Supporting Information

Iron-Catalyzed Asymmetric Hydrosilylation of Ketones

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1. General information

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification**.** All manipulations were carried out using standard Schlenk, high-vacuum and glovebox techniques. Tetrahydrofuran (THF) and toluene were distilled from sodium benzophenone ketyl prior to use. The following compounds were prepared according to literature procedures[1]: *i*Pr-(*S*)-*i*Pr-IPO ((*S*)-**2a**), *i*Pr-(*S*)-*t*Bu-IPO ((*S*)-**2b**), *i*Pr-(*S*)-Bn-IPO ((*S*)-**2c**), [*i*Pr-(S)-*i*Pr-IPO]$CoCl_2$ ((*S*)-**3e**).

NMR spectra were recorded on Agilent 400 MHz or Varian Mercury 400 MHz. ^{1}H NMR chemical shifts were referenced to residual protio solvent peaks or tetramethylsilane signal (0 ppm), and ^{13}C NMR chemical shifts were referenced to the solvent resonance. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, quint = quintuplet, sext = sextuplet, m = multiplet or unresolved, coupling constant (s) in Hz, integration). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). Enantiomeric excesses were determined by high-performance liquid chromatograpy (HPLC) with a Dionex or Agilent chromatography [Phenomenex Lux 5u Cellulose-1 (0.46 x 25 cm), Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), Daicel Chiralpak AD-H (0.46 x 25 cm), Daicel Chiralpak OD-H (0.46 x 25 cm), CHIRALPAK IC (0.46 x 25 cm), Lux 5u Amylose-2 (0.46 x 25 cm)] in comparison with authentic racemic materials. Optical rotations were measured on a Rudolph Research Analytical Autopol I Polarimeter. Elemental analyses and high resolution mass spectrometer (HR-MS) were carried out by the Analytical Laboratory of Shanghai Institute of Organic Chemistry (CAS).

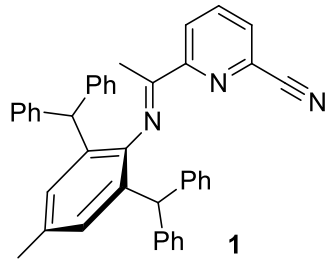
X-ray Data Collection and Structure Determinations. Single crystals of complex (*S*)-**3a** suitable for single crystal X-ray diffraction were grown from the diffusion of diethyl ether into a DMF solution of (*S*)-**3a**, while single crystals of (*S*)-**3d** suitable for single crystal X-ray diffraction were grown by slow evaporation of a THF solution of (*S*)-**3d**. The single crystals of (*S*)-**3a** and (*S*)-**3d** were mounted

under nitrogen atmosphere on a glass fiber, and data collection was performed on a Bruker APEX DUE diffractometer. The SMART program package was used to determine the unit cell parameters. The absorption correction was applied using SADABS. Using Olex2,[1] the structures were solved with the ShelXS[2] structure solution program using Direct Methods and refined with the XL[2] refinement package using Least Squares minimisation. Crystallographic data for (*S*)-**3a** and (*S*)-**3d** are listed in Table S4.1 and Table S4.2 (Supporting Information), respectively.

Crystal Data for (*S*)-**3a** (*M* =1287.52 g/mol): monoclinic, space group $P2_1$ (no. 4), *a* = 15.777(4) Å, *b* = 10.030(3) Å, *c* = 17.685(5) Å, *β* = 100.090(4)°, *V* = 2755.3(12) $Å^3$, *Z* = 2, *T* = 133.15 K, μ(MoKα) = 3.475 mm^{-1}, *Dcalc* = 1.552 g/cm^3, 26394 reflections measured (2.338° ≤ 2Θ ≤ 60.648°), 15709 unique (R_{int} = 0.1132, R_{sigma} = 0.2432) which were used in all calculations. The final R_1 was 0.0715 (I > 2σ(I)) and wR_2 was 0.1556 (all data).

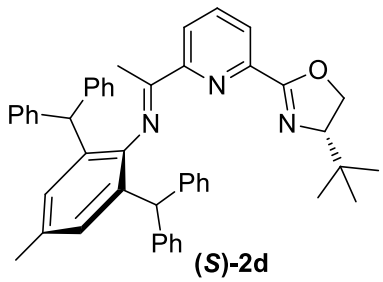
Crystal Data for (*S*)-**3d** (*M* =883.53 g/mol): tetragonal, space group P4 (no. 75), *a* = 33.2315(4) Å, *c* = 18.2906(3) Å, *V* = 20198.9(6) $Å^3$, *Z* = 16, *T* = 130 K, μ(CuKα) = 4.490 mm^{-1}, *Dcalc* = 1.162 g/cm^3, 112205 reflections measured (2.658° ≤ 2Θ ≤ 139.506°), 34361 unique (R_{int} = 0.1082, R_{sigma} = 0.1085) which were used in all calculations. The final R_1 was 0.0714 (I > 2σ(I)) and wR_2 was 0.2029 (all data).

2. **Procedure for Preparation of Fe complexes**



1

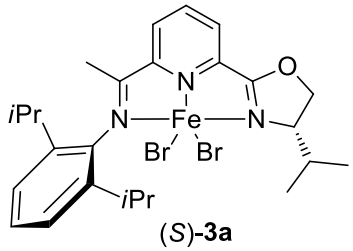
(E)-6-(1-((2,6-dibenzhydryl-4-methylphenyl)imino)ethyl)picolinonitrile (1). To a solution of 6-acetylpicolinonitrile (2.06 g, 14.1 mmol) in toluene (35 mL) was added 2,6-dibenzhydryl-4-methylaniline (6.82 g, 15.5 mmol) and *p*-toluenesulfonic acid monohydrate (135 mg, 0.71 mmol). The reaction was set to reflux and the water was removed using a Dean-Stark apparatus. After 48 h, the reaction mixture was concentrated under reduced pressure and the residue was purified by flash chromatography on silica gel eluting with EtOAc/petroleum ether 30：1 (v/v) to afford the title compound as a yellow solid (6.83 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.0 Hz, 1H), 7.82 (t, J = 7.8 Hz, 1H), 7.71 (d, J = 7.5 Hz, 1H), 7.30 – 7.13 (m, 12H), 7.04 – 6.95 (m, 8H), 6.67 (s, 2H), 5.18 (s, 2H), 2.17 (s, 3H), 1.09 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 157.3, 145.3, 143.4, 142.2, 137.1, 132.5, 132.1, 131.9, 129.7, 129.4, 129.3, 128.7, 128.4, 128.1, 126.4, 126.1, 124.5, 117.3, 52.2, 21.4, 16.6. HRMS-ESI (*m/z*): Calcd for $C_{41}H_{34}N_3$ $[M+H]^+$, 568.2747; found: 568.2750.



(*S*)-2d

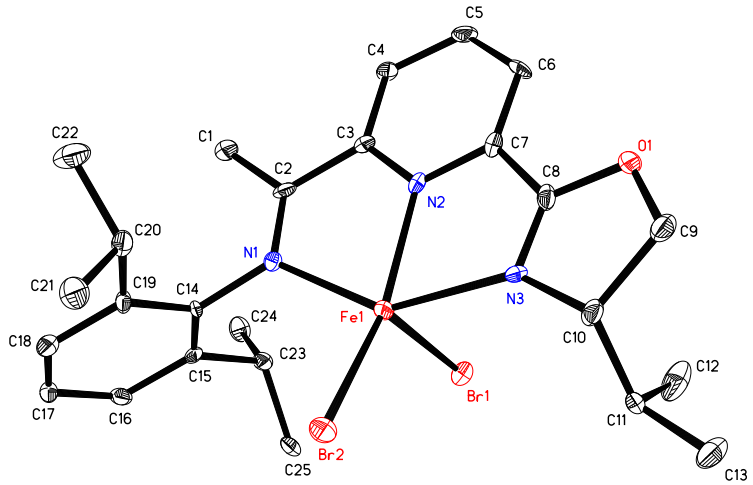
Preparation of dibenzhydryl-(*S*)- *t*Bu -IPO ((*S*)-2d). To an oven-dried 100 mL two-necked flask fitted with a reflux condenser was charged with (E)-6-(1-((2,6-dibenzhydryl-4-methylphenyl)imino)ethyl)picolinonitrile (**1**) (1.0 g, 1.76 mmol) and zinc triflate (32 mg, 0.09 mmol). The system was purged with argon and anhyd toluene (15 mL) was added. The solution was stirred during 5 min and a

solution of L-tert-Leucinol (310 mg, 2.64 mmol) in anhydrous toluene (20 mL) was added. The reaction was set to reflux for 48 h. The system was allowed to cool, and the reaction was diluted with 20 mL of EtOAc, then washed with saturated aq. $NaHCO_3$ (3×15 mL) and brine (20 mL), dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The residue so obtained was purified by flash column chromatography with EtOAc/petroleum ether (1:20 → 1:15) to give the title compound as a yellow solid **((*S*)-2a)** (525 mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.6 Hz, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.26 – 7.12 (m, 12H), 7.03 (d, *J* = 6.9 Hz, 8H), 6.70 (s, 2H), 5.27 (s, 2H), 4.47 (t, *J* = 9.5 Hz, 1H), 4.34 (t, *J* = 8.4 Hz, 1H), 4.18 – 4.11 (m, 1H), 2.18 (s, 3H), 1.42 (s, 3H), 1.01 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 162.8, 155.9, 145.9, 145.8, 143.5, 143.4, 142.7, 142.5, 136.5, 132.2, 132.0, 131.6, 129.8, 129.7, 129.4, 128.6, 128.3, 128.2, 127.9, 126.1, 125.9, 125.2, 123.0, 76.2, 69.4, 52.0, 51.9, 34.0, 25.9, 21.3, 17.0. Anal. Calcd. ($C_{47}H_{45}N_3O$): C, 84.52; H, 6.79; N, 6.29. Found: C, 84.60; H, 6.99; N, 6.15. Optical Rotation: $[\alpha]_D^{27}$ = - 40.87 (c = 0.51, CH_2Cl_2).



(*S*)-**3a**

Preparation of [(*S*)-*i*Pr-IPO]FeBr$_2$ ((*S*)-3a). To a yellow solution of (*S*)-**2a** (392 mg, 1.0 mmol) in approximately 30 mL of THF, 216 mg (1.0 mmol) of $FeBr_2$ were added. The resulting mixture was stirred at room temperature for 10 hours. The solvent was removed under vacuum and the resulting solid was washed with diethyl ether, collected by filtration and dried under vacuum to yield 580 mg (95%) of a dark blue solid identified as (*S*)-**3a**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 70.14, 60.37, 48.88, 18.28, 14.17, 14.04, 9.59, 5.31, 3.77, 3.75, 3.73, 3.38, 1.86, 1.64, 1.25, 0.33, 0.07, -1.51, -6.01, -6.90, -8.10, -11.76, -27.20. Anal. Calcd. ($C_{25}H_{33}Br_2FeN_3O$): C, 49.45; H, 5.48; N, 6.92. Found: C, 49.72; H, 5.63; N, 6.57.

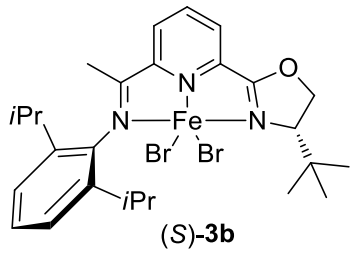


Selected Bond Length for Complex (*S*)-3a

Selected Bond Length	Distance(Å)
Fe1–N2	2.111(11)
Fe1–N3	2.240(10)
Fe1–N1	2.252(9)
Fe1–Br2	2.429(2)
Fe1–Br1	2.544(2)

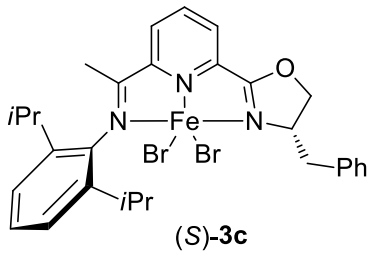
Selected Bond Angles for Complex (*S*)-3a

Selected Bond Angles	(deg)
N(2)-Fe(1)-N(3)	74.0(4)
N(2)-Fe(1)-N(1)	73.2(4)
N(3)-Fe(1)-N(1)	146.2(4)
N(2)-Fe(1)-Br(2)	156.4(3)
N(3)-Fe(1)-Br(2)	99.3(3)
N(1)-Fe(1)-Br(2)	107.5(3)
N(2)-Fe(1)-Br(1)	90.8(3)
N(3)-Fe(1)-Br(1)	92.6(3)
N(1)-Fe(1)-Br(1)	95.6(3)
Br(2)-Fe(1)-Br(1)	112.32(9)



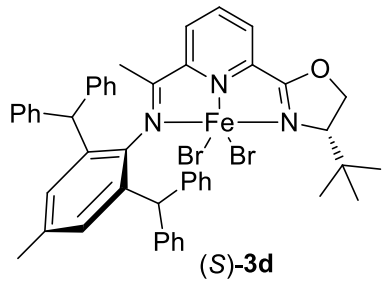
(*S*)-**3b**

Preparation of [(*S*)-*t*Bu-IPO]FeBr$_2$ ((*S*)-3b). This compound was prepared in a similar manner to (*S*)-**3a** with 150 mg (0.37 mmol) of *(S)*-**2b** and 80 mg of $FeBr_2$ (0.37 mmol) and approximately 15 mL of THF. This procedure yielded 206 mg (90%) of a dark blue identified as (*S*)-**3b**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 73.12, 62.04, 36.57, 20.60, 15.40, 14.80, 8.21, 5.31, 3.91, 1.93, 1.33, 1.25, 0.06, -6.15, -10.32, -11.41, -12.17, -19.32. Anal. Calcd. ($C_{26}H_{35}Br_2FeN_3O$): C, 50.27; H, 5.68; N, 6.67. Found: C, 50.35; H, 5.76; N, 6.70.



