74719e4	723.56659	49.7308

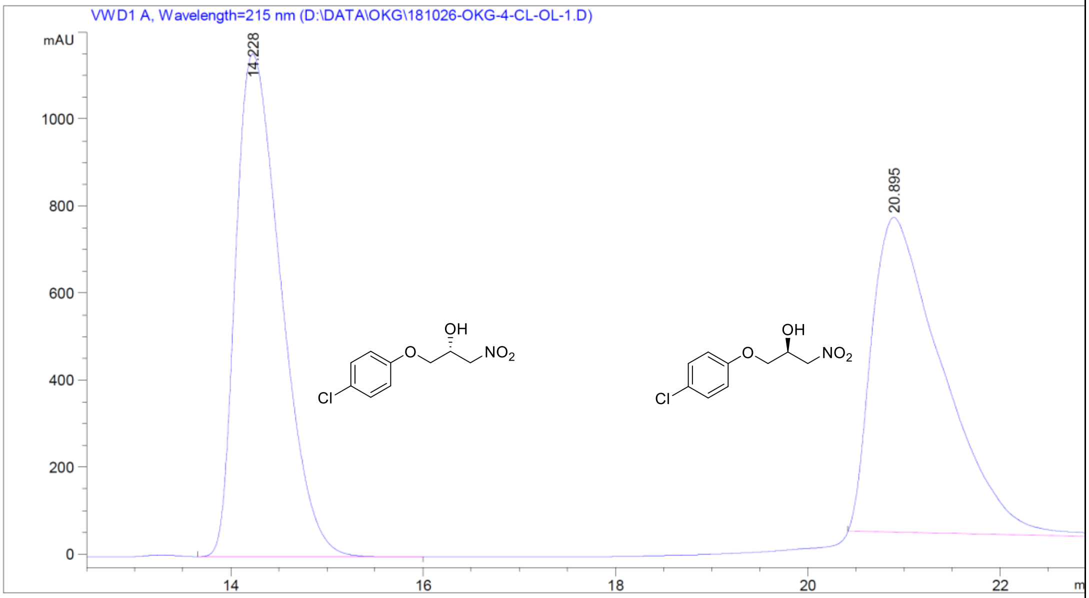


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.239	BB	0.7407	7.72183e4	1629.86804	96.5514
2	25.188	BBA	0.8396	2758.04272	51.19249	3.4486

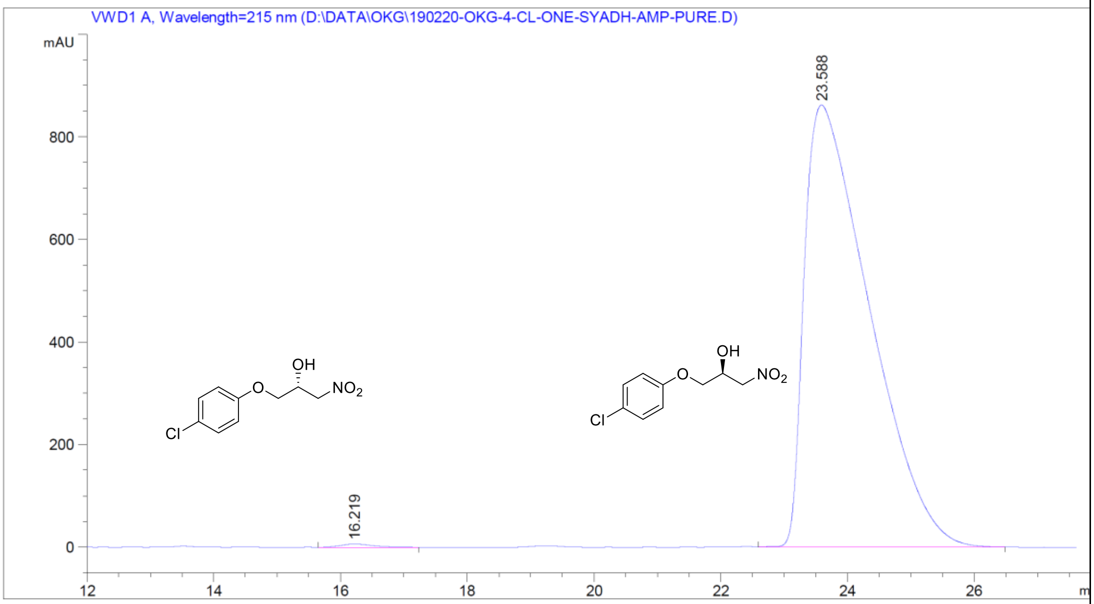
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(S)-1-(4-chlorophenoxy)-3-nitropropan-2-ol (5h)

Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=14.2 min (minor), t_R'=20.9 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	14.228	VB	0.5133	3.78776e4	1155.97607	50.2692
2	20.895	BBA	0.7142	3.74719e4	723.56659	49.7308

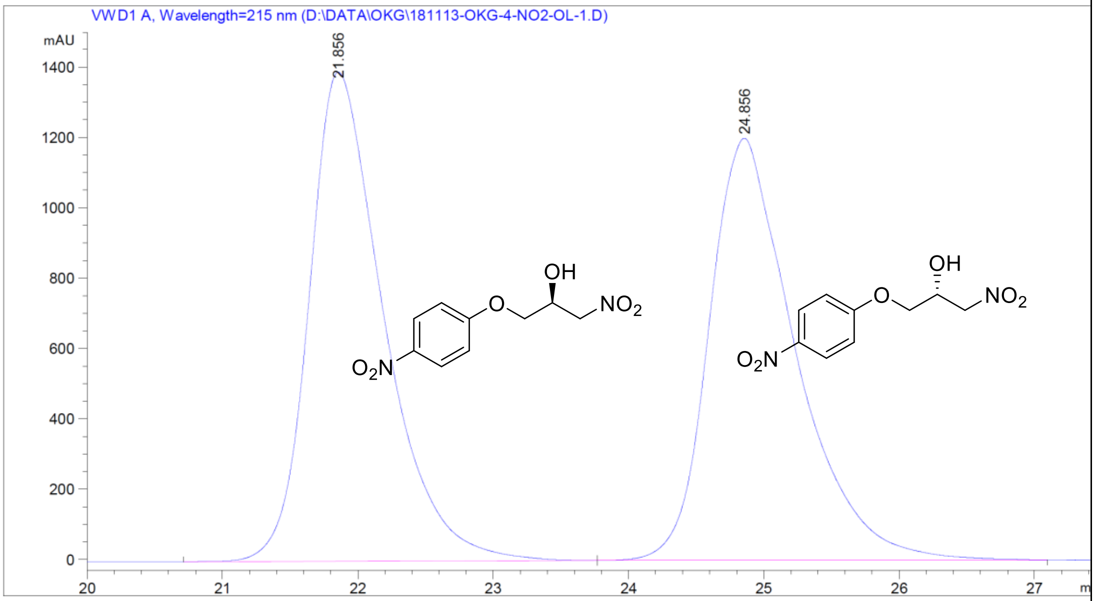


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.219	BB	0.4211	226.41188	6.31712	0.3678
2	23.588	BB	0.9972	6.13271e4	861.77277	99.6322

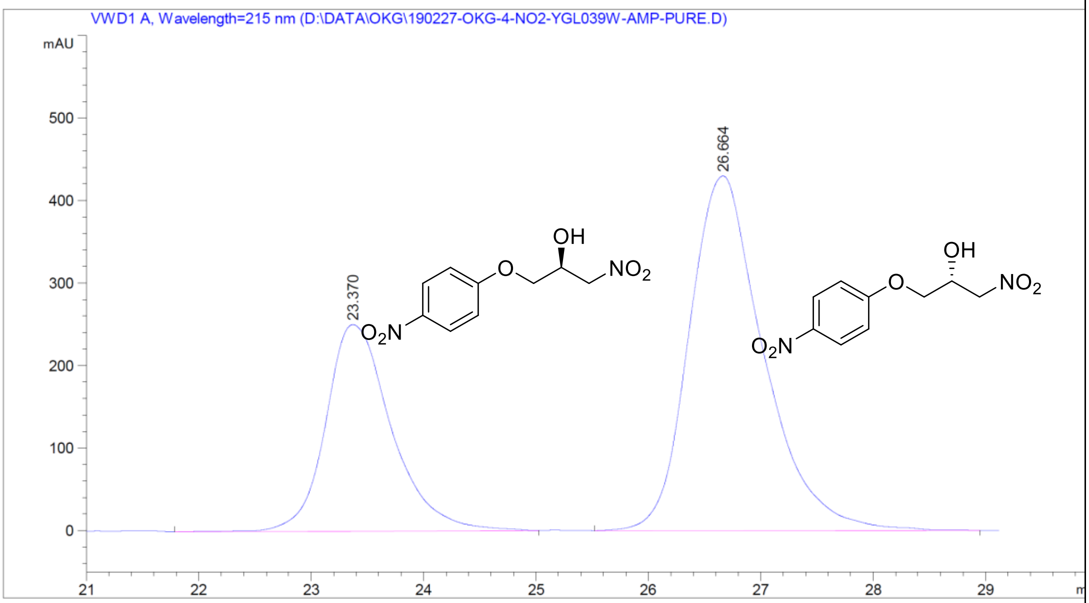
The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