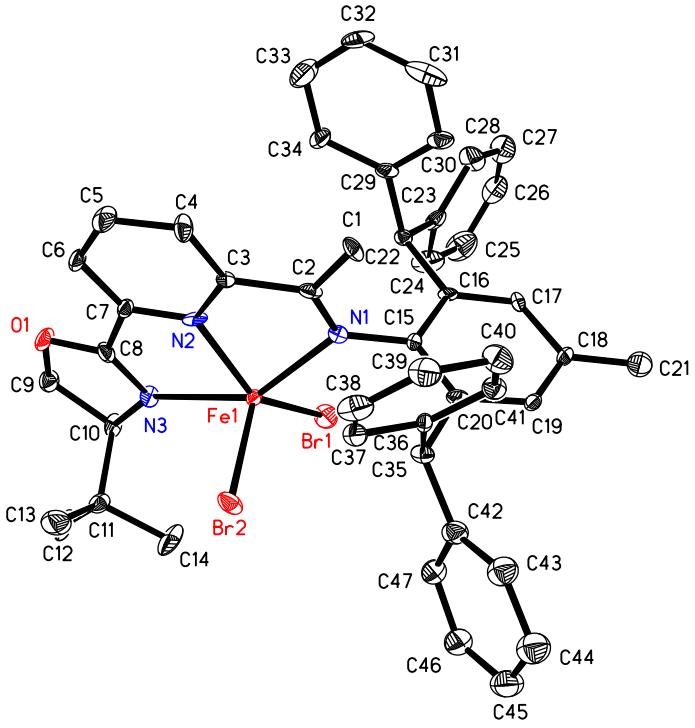
(*S*)-**3c**

Preparation of [(*S*)-Bn-IPO]FeBr$_2$ ((*S*)-3c). This compound was prepared in a similar manner to (*S*)-**3a** with 250 mg (0.57 mmol) of *(S)*-**2c** and 123 mg of $FeBr_2$(0.57 mmol) and approximately 20 mL of THF. This procedure yielded 339 mg (91 %) of a dark blue solid identified as (*S*)-**3c**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 69.92, 59.50, 55.90, 16.91, 15.40, 10.34, 10.15, 5.20, 4.89, 3.07, 1.56, 1.25, 1.15, 0.87, 0.07, -1.20, -6.47, -7.72, -27.32. Anal. Calcd. ($C_{29}H_{33}Br_2FeN_3O$): C, 53.16; H, 5.08; N, 6.41. Found: C, 52.87; H, 5.20; N, 6.38.



(*S*)-**3d**

Preparation of [dibenzhydryl-(*S*)-*t*Bu-IPO]FeBr$_2$ ((*S*)-3d). This compound was prepared in a similar manner to (*S*)-**3a** with 250 mg (0.37 mmol) of *(S)*-**2d** and 80 mg of $FeBr_2$(0.37 mmol) and approximately 20 mL of THF. This procedure yielded 278 mg (84 %) of a dark blue solid identified as (*S*)-**3c**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 69.68, 65.02, 28.14, 25.46, 21.73, 19.01, 16.97, 16.72, 12.11, 11.02, 9.78, 8.80, 8.70, 8.49, 8.40, 5.62, 4.52, 3.59, 3.07, 2.88, 2.50, 2.10, 1.23, 1.02, -1.69, -8.06, -11.80, -16.46. Anal. Calcd. ($C_{29}H_{33}Br_2FeN_3O$): C, 63.89; H, 5.13; N, 4.76. Found: C, 63.41; H, 5.20; N, 4.54.



Selected Bond Length for Complex (*S*)-3d

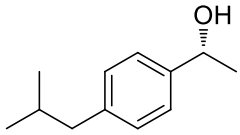
Selected Bond Length	Distance(Å)
Fe1–N3	2.205(9)
Fe1–N2	2.067(9)
Fe1–N1	2.294(9)
Fe1–Br2	2.471(2)
Fe1–Br1	2.407(2)

Selected Bond Angles for Complex (*S*)-3d

Selected Bond Angles	(deg)
N(2)-Fe(1)-N(3)	75.4(4)

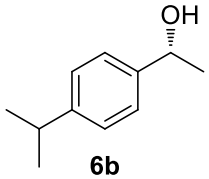
N(2)-Fe(1)-N(1)	73.6(4)
N(3)-Fe(1)-N(1)	146.6(3)
N(2)-Fe(1)-Br(2)	97.4(3)
N(3)-Fe(1)-Br(2)	97.1(3)
N(1)-Fe(1)-Br(2)	98.7(2)
N(2)-Fe(1)-Br(1)	143.9(3)
N(3)-Fe(1)-Br(1)	99.9(2)
N(1)-Fe(1)-Br(1)	98.0(2)
Br(2)-Fe(1)-Br(1)	118.68(8)

3. **Procedure for Hydrosilylation of Ketones**



6a

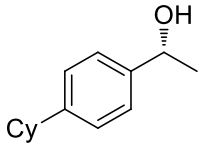
Representative procedure for hydrosilylation with iron complex. **(*R*)-1-(4-isobutylphenyl)ethanol (6a).** In a Nitrogen filled glovebox, to a solution of (*S*)-**3d** (0.005mmol, 4.4 mg) in 2 mL of THF, a solution (1.0 M in THF) of $NaBHEt_3$ (10 μL, 0.01 mmol) was slowly added at 25 ºC. After stirring for 1 min, Ph_2SiH_2 (92 mg, 0.5 mmol, 1 equiv), 1-(4-isobutylphenyl)ethanone **5a** (88.0 mg, 0.5 mmol) were sequentially added. The reaction mixture stirred for 3 h at 25 ºC and then was quenched by exposing the solution to air. Then MeOH (1.5 mL) and 10 % NaOH (2 mL) were added with vigorously stirring for 10 h. The resulting solution was extracted with EtOAc and washed with brine (15 mL), dried over anhydrous Na_2SO_4. After filtration and evaporation of the solvent, the residue was purified by flash column chromatography with EtOAc/petroleum ether (1:20) to give the title compound **6a** (86 mg, 97 %) as colorless oil. 93% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), CH_3CN/H_2O = 70/30, v = 0.7 mL·min^{-1}, λ = 230 nm, t (minor) = 20.605 min, t (major) = 22.408 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.86 (q, *J* = 6.4 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 2.04 (br s, 1H), 1.93 – 1.78 (m, 1H), 1.49 (d, *J* = 6.5 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 140.9, 129.2, 125.2, 70.2, 45.1, 30.2, 25.0, 22.3. Rotation: $[\alpha]_D^{28}$ = +31.56 (c = 0.33, CH_2Cl_2). These spectroscopic data correspond to reported data[4].



6b

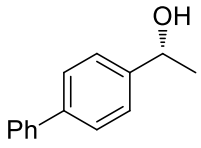
(*R*)-1-(4-isopropylphenyl)ethanol (6b). Colorless oil (65 mg, 79%). 77% ee

[Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 98/2, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 12.68 min, t (major) = 13.19 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32– 7.30 (m, 2H), 7.25 – 7.20 (m, 2H), 4.87 (q, *J* = 6.4 Hz, 1H), 2.99 – 2.84 (m, 1H), 1.98 (br s, 1H), 1.50 (d, *J* = 6.5 Hz, 3H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 143.2, 126.5, 125.4, 70.2, 33.8, 24.9, 24.0. Optical Rotation: $[\alpha]_D^{28}$ = +28.55 (c = 0.50, CH_2Cl_2). These spectroscopic data correspond to reported data[5].



6c

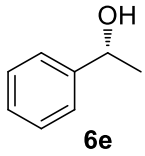
(*R*)-1-(4-cyclohexylphenyl)ethanol (6c). White solid (98 mg, 96%). 86% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 90/10, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 6.96 min, t (major) = 7.25 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.87 (q, *J* = 6.4 Hz, 1H), 2.52 – 2.47 (m, 1H), 1.88 – 1.85 (m, 4H), 1.76 (d, *J* = 12.2 Hz, 1H), 1.66 (br s, 1H), 1.50 (d, *J* = 6.4 Hz, 3H), 1.44 – 1.35 (m, 4H), 1.31 – 1.22 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.4, 143.2, 126.9, 125.4, 70.3, 44.2, 34.5, 26.9, 26.2, 24.9. Optical Rotation: $[\alpha]_D^{28}$ = +26.68 (c = 0.45, CH_2Cl_2). These spectroscopic data correspond to reported data[6].



6d

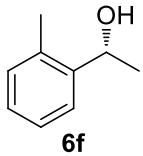
(*R*)-1-([1,1'-biphenyl]-4-yl)ethanol (6d). White solid (94 mg, 95%). 86% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 13.72 min, t (major) = 14.89 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 –7.58 (m, 4H), 7.46 –7.42 (m, 4H), 7.37 –7.33 (m, 1H), 4.96 (q, *J* = 6.4, 1H), 1.88 (br s, 1H), 1.55 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.8, 140.8, 140.4, 128.8, 127.3, 127.1, 125.8, 70.2, 25.2. Optical Rotation: $[\alpha]_D^{28}$ =

+29.81 (c = 0.37, CH_2Cl_2). These spectroscopic data correspond to reported data[7].



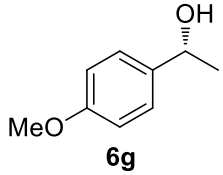
6e

(*R*)-1-phenylethanol (6e). Colorless oil (60 mg, 98%). 83% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 10.21 min, t (major) = 11.11 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.23 (m, 5H), 4.86 (q, *J* = 6.4 Hz, 1H), 2.14 (br s, 1H), 1.48 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.7, 128.4, 127.4, 125.3, 70.37, 25.1. Optical Rotation: $[\alpha]_D^{28}$ = +30.15 (c = 0.36, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



6f

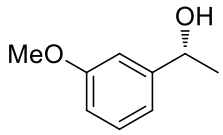
(*R*)-1-(o-tolyl)ethanol (6f). Colorless oil (55 mg, 81%). 76% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 9.98 min, t (major) = 10.57 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.14 (m, 3H), 5.13 (q, *J* = 6.3 Hz, 1H), 2.36 (s, 3H), 1.99 (s, 1H), 1.48 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 134.2, 130.3, 127.1, 126.3, 124.4, 66.7, 23.9, 18.9. Optical Rotation: $[\alpha]_D^{29}$ = +44.06 (c = 0.54, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



6g

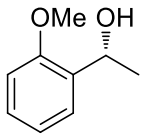
(*R*)-1-(4-methoxyphenyl)ethanol (6g). Colorless oil (63 mg, 83%). 91% ee [Daicel Chiralpak OD-H (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 15.51 min, t (major) = 17.25 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.32 – 7.27 (m, 2H), 6.91 – 6.85 (m, 2H), 4.84 (q, *J* = 6.4 Hz, 1H), 3.80 (s, 3H), 1.87 (br s, 1H), 1.47 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 138.0, 126.6, 113.8, 70.0, 55.3, 25.0. Optical Rotation: $[\alpha]_D^{29}$ = +33.80 (c = 0.60, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



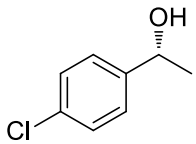
6h

(*R*)-1-(3-methoxyphenyl)ethanol (6h). Colorless oil (75 mg, 98%). 64% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 90/10, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 9.75 min, t (major) = 10.21 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 1H), 6.97 – 6.91 (m, 2H), 6.81 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 4.86 (q, *J* = 6.4 Hz, 1H), 3.81 (s, 3H), 2.04 (br s, 1H), 1.48 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 147.6, 129.5, 117.7, 112.9, 110.9, 70.3, 55.2, 25.1. Optical Rotation: $[\alpha]_D^{29}$ = +20.79 (c = 0.49, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



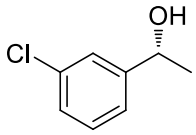
6i

(*R*)-1-(2-methoxyphenyl)ethanol (6i). Colorless oil (54 mg, 71%). 19% ee [Daicel Chiralpak OD-H (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 13.55 min, t (major) = 14.57 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 7.2 Hz, 1H), 7.24 (t, *J* = 7.8 Hz, 1H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 5.08 (q, *J* = 6.5 Hz, 1H), 3.85 (s, 3H), 2.73 (br s, 1H), 1.49 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $cdcl_3$) δ 156.5, 133.3, 128.3, 126.1, 120.7, 110.3, 66.5, 55.2, 22.8. Optical Rotation: $[\alpha]_D^{28}$ = +2.22 (c = 0.62, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



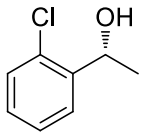
6j

(*R*)-1-(4-chlorophenyl)ethanol (6j). Colorless oil (75 mg, 96%). 61% ee [Daicel Chiralpak OD-H (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 10.69 min, t (major) = 11.76 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.23 (m, 4H), 4.84 (q, *J* = 6.4 Hz, 1H), 2.06 (br s, 1H), 1.44 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.2, 133.0, 128.6, 126.8, 69.7, 25.2. Optical Rotation: $[\alpha]_D^{29}$ = +21.94 (c = 0.58, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



6k

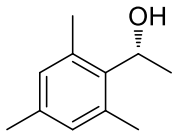
(*R*)-1-(3-chlorophenyl)ethanol (6k). Colorless oil (75 mg, 96%). 63% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 10.08 min, t (major) = 10.81 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.36 (m, 1H), 7.29 – 7.26 (m, 1H), 7.26 – 7.21 (m, 2H), 4.86 (q, *J* = 6.5 Hz, 1H), 2.08 (br s, 1H), 1.47 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 134.3, 129.8, 127.5, 125.6, 123.5, 69.8, 25.2. Optical Rotation: $[\alpha]_D^{29}$ = +17.65 (c = 0.58, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



6l

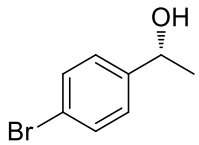
(*R*)-1-(2-chlorophenyl)ethanol (6l). Colorless oil (74 mg, 95%). 75% ee [Lux 5u Amylose-2 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 98.5/1.5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 13.91 min, t (major) = 14.83 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.6 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.21 – 7.15 (m, 1H), 5.28 (q, *J* = 6.4 Hz,

1H), 2.05 (br s, 1H), 1.47 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 131.6, 129.4, 128.4, 127.2, 126.4, 67.0, 23.5. Optical Rotation: $[\alpha]_D^{29}$ = +37.70 (c = 0.47, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



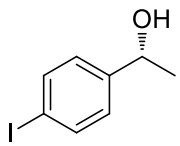
6m

(*R*)-1-mesitylethanol (6m). White solid (80 mg, 97%). 93% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 90/10, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 5.97 min, t (major) = 6.69 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (s, 2H), 5.36 (q, *J* = 6.7 Hz, 1H), 2.43 (s, 6H), 2.27 (s, 3H), 1.82 (br s, 1H), 1.53 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6, 136.4, 135.6, 130.1, 67.4, 21.5, 20.7, 20.5. Optical Rotation: $[\alpha]_D^{28}$ = +46.93 (c = 0.32, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



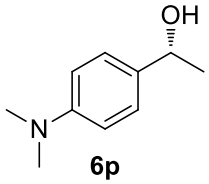
6n

(*R*)-1-(4-bromophenyl)ethanol (6n). Colorless oil (97 mg, 96%). 76% ee [Daicel Chiralpak AD-H (0.46 x 25 cm), $scCO_2$ /*i*-propanol = 90/10, v = 1.3 mL·min^{-1}, λ = 214 nm, t (minor) = 9.481 min, t (major) = 10.165 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 4.76 (q, *J* = 6.5 Hz, 1H), 2.84 (s, 1H), 1.40 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 131.4, 127.1, 120.9, 69.5, 25.1. Optical Rotation: $[\alpha]_D^{28}$ = +23.79 (c = 0.55, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



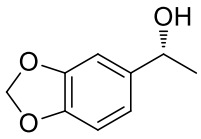
6o

(*R*)-1-(4-iodophenyl)ethanol (6o). White solid (120 mg, 97%). 88% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 80/20, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 5.98 min, t (major) = 6.40 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.11 – 7.06 (m, 2H), 4.80 (q, J = 6.4 Hz, 1H), 2.19 (br s, 1H), 1.44 (d, *J* = 6.4, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 137.4, 127.4, 92.7, 69.7, 25.2. Optical Rotation: $[\alpha]_D^{28}$ = +24.96 (c = 0.54, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



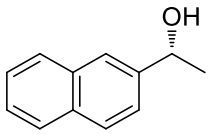
6p

(R)-1-(4-(dimethylamino)phenyl)ethanol (6p). Colorless oil (82 mg, 98%). 87% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 80/20, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 8.56 min, t (major) = 10.79 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (m, 2H), 6.77 – 6.70 (m, 2H), 4.80 (q, *J* = 6.4 Hz, 1H), 2.95 (s, 6H), 2.11 (br s, 1H), 1.48 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 133.8, 126.4, 112.6, 70.0, 40.7, 24.6. Optical Rotation: $[\alpha]_D^{28}$ = +49.45 (c = 0.50, CH_2Cl_2). These spectroscopic data correspond to reported data[10].



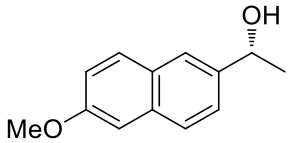
6q

(*R*)-1-(benzo[d][1,3]dioxol-5-yl)ethanol (6q). Colorless oil (81 mg, 97%). 75% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 80/20, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 8.21 min, t (major) = 9.11 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, *J* = 1.4 Hz, 1H), 6.81 – 6.73 (m, 2H), 5.92 (s, 2H), 4.78 (q, *J* = 6.4 Hz, 1H), 2.15 (br s, 1H), 1.43 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 146.7, 139.9, 118.6, 108.0, 106.0, 100.9, 70.1, 25.1. Optical Rotation: $[\alpha]_D^{28}$ = +26.55 (c = 0.43, CH_2Cl_2). These spectroscopic data correspond to reported data[11].



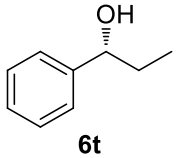
6r

(*R*)-1-(naphthalen-2-yl)ethanol (6r). White solid (85 mg, 98%). 92% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 90/10, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 16.62 min, t (major) = 20.54 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.80 (m, 4H), 7.52 – 7.45 (m, 3H), 5.05 (q, *J* = 6.3 Hz, 1H), 2.13 (br s, 1H), 1.58 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.1, 133.3, 132.9, 128.3, 127.9, 127.6, 126.1, 125.8, 123.8, 123.8, 77.0, 70.5, 25.1. Optical Rotation: $[\alpha]_D^{29}$ = +33.71 (c = 0.53, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



6s

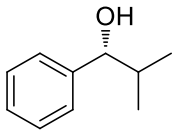
(*R*)-1-(6-methoxynaphthalen-2-yl)ethanol (6s). White solid (100 mg, 99%). 75% ee [Daicel Chiralpak OD-H (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 23.77 min, t (major) = 33.76 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.71 (m, 3H), 7.47 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.17 – 7.13 (m, 2H), 5.03 (q, *J* = 6.5 Hz, 1H), 3.92 (s, 3H), 1.95 (br s, 1H), 1.57 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 140.9, 134.0, 129.4, 128.7, 127.1, 124.3, 123.7, 118.9, 105.6, 70.5, 55.3, 25.0. Optical Rotation: $[\alpha]_D^{29}$ = +31.52 (c = 0.40, CH_2Cl_2). These spectroscopic data correspond to reported data[10].



6t

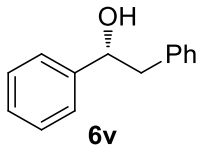
(*R*)-1-phenylpropan-1-ol (6t). Colorless oil (54 mg, 79%). 86% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ =

214 nm, t (minor) = 9.37 min, t (major) = 9.80 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.26 (m, 5H), 4.60 (t, *J* = 6.5 Hz, 1H), 2.04 (br s, 1H), 1.88 – 1.72 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.6, 128.4, 127.4, 125.9, 76.0, 31.8, 10.1. Optical Rotation: $[\alpha]_D^{29}$ = +26.28 (c = 0.56, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



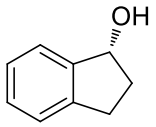
6u

(*R*)-2-methyl-1-phenylpropan-1-ol (6u). Colorless oil (57 mg, 76%). 71% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), CH_3CN/H_2O = 90/10, v = 0.4 mL·min^{-1}, λ = 214 nm, t (minor) = 14.701 min, t (major) = 15.532 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 5H), δ 4.34 (d, J = 6.9 Hz, 1H), 2.04 – 1.90 (m, 2H), 1.01 (d, *J* = 6.7 Hz, 3H), 0.80 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 128.1, 127.4, 126.5, 80.0, 35.2, 19.0, 18.3. Optical Rotation: $[\alpha]_D^{28}$ = +21.67 (c = 0.42, CH_2Cl_2). These spectroscopic data correspond to reported data[8].



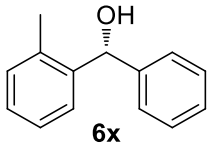
6v

(*S*)-1,2-diphenylethanol (6v). White solid (93 mg, 94%). 11% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 12.22 min, t (major) = 14.40 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.19 (m, 10H), 4.96 – 4.87 (m, 1H), 3.11 – 2.97 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 138.0, 129.5, 128.5, 128.4, 127.6, 126.6, 125.9, 102.4, 75.3, 46.1. Optical Rotation: $[\alpha]_D^{23}$ = +0.5932 (c = 0.48, CH_2Cl_2). These spectroscopic data correspond to reported data. [8]



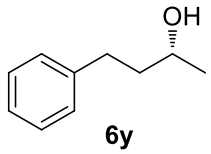
6w

(*R*)-2,3-dihydro-1H-inden-1-ol (6w). White solid (43 mg, 64%). 76% ee [CHIRALPAK IC (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 11.09 min, t (major) = 11.83 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 6.2 Hz, 1H), 7.30 – 7.24 (m, 3H), 5.25 (t, *J* = 6.0 Hz, 1H), 3.13 – 3.01 (m, 1H), 2.89 – 2.78 (m, 1H), 2.57 – 2.44 (m, 1H), 1.96 – 1.88 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9, 143.3, 128.3, 126.6, 124.8, 124.2, 76.4, 35.9, 29.7. Optical Rotation: $[\alpha]_D^{29}$ = –14.82 (c = 0.58, CH_2Cl_2). These spectroscopic data correspond to reported data[12].



6x

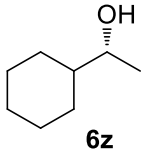
(*R*)-phenyl(o-tolyl)methanol (6x). White solid (96 mg, 97%). 24% ee [Phenomenex Lux 5u Cellulose-3 (0.46 x 25 cm), CH_3CN/H_2O = 90/10, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 8.389 min, t (major) = 9.872 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.37 – 7.31 (m, 4H), 7.30 – 7.20 (m, 3H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.00 (d, *J* = 3.4 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8, 141.4, 135.3, 130.5, 128.4, 127.5, 127.5, 127.1, 126.2, 126.1, 73.3, 19.4. Optical Rotation: $[\alpha]_D^{28}$ = –0.22 (c = 0.66, CH_2Cl_2). These spectroscopic data correspond to reported data[9].



6y

(*R*)-4-phenylbutan-2-ol (**6y**)**.** Colorless oil (60 mg, 80%). 1.1% ee [Phenomenex Lux 5u Cellulose-4 (0.46 x 25 cm), *n*-hexane/*i*-propanol = 95/5, v = 0.7 mL·min^{-1}, λ = 214 nm, t (minor) = 10.53 min, t (major) = 9.44 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.24 – 7.17 (m, 3H), 3.88 – 3.79 (m, 1H), 2.82 – 2.63 (m, 2H), 1.83 –

1.74 (m, 2H), 1.52 (s, 1H), 1.24 (d, J = 6.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 128.4, 125.8, 67.5, 40.9, 32.2, 23.7. Optical Rotation: $[\alpha]_D^{29}$ = –1.5420 (c = 0.45, CH_2Cl_2). These spectroscopic data correspond to reported data[13].



6z

(*R*)-1-cyclohexylethanol (6z). Colorless oil (58 mg, 90%). 9.5% ee [Gas chromatograpy, CP-Cyclodextrin (25 m x 0.25 mm x 0.25 um)], Oven: 80 °C (65 min), 20 °C /min to 220 °C (10 min), Injection: 300°C, He: 1.0 mL/min, split: 200:1, FID, H_2: 40.0 mL/min, air flow: 450.0 mL/min, t (minor) = 43.771 min, t (major) = 44.901 min]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56 – 3.49 (m, 1H), 1.89 – 1.61 (m, 5H), 1.56 (s, 1H), 1.30 – 1.15 (m, 4H), 1.13 (d, J = 6.3 Hz, 3H), 1.04 – 0.89 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 72.2, 45.1, 28.7, 28.4, 26.5, 26.2, 26.1, 20.4. Optical Rotation: $[\alpha]_D^{29}$ = –1.1993 (c = 0.48, CH_2Cl_2). These spectroscopic data correspond to reported data[9].

4. Crystallographic Data of Complex (*S*)-**3a** and (*S*)-**3d**

Table S4.1 Crystal data and structure refinement for (*S*)-3a

Identification code	mo_dm14439_0m	
Empirical formula	C53 H73 Br4 Fe2 N7 O3	
Formula weight	1287.52	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 15.777(4) Å	a= 90°.
	b = 10.030(3) Å	b=100.090(4)°.
	c = 17.685(5) Å	g = 90°.
Volume	2755.3(12) $Å^3$	
Z	2	
Density (calculated)	1.552 Mg/m^3	
Absorption coefficient	3.475 mm^{-1}	
F(000)	1312	
Crystal size	0.120 x 0.080 x 0.010 mm^3	
Theta range for data collection	1.169 to 30.324°.	
Index ranges	-19<=h<=22, -12<=k<=14, -25<=l<=24	
Reflections collected	26394	
Independent reflections	15709 [R(int) = 0.1132]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.746 and 0.418	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15709 / 7 / 638	
Goodness-of-fit on F^2	0.973	
Final R indices [I>2sigma(I)]	R1 = 0.0715, wR2 = 0.1144	
R indices (all data)	R1 = 0.1988, wR2 = 0.1556	
Absolute structure parameter	0.019(14)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.451 and -1.669 $e.Å^{-3}$	

Table S4.2 Crystal data and structure refinement for (*S*)-3d

Identification code	cu_dm14700_0m	
Empirical formula	C47 H45 Br2 Fe N3 O	
Formula weight	883.53	
Temperature	130 K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	P 4	
Unit cell dimensions	a = 33.2315(4) Å	a= 90°.
	b = 33.2315(4) Å	b= 90°.
	c = 18.2906(3) Å	g = 90°.
Volume	20198.9(6) $Å^3$	
Z	16	
Density (calculated)	1.162 Mg/m^3	
Absorption coefficient	4.490 mm^{-1}	
F(000)	7232	
Crystal size	0.25 x 0.22 x 0.16 mm^3	
Theta range for data collection	1.329 to 69.753°.	
Index ranges	-39<=h<=39, -40<=k<=38, -21<=l<=22	
Reflections collected	112205	
Independent reflections	34361 [R(int) = 0.1082]	
Completeness to theta = 67.679°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7532 and 0.3163	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	34361 / 752 / 1953	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0714, wR2 = 0.1873	
R indices (all data)	R1 = 0.0978, wR2 = 0.2029	
Absolute structure parameter	0.082(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.258 and -1.201 $e.Å^{-3}$	