(R)-1-nitro-3-(4-nitrophenoxy)propan-2-ol (5i)

Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.8 min (minor), t_R'=24.8 min (major)



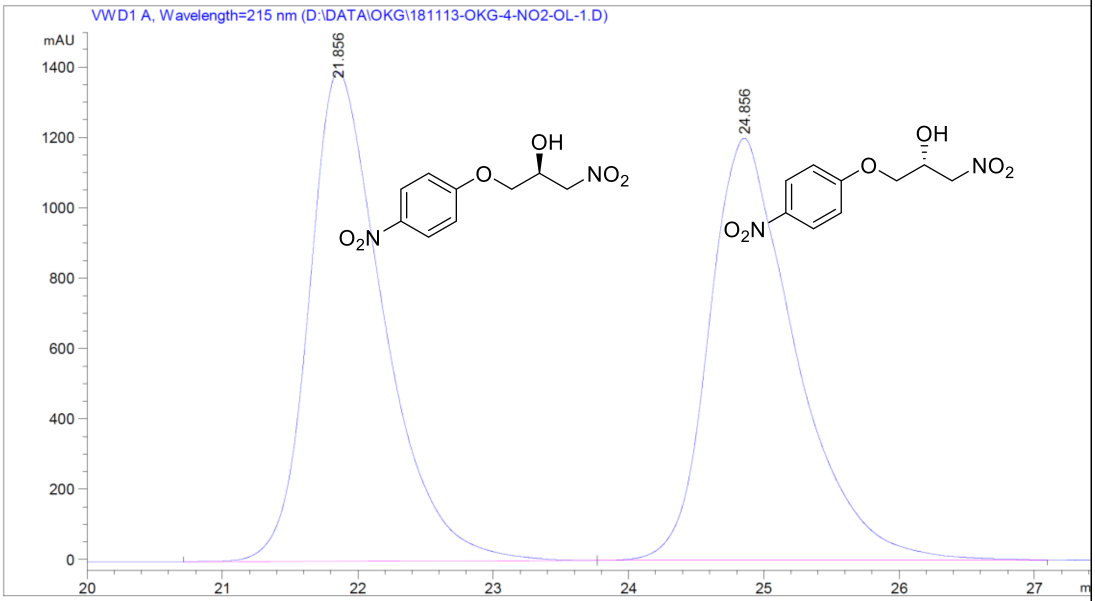
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.856	BB	0.5751	5.33469e4	1392.03748	50.0170
2	24.856	BV	0.6345	5.33107e4	1201.77563	49.9830