5. References

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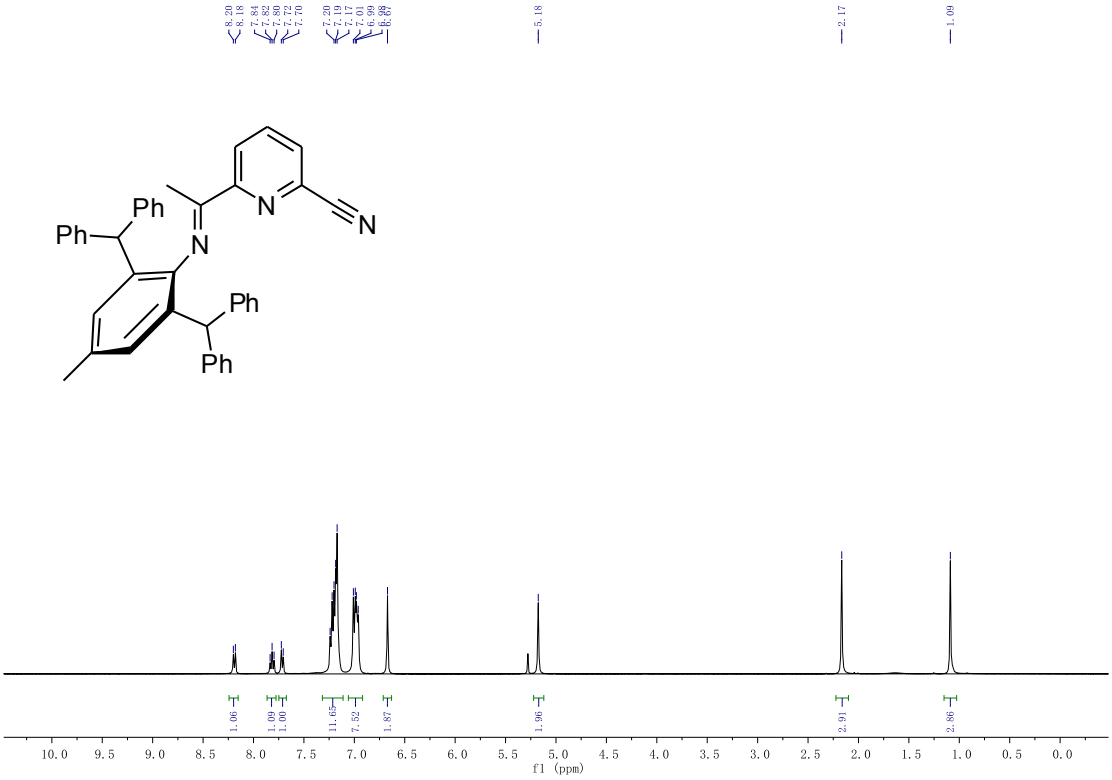
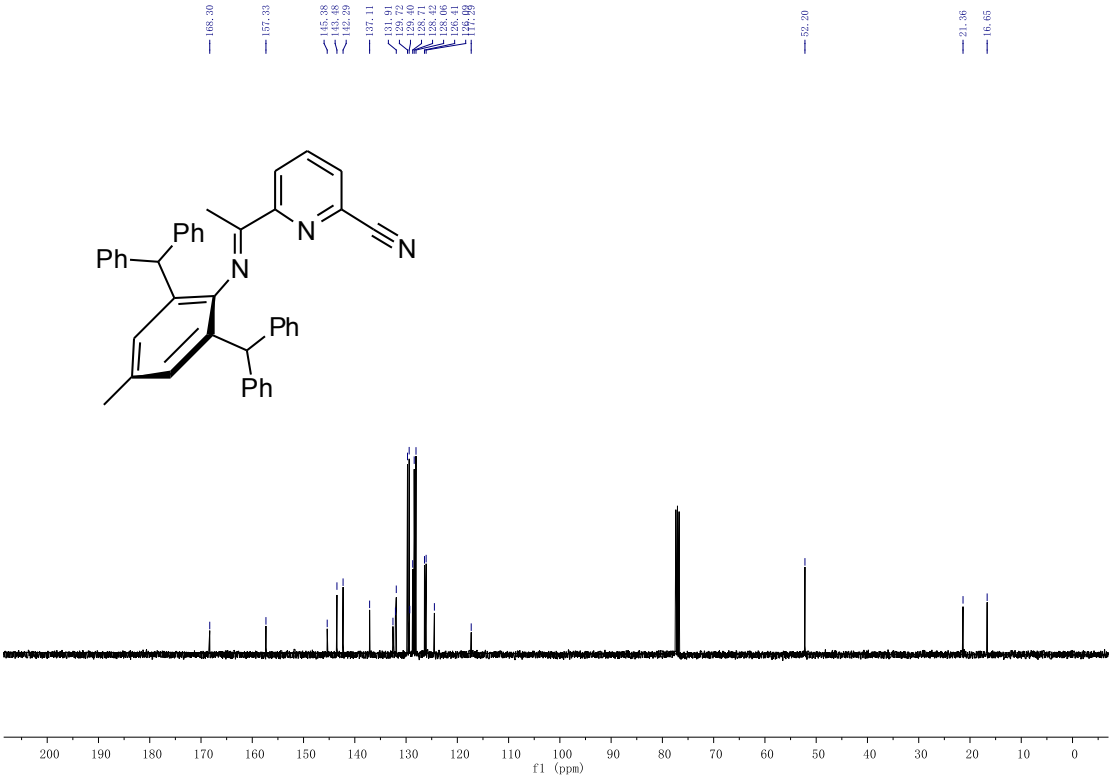
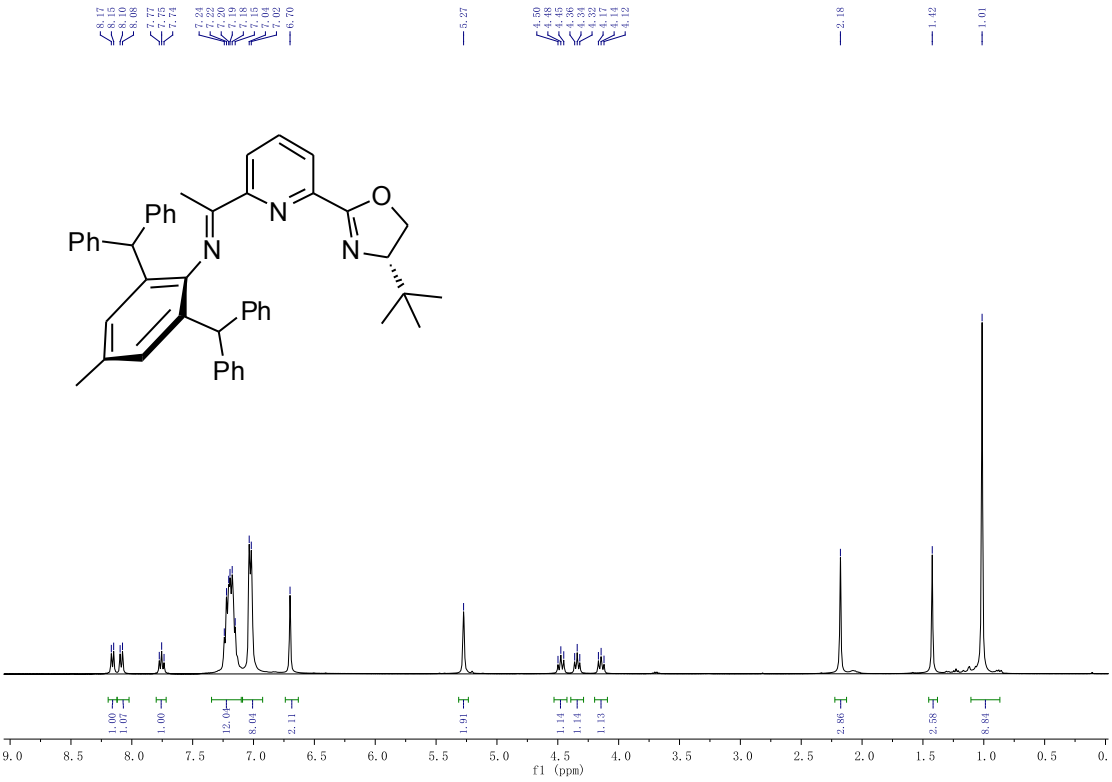
6. NMR Spectra



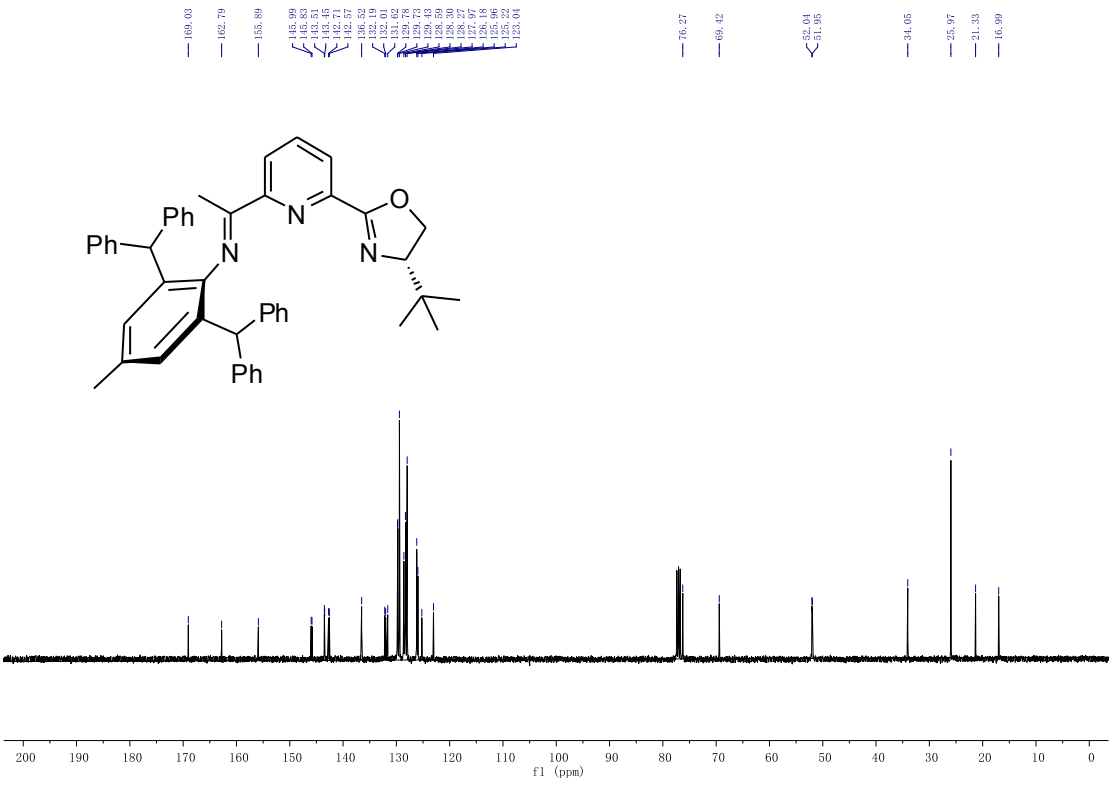
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **1**



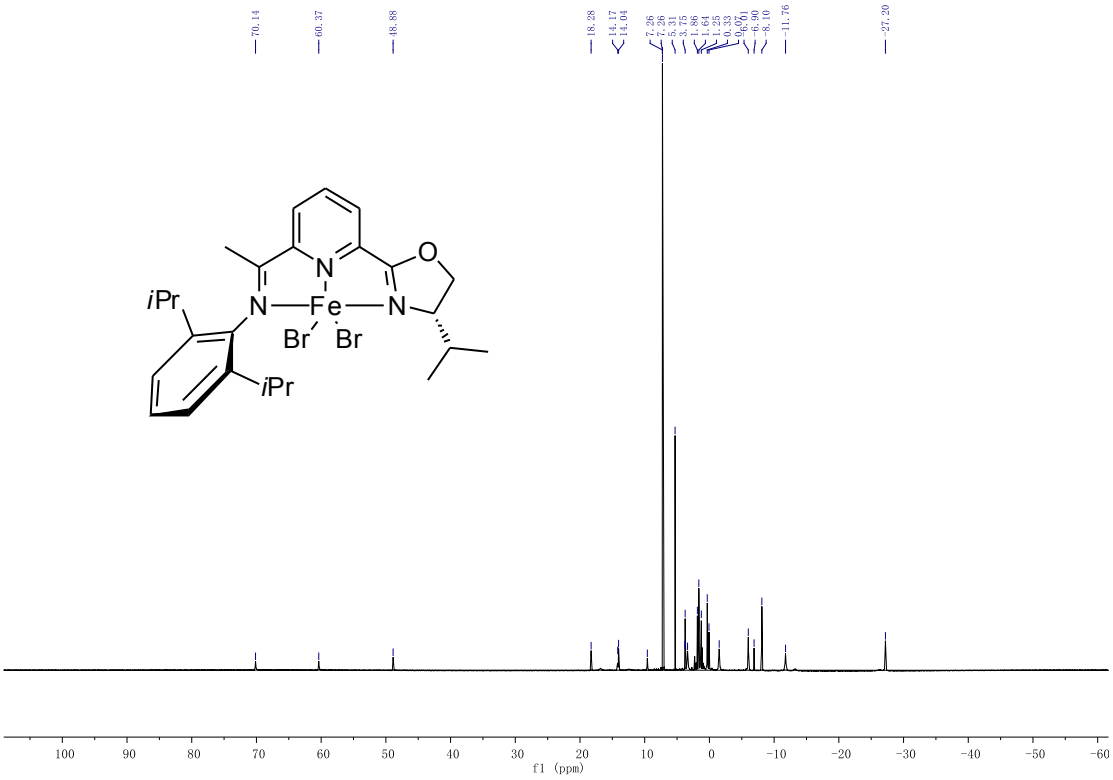
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **1**



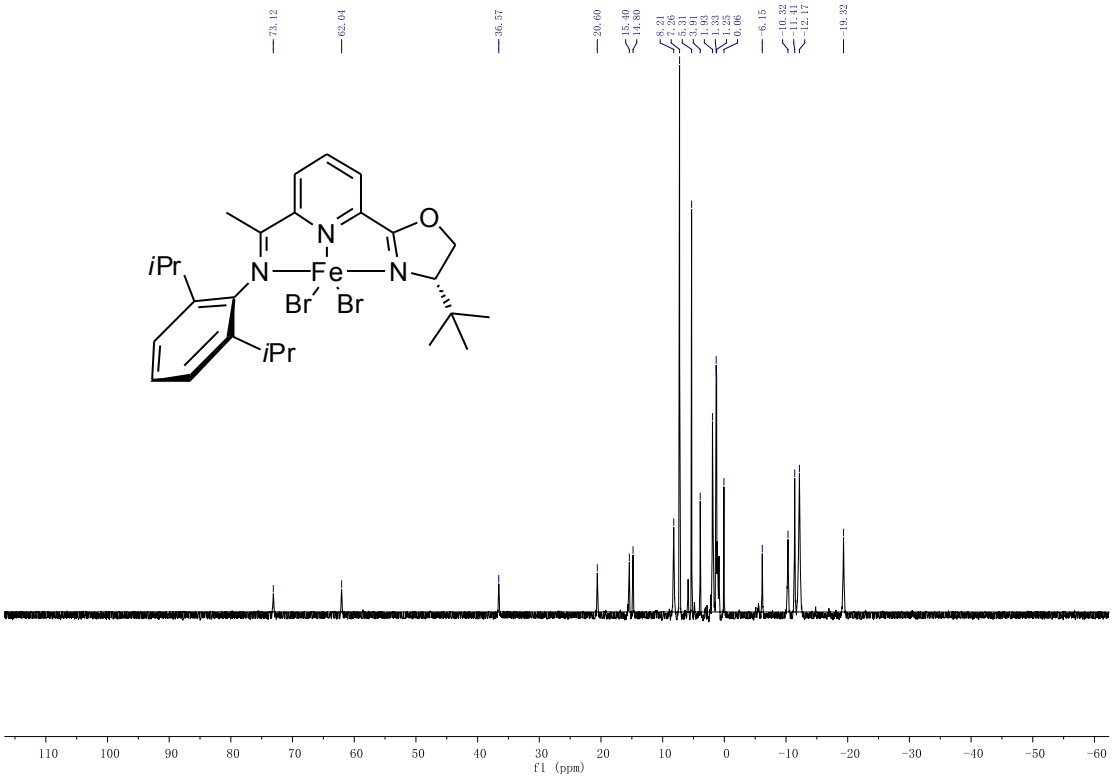
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*S*)-**2d**



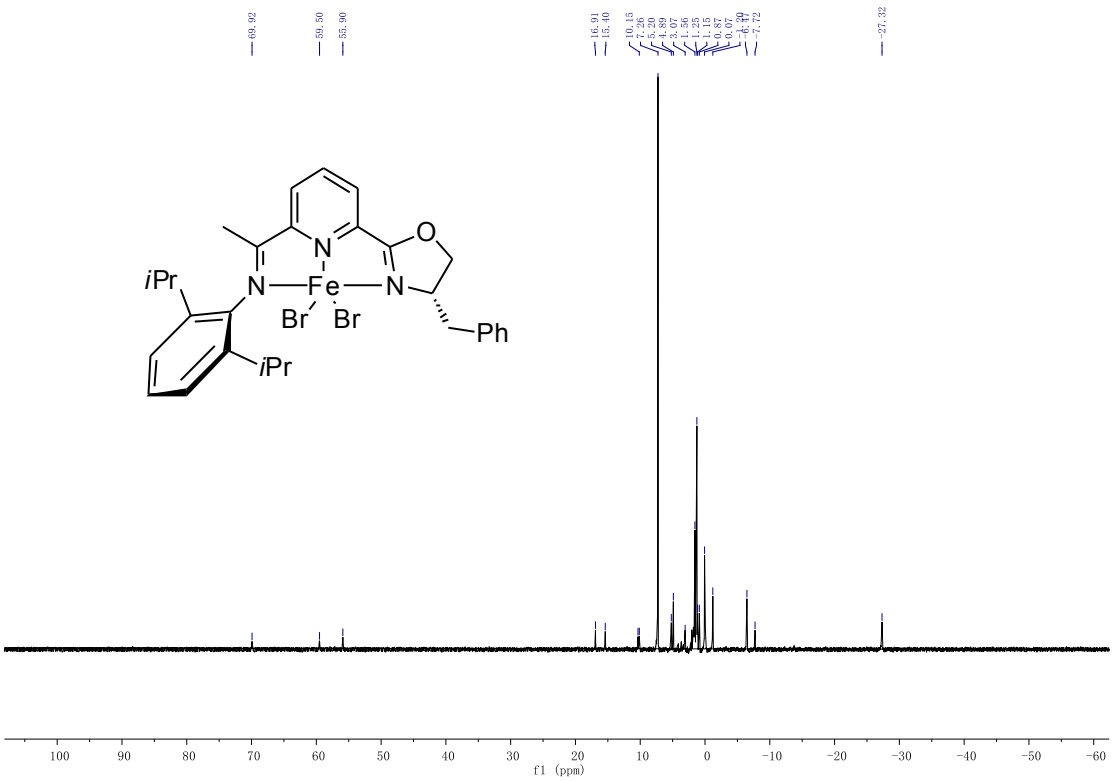
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of (*S*)-**2d**



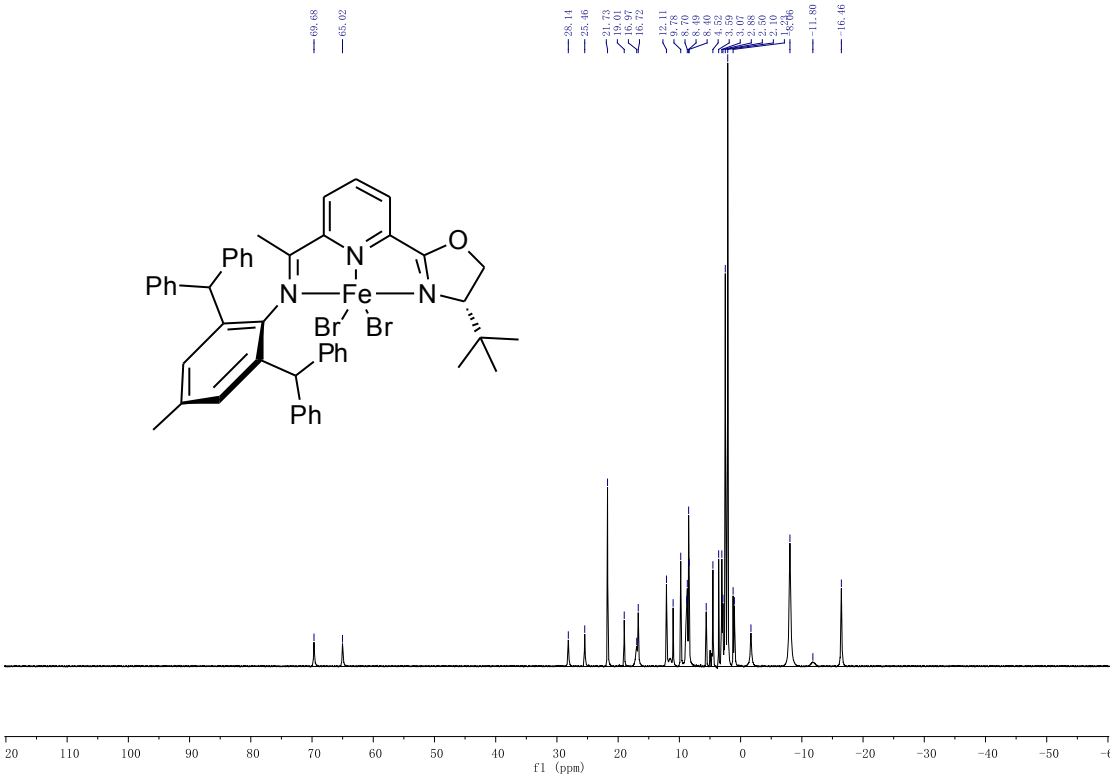
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*S*)-**3a**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*S*)-**3b**



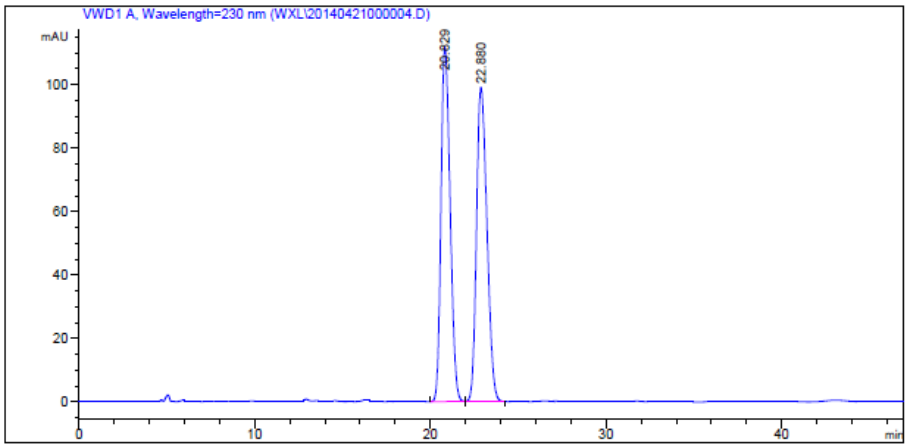
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*S*)-**3c**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of (*S*)-**3d**

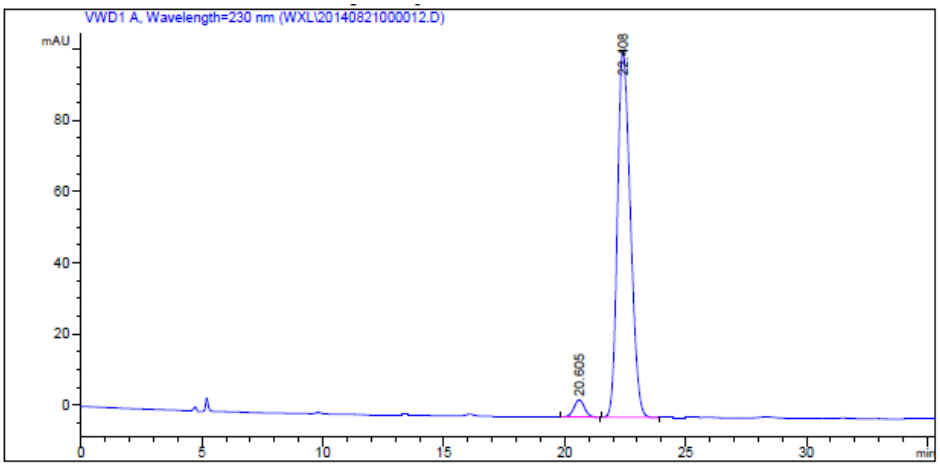
7. HPLC chromatographs

6a



Area Percent Report

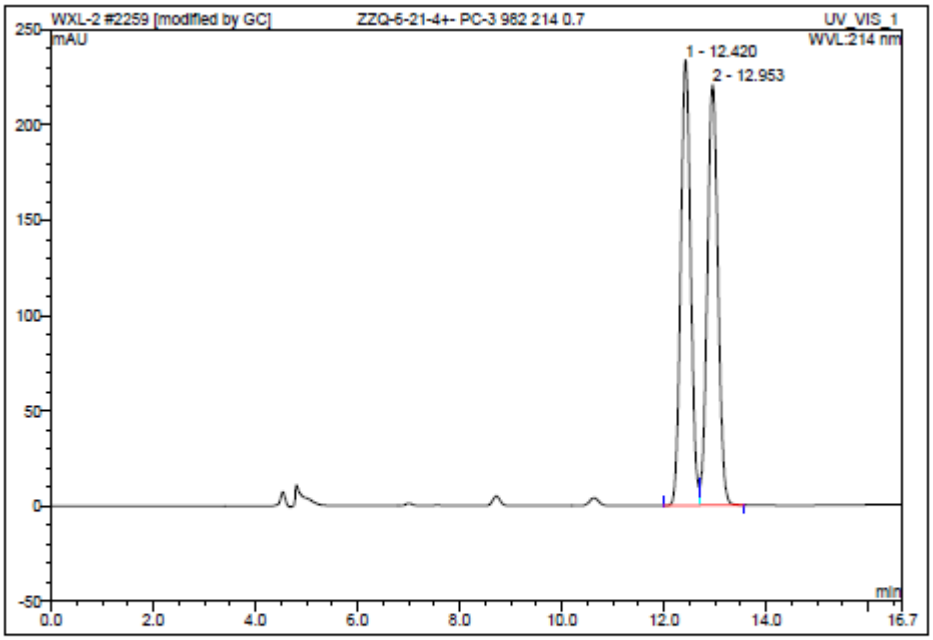
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.829	BB	0.5643	4021.67896	111.76553	49.5905
2	22.880	BB	0.6482	4088.10083	99.00758	50.4095
Totals :				8109.77979	210.77312	



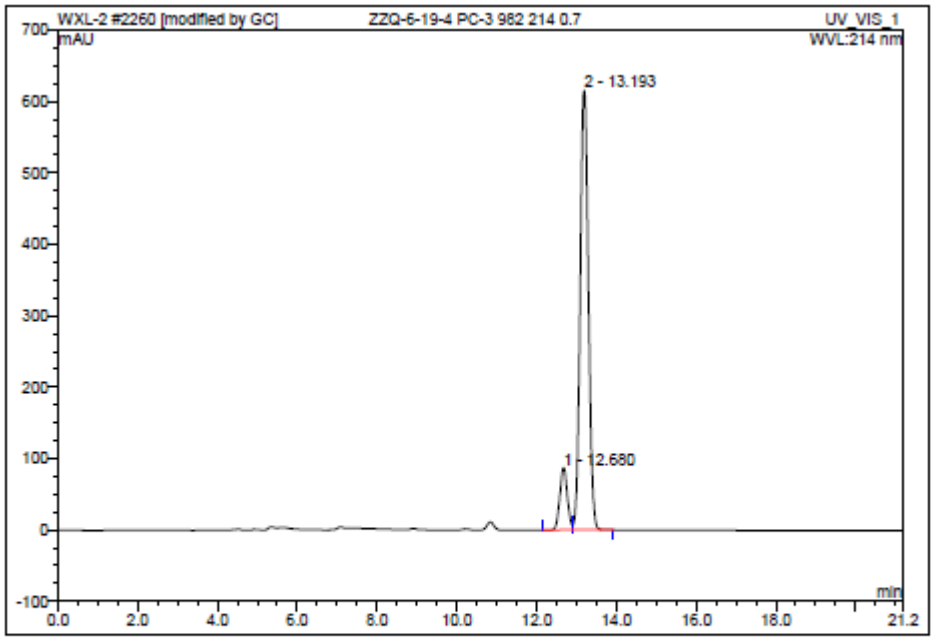
Area Percent Report

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.605	BB	0.4732	144.89261	4.77198	3.6523
2	22.408	BB	0.5835	3822.25732	102.63398	96.3477
Totals :				3967.14993	107.40596	

6b



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.42	n.a.	233.914	52.859	49.77	n.a.	BM *
2	12.95	n.a.	220.638	53.343	50.23	n.a.	MB*
Total:			454.552	106.202	100.00	0.000	