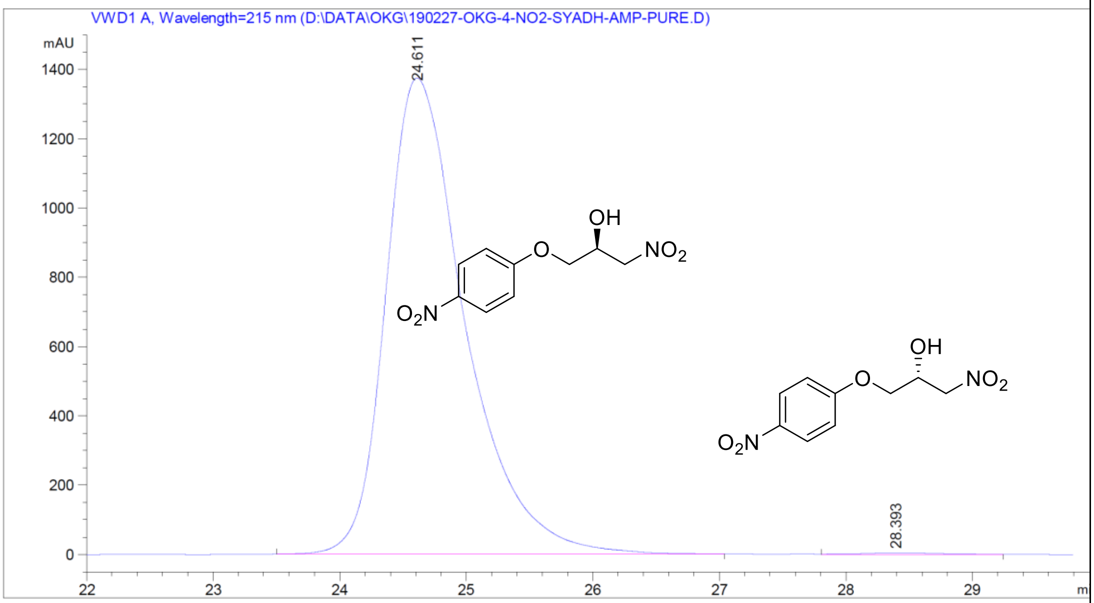
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.370	BV	0.6110	1.01972e4	250.47353	33.9715
2	26.664	BV	0.6920	1.98198e4	429.76294	66.0285

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

(S)-1-nitro-3-(4-nitrophenoxy)propan-2-ol (5i)
Chiracel® IA, 250 × 4.6 mm column, hexane/2-propanol 80:20, 1 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=21.8 min (major), t_R'=24.8 min (minor)



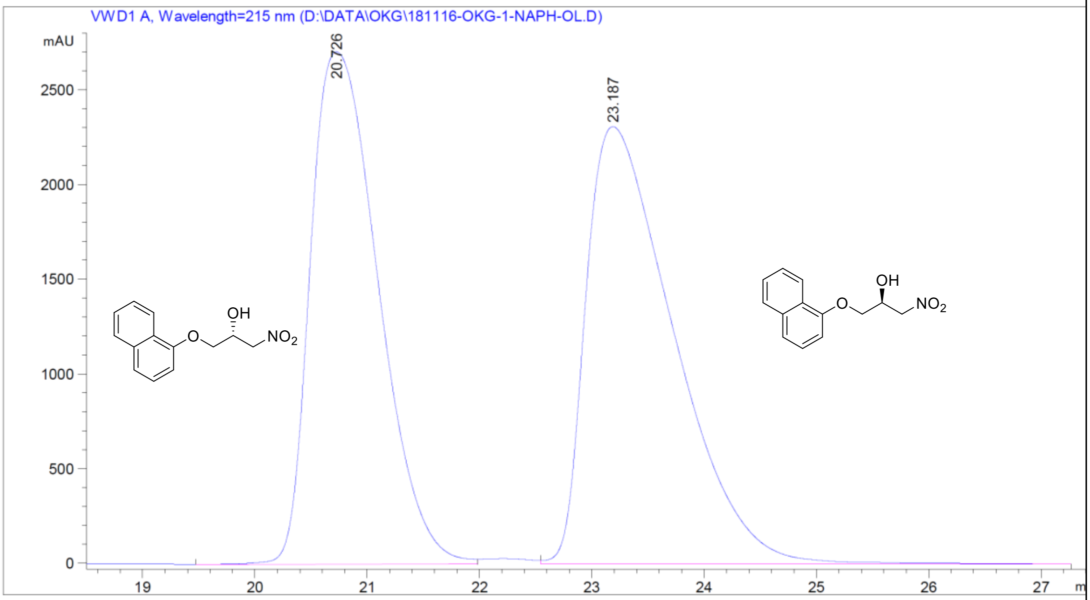
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	21.856	BB	0.5751	5.33469e4	1392.03748	50.0170
2	24.856	BV	0.6345	5.33107e4	1201.77563	49.9830