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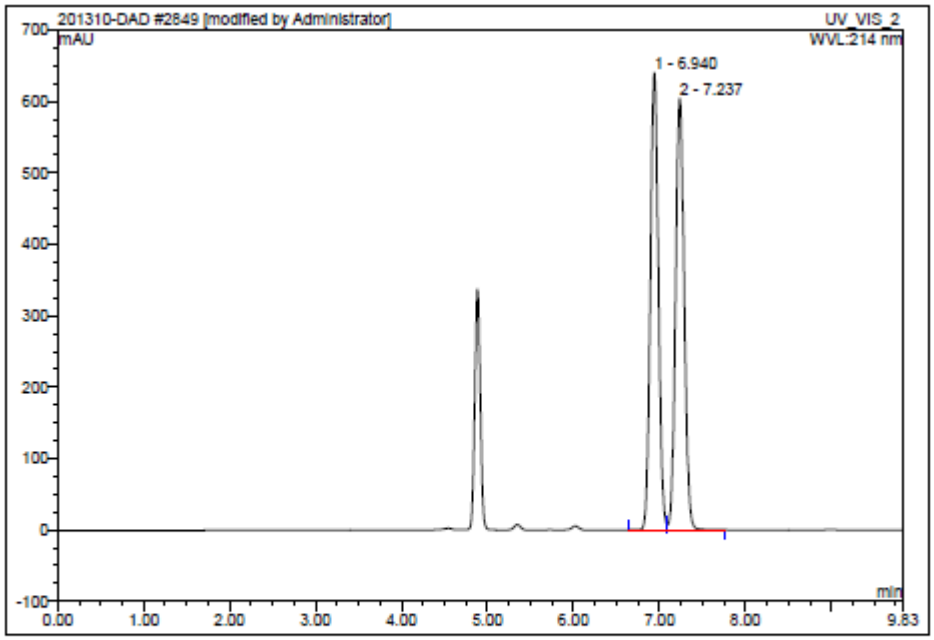
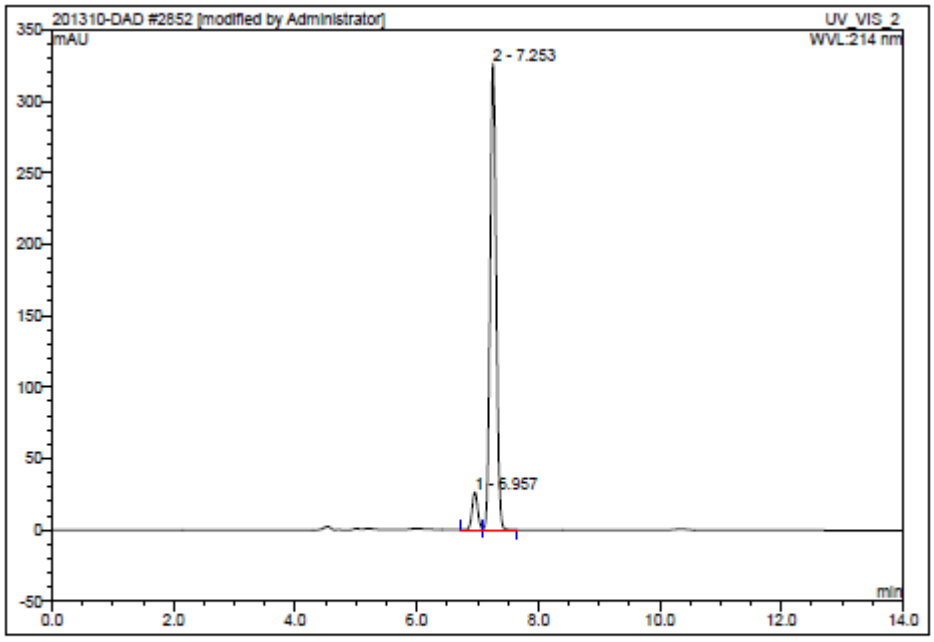
1	12.68	n.a.	87.152	18.862	11.39	n.a.	BM *
2	13.19	n.a.	614.674	146.671	88.61	n.a.	MB*
Total:			701.826	165.534	100.00	0.000	

6c



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.94	n.a.	639.611	69.457	49.67	n.a.	BM *
2	7.24	n.a.	603.613	70.366	50.33	n.a.	MB*
Total:			1243.224	139.823	100.00	0.000	



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1	6.96	n.a.	26.134	2.828	6.94	n.a.	BM *
2	7.25	n.a.	326.164	37.926	93.06	n.a.	MB*
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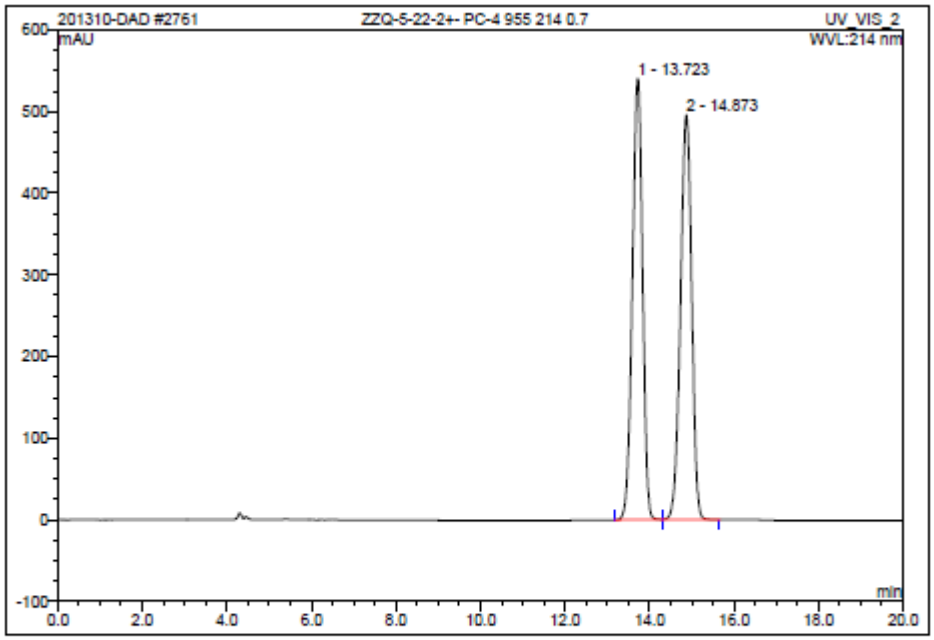
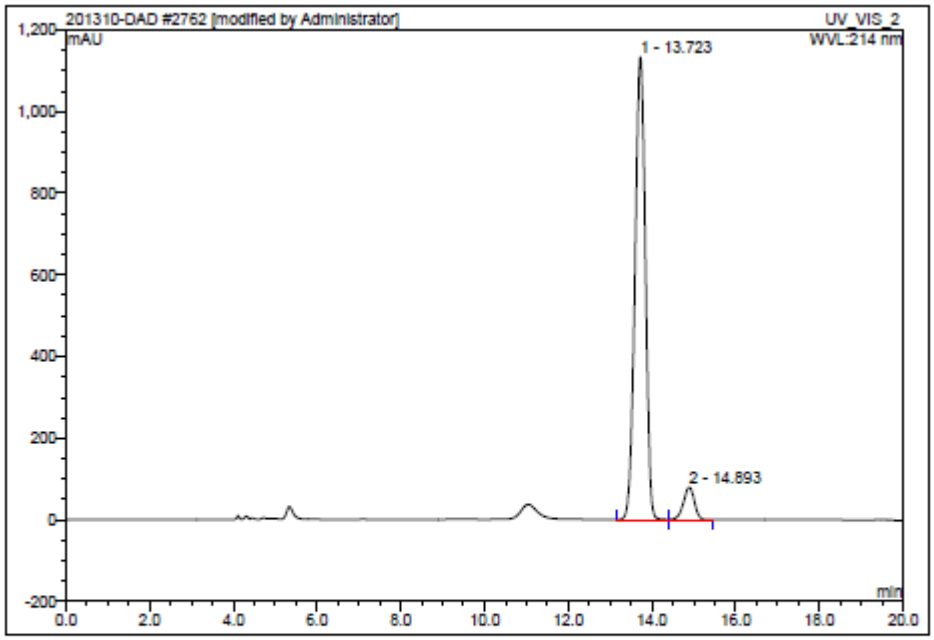
6d

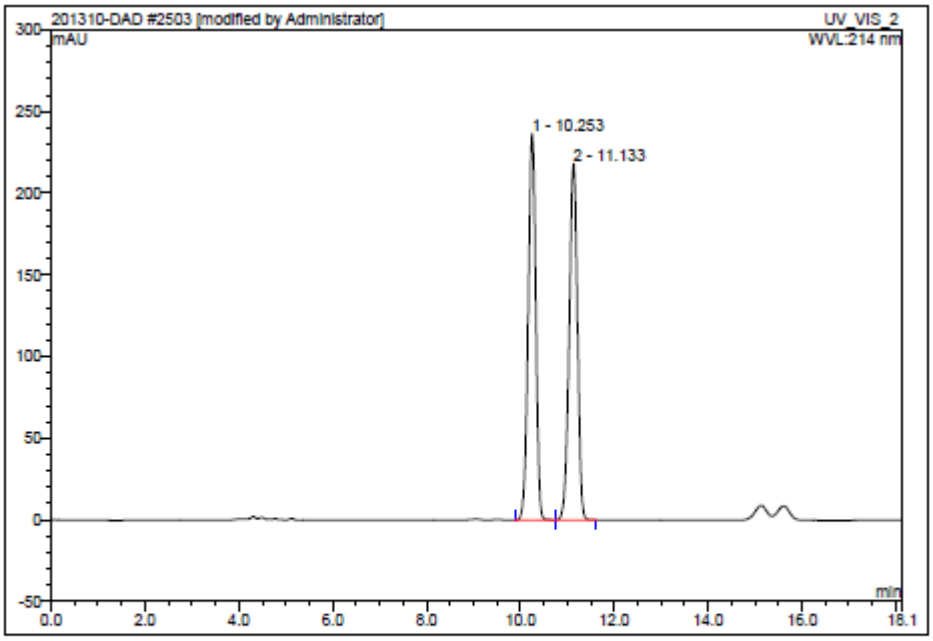


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.72	n.a.	540.465	151.213	49.81	n.a.	BM
2	14.87	n.a.	495.562	152.392	50.19	n.a.	MB
Total:			1036.026	303.605	100.00	0.000	

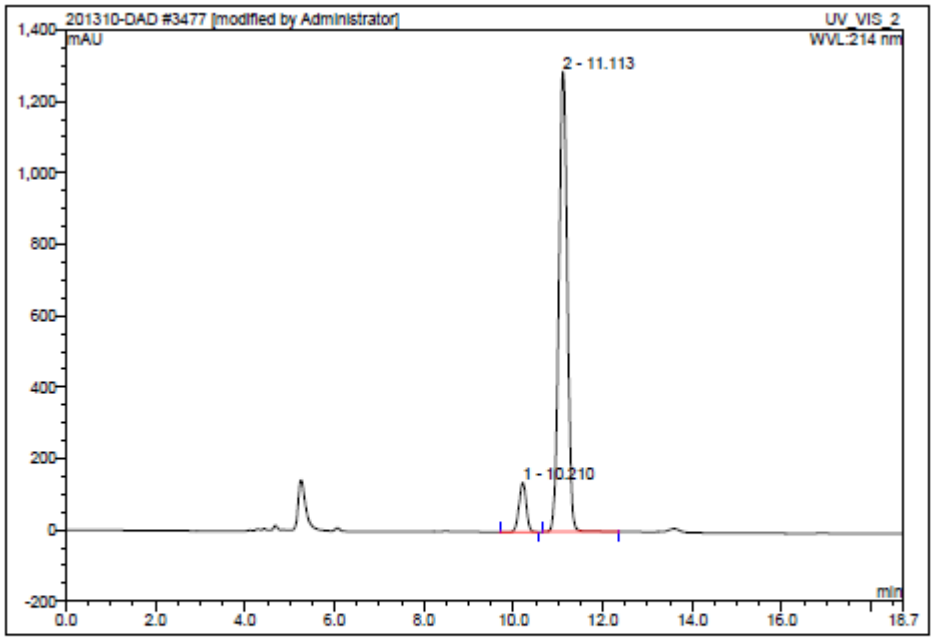


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.72	n.a.	1132.571	326.344	93.19	n.a.	BM
2	14.89	n.a.	79.021	23.867	6.81	n.a.	MB
Total:			1211.592	350.211	100.00	0.000	

6e

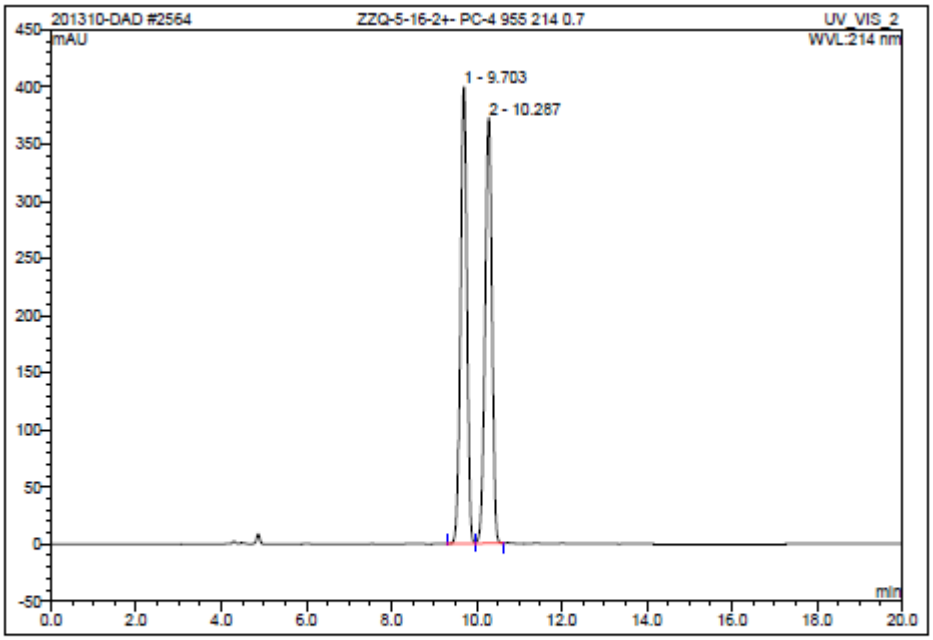


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.25	n.a.	236.749	44.461	49.96	n.a.	BM
2	11.13	n.a.	217.963	44.540	50.04	n.a.	MB
Total:			454.711	89.001	100.00	0.000	