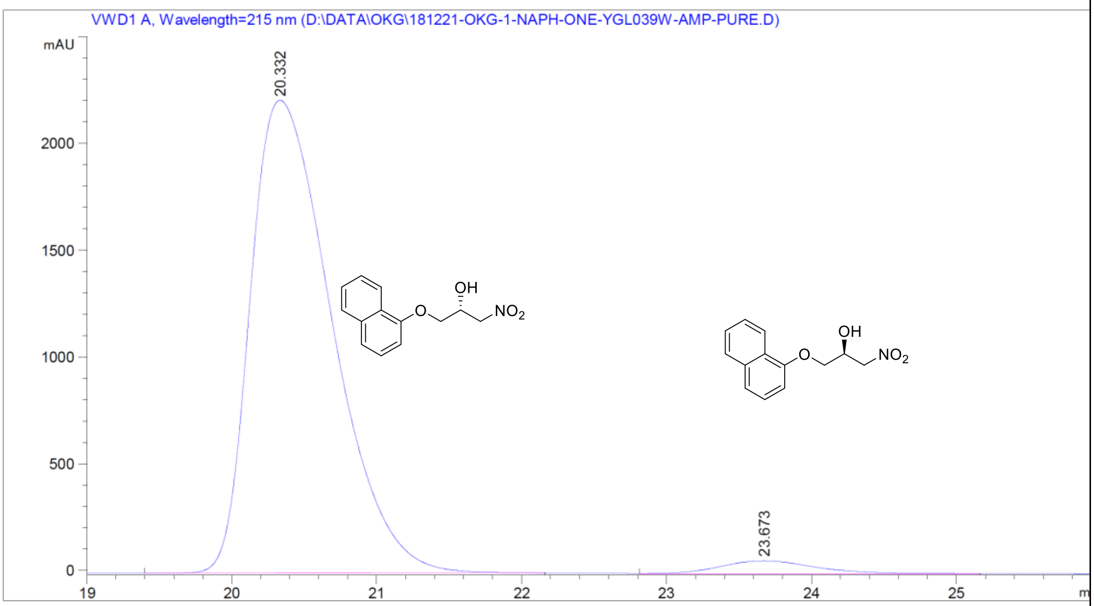
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.611	BB	0.6500	5.96688e4	1374.29236	99.7033
2	28.393	BB	0.5007	177.54893	4.17074	0.2967

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH (CFE) catalyzed biotransformation.

***(R)*-1-(naphthalen-1-yloxy)-3-nitropropan-2-ol (5j)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=20.7 min (major), t_R'=23.2 min (minor)



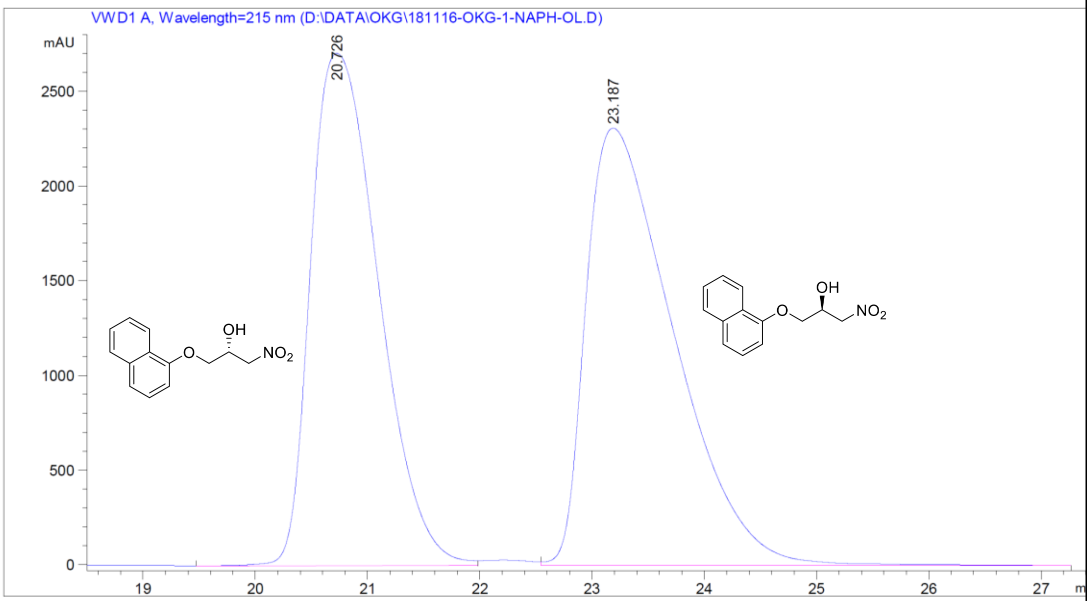
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.726	BV	0.5722	1.13360e5	2706.28735	47.4350
2	23.187	VBA	0.7922	1.25620e5	2310.82715	52.5650