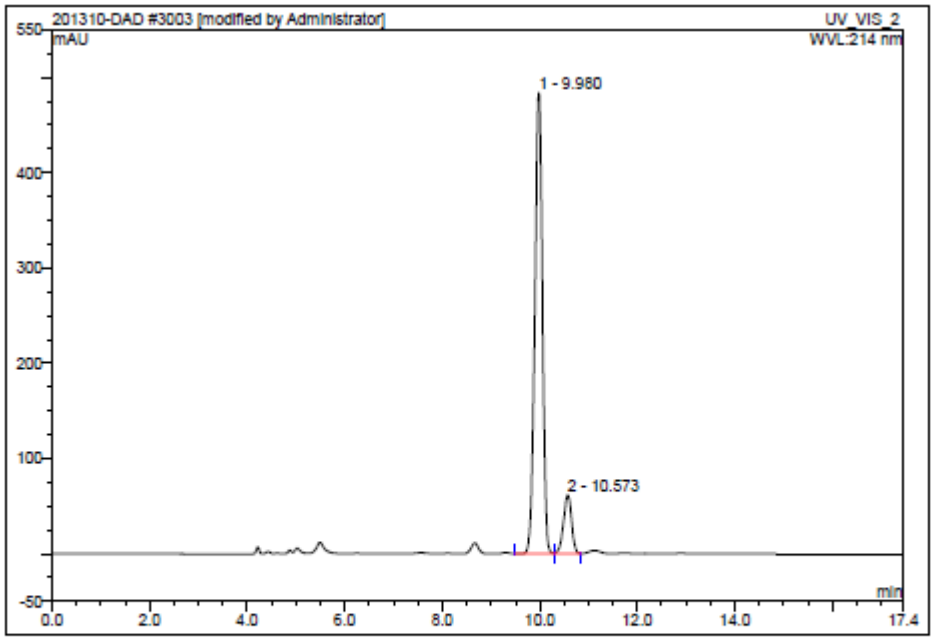


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.21	n.a.	138.603	26.034	8.44	n.a.	BMB*
2	11.11	n.a.	1288.849	282.272	91.56	n.a.	BMB*
Total:			1427.452	308.306	100.00	0.000	

6f

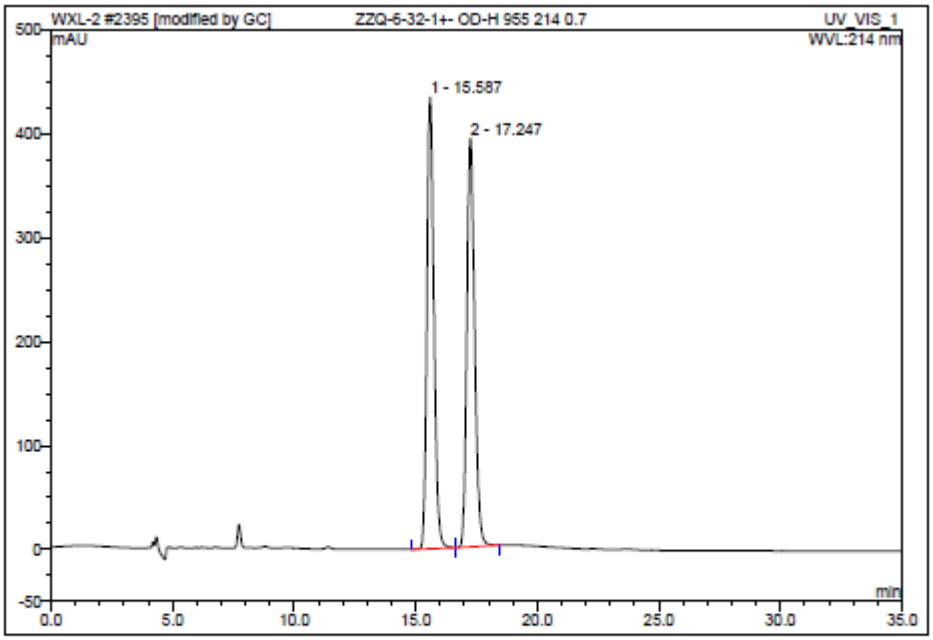


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.70	n.a.	399.671	70.486	50.01	n.a.	BM
2	10.29	n.a.	372.287	70.453	49.99	n.a.	MB
Total:			771.957	140.939	100.00	0.000	

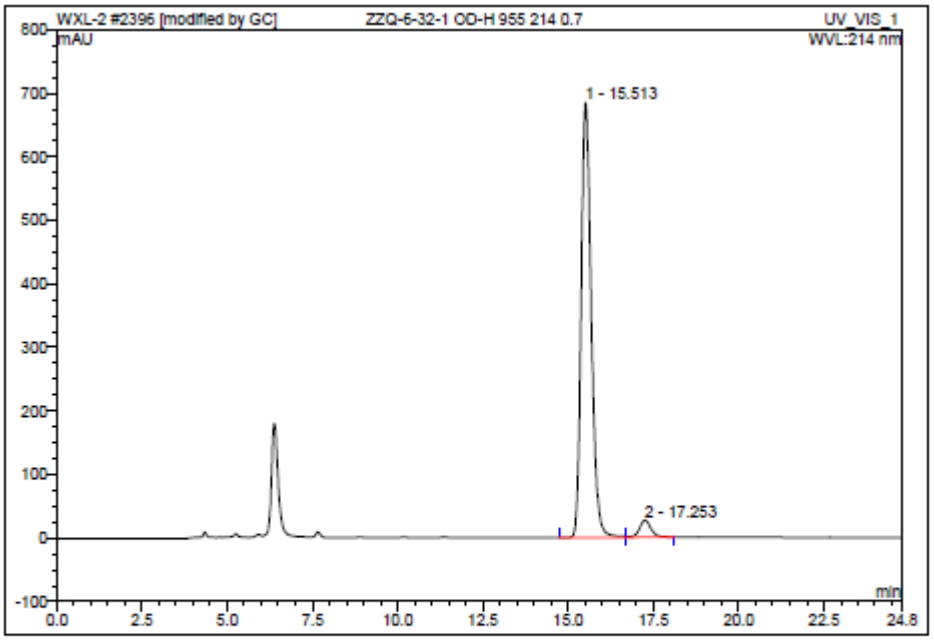


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.98	n.a.	483.869	87.531	88.09	n.a.	BM *
2	10.57	n.a.	61.401	11.839	11.91	n.a.	MB*
Total:			545.269	99.369	100.00	0.000	

6g

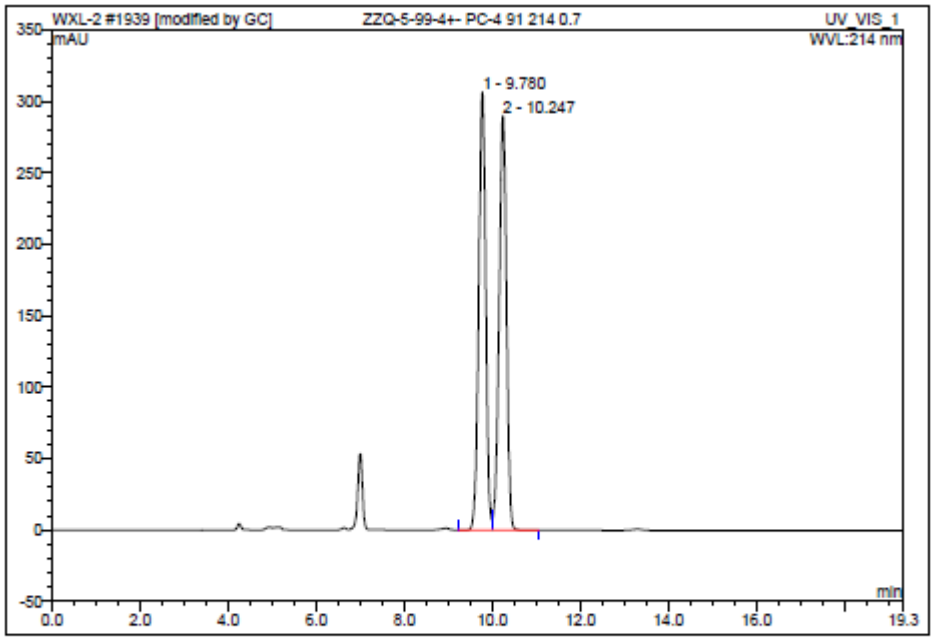


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.59	n.a.	434.417	145.101	49.97	n.a.	BMb*
2	17.25	n.a.	393.028	145.251	50.03	n.a.	bMB*
Total:			827.444	290.351	100.00	0.000	

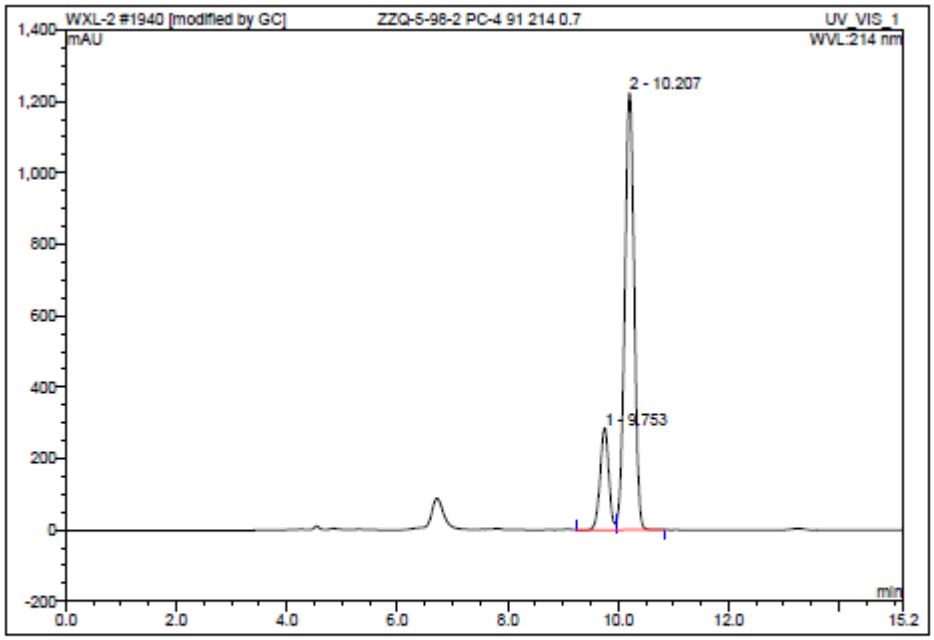


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	15.51	n.a.	684.481	235.005	95.64	n.a.	BM *
2	17.25	n.a.	26.989	10.724	4.36	n.a.	MB*
Total:			711.470	245.729	100.00	0.000	

6h

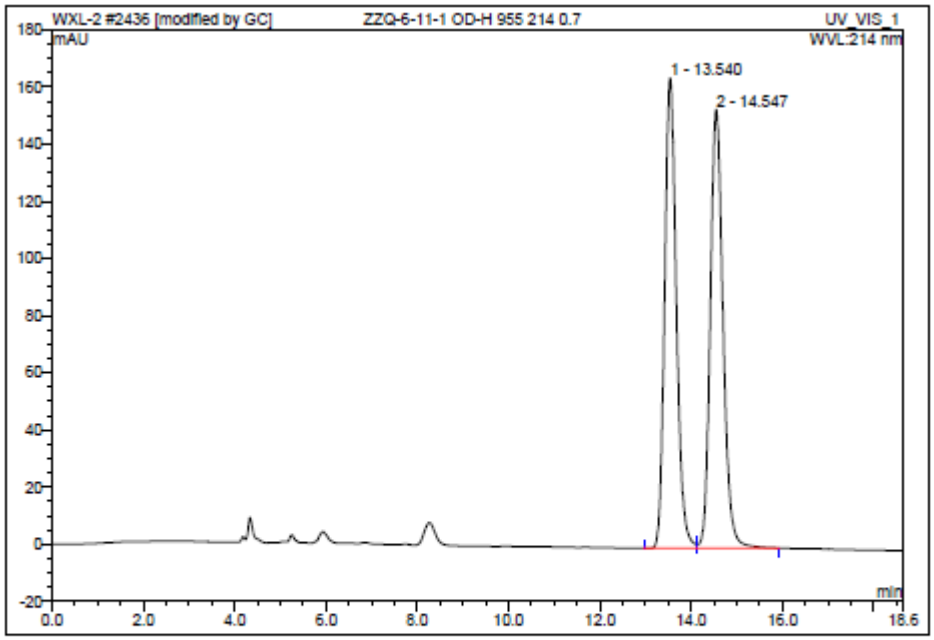


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.78	n.a.	306.471	56.364	49.91	n.a.	BM *
2	10.25	n.a.	290.085	56.572	50.09	n.a.	MB*
Total:			596.556	112.937	100.00	0.000	

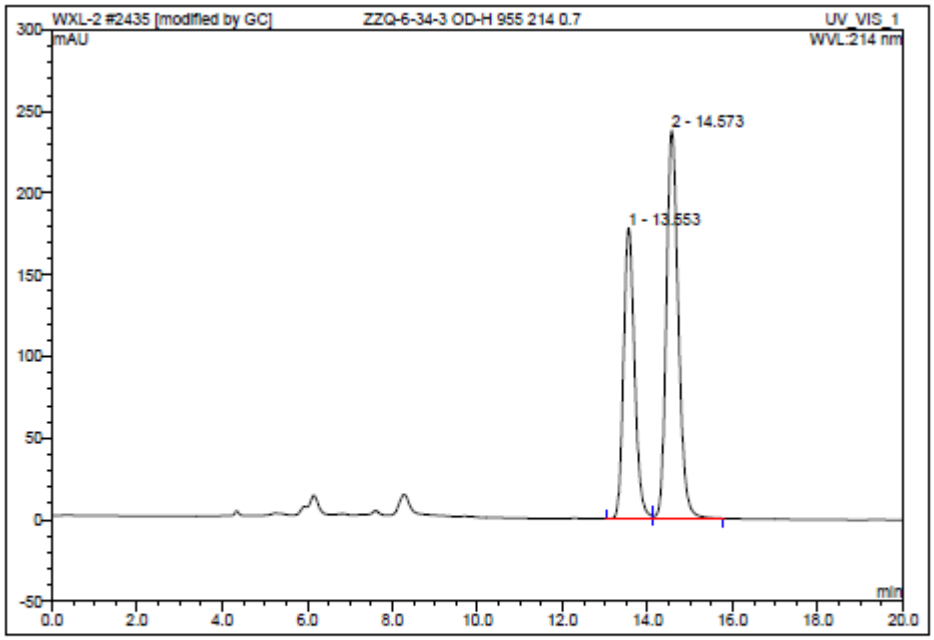


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.75	n.a.	285.639	52.191	17.79	n.a.	BM *
2	10.21	n.a.	1223.142	241.109	82.21	n.a.	MB*
Total:			1508.781	293.301	100.00	0.000	