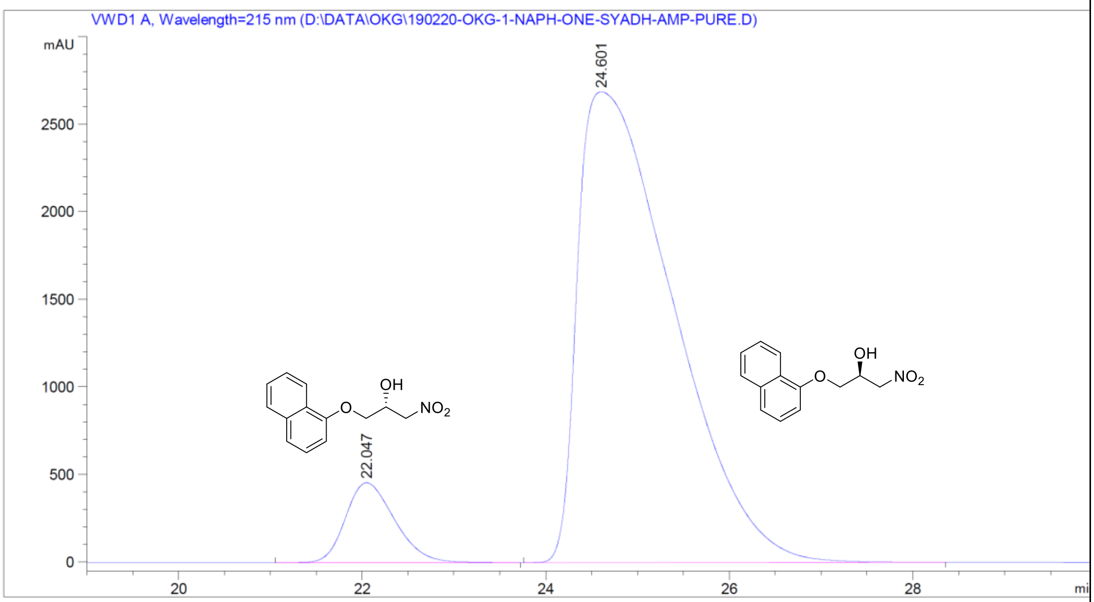
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.332	BB	0.6007	8.62263e4	2212.49756	97.0656
2	23.673	BB	0.6449	2606.67529	58.78125	2.9344

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of YGL039w (CFE) catalyzed biotransformation.

***(S)*-1-(naphthalen-1-yloxy)-3-nitropropan-2-ol (5j)**
Chiracel® AS-H, 250 × 4.6 mm column, hexane/2-propanol 80:20, 0.6 mL/min flow rate, 215 nm UV lamp, 24 °C, t_R=20.7 min (minor), t_R'=23.2 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	20.726	BV	0.5722	1.13360e5	2706.28735	47.4350
2	23.187	VBA	0.7922	1.25620e5	2310.82715	52.5650



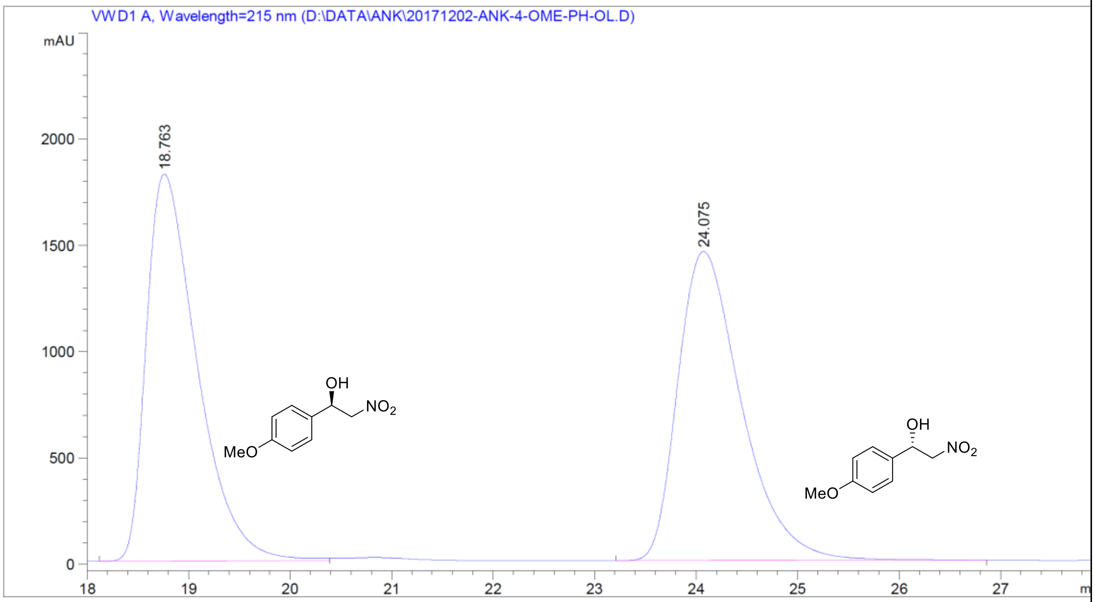
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.047	BB	0.5764	1.69630e4	455.57794	8.0320
2	24.601	BB	0.8482	1.94230e5	2687.51782	91.9680

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of SyADH-catalyzed biotransformation.

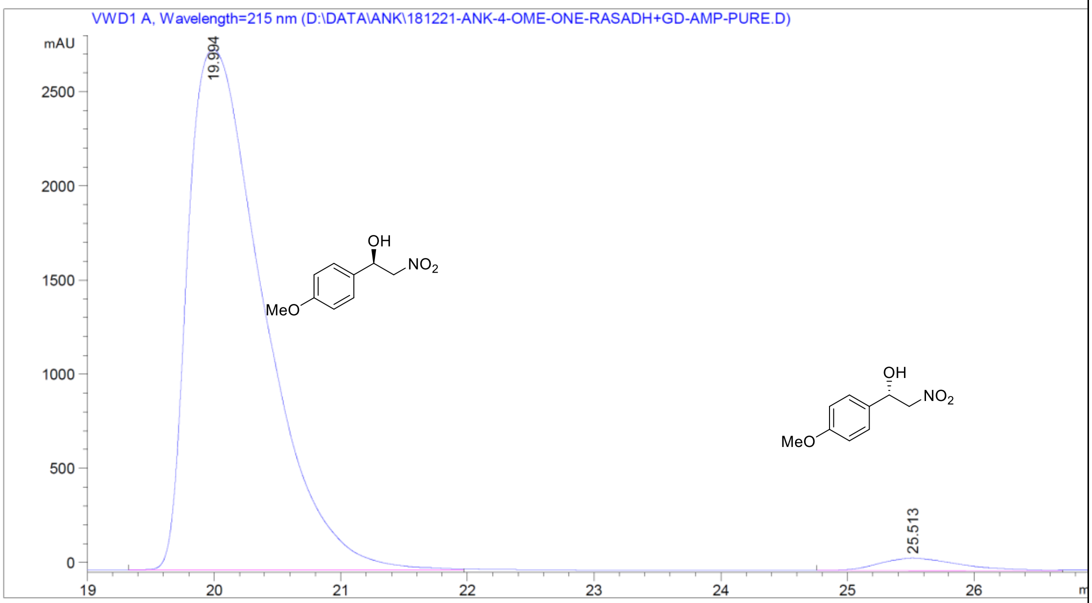
HPLC spectra of **2k** from whole-cell catalysis

***(S)*-1-(4-methoxyphenyl)-2-nitroethan-1-ol (2k)**

Chiracel® OD-H, 250 × 4.6 mm column, hexane/2-propanol 90:10, 1 mL/min flow rate, 215 nm UV lamp, 22 °C, t_R=18.8 min (minor), t_R'=24.1 min (major)



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.763	BV	0.5293	6.30614e4	1819.79443	49.9132
2	24.075	BB	0.6718	6.32808e4	1453.74915	50.0868



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.994	VV	0.5522	1.14416e5	2762.62231	97.5558
2	25.513	VV	0.6321	2866.66040	66.28095	2.4442

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of whole-cell mediated biotransformation.