6i

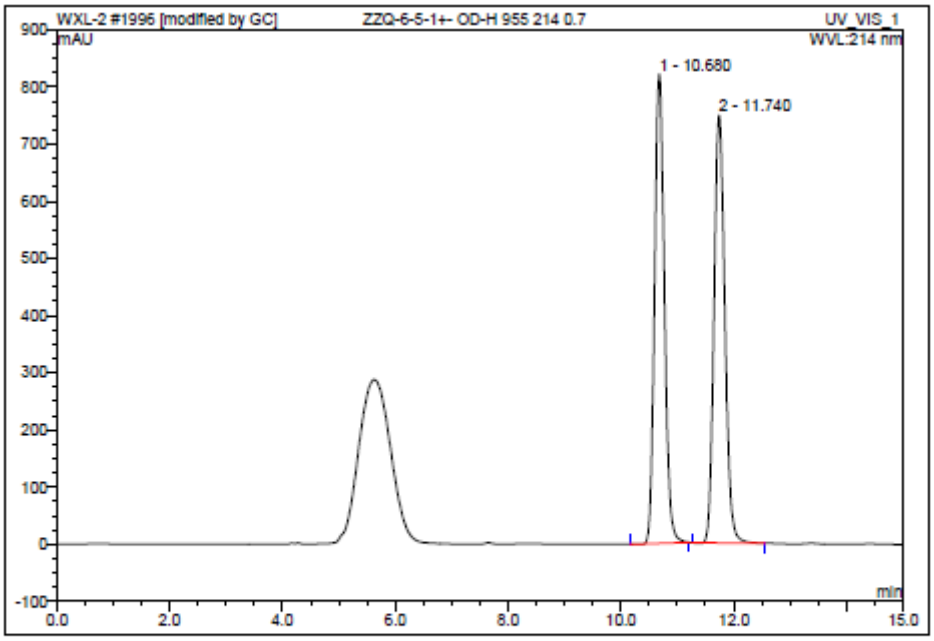


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.54	n.a.	164.624	48.750	49.53	n.a.	BM *
2	14.55	n.a.	153.517	49.666	50.47	n.a.	MB*
Total:			318.141	98.416	100.00	0.000	

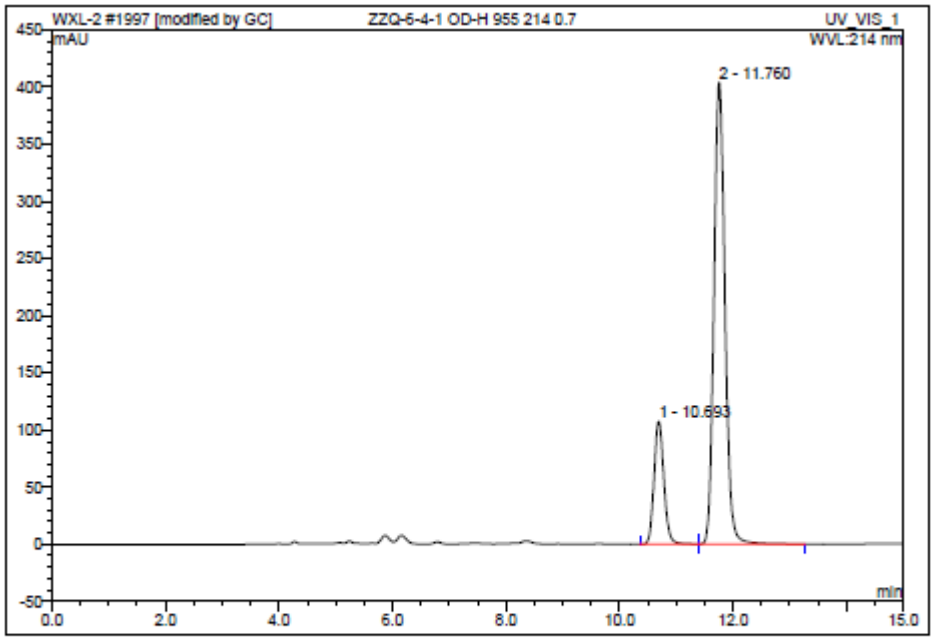


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.55	n.a.	177.775	53.284	40.74	n.a.	BM *
2	14.57	n.a.	237.660	77.513	59.26	n.a.	MB*
Total:			415.435	130.797	100.00	0.000	

6j

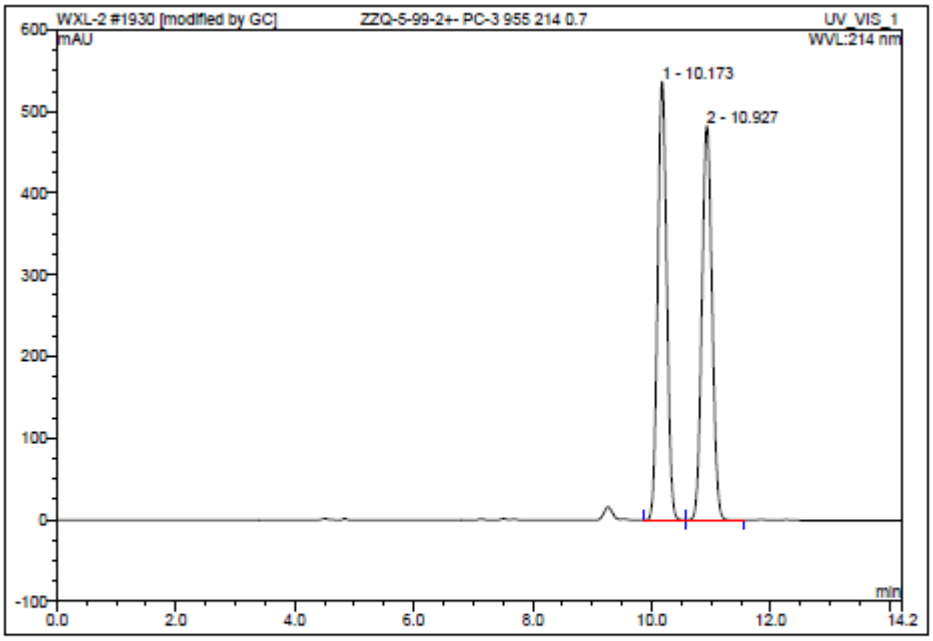


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.68	n.a.	820.718	165.410	49.75	n.a.	BMB*
2	11.74	n.a.	748.355	167.047	50.25	n.a.	BMB*
Total:			1569.074	332.456	100.00	0.000	

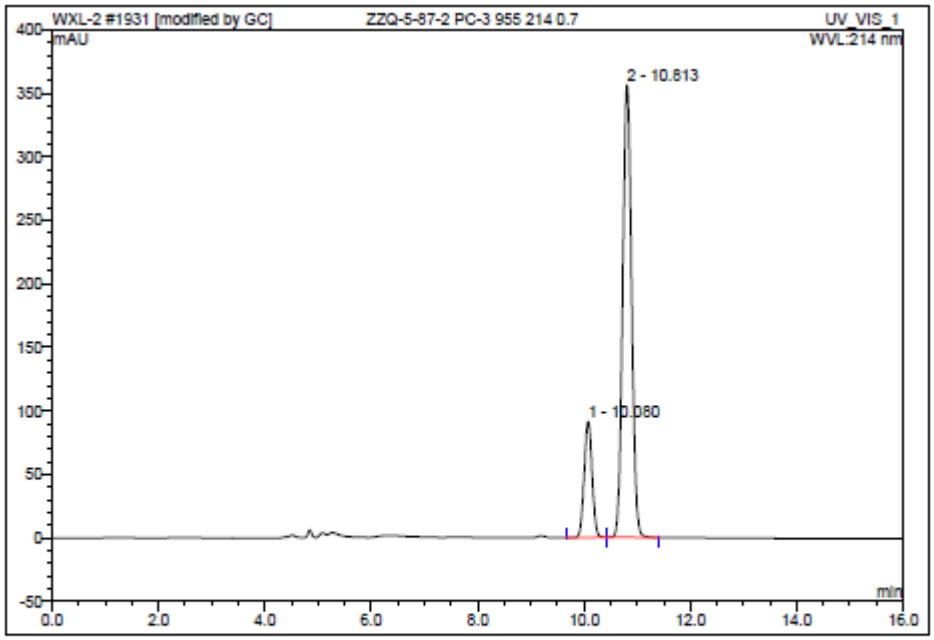


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.69	n.a.	107.562	21.660	19.28	n.a.	BM *
2	11.76	n.a.	404.168	90.707	80.72	n.a.	MB*
Total:			511.730	112.368	100.00	0.000	

6k

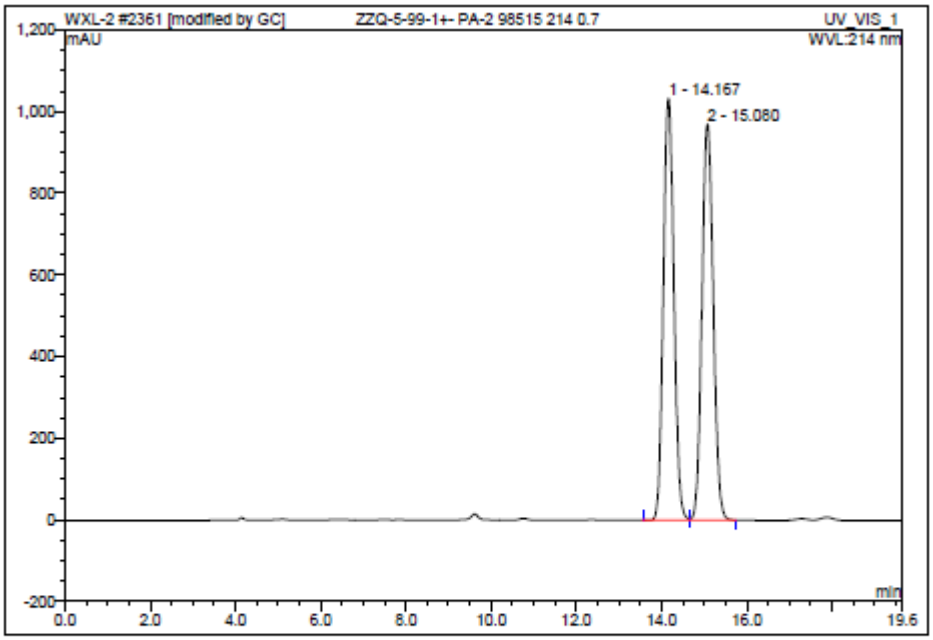


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.17	n.a.	536.852	95.128	49.86	n.a.	BM
2	10.93	n.a.	483.009	95.651	50.14	n.a.	MB
Total:			1019.861	190.778	100.00	0.000	

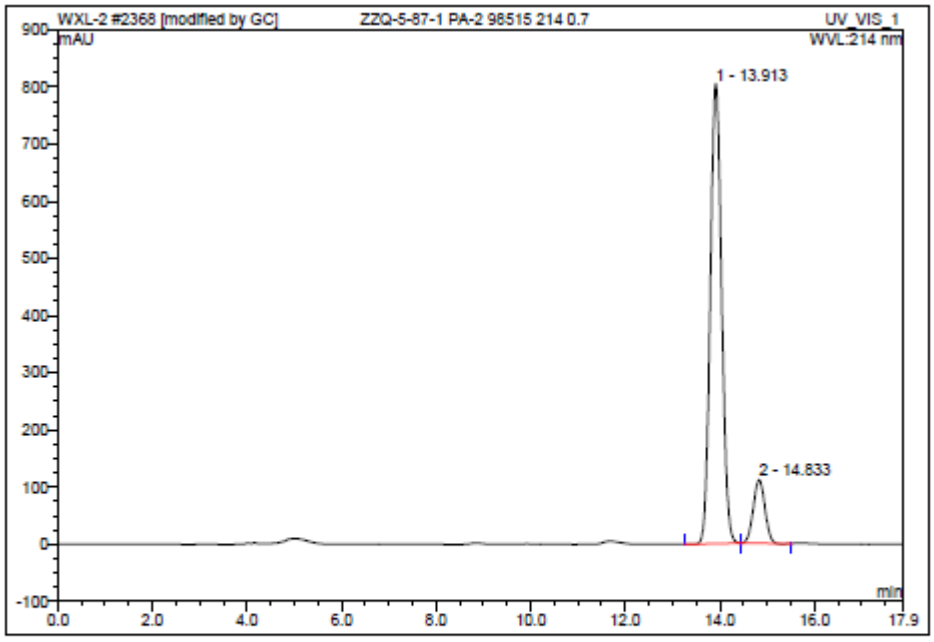


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.08	n.a.	91.390	15.732	18.50	n.a.	BMB*
2	10.81	n.a.	356.270	69.289	81.50	n.a.	BMB*
Total:			447.659	85.022	100.00	0.000	

6l

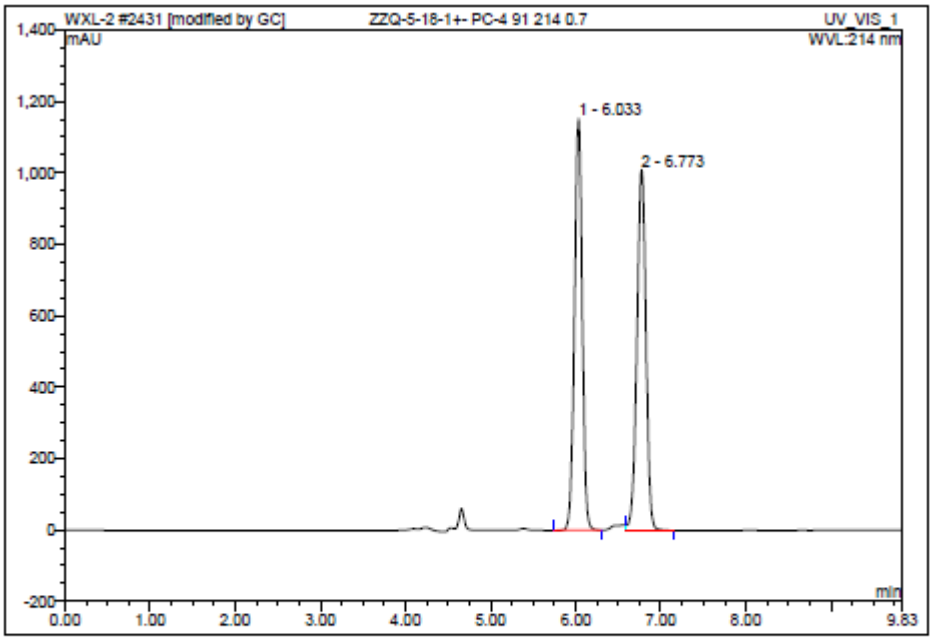


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	14.17	n.a.	1032.777	295.991	49.82	n.a.	BM *
2	15.08	n.a.	970.136	298.177	50.18	n.a.	MB*
Total:			2002.912	594.167	100.00	0.000	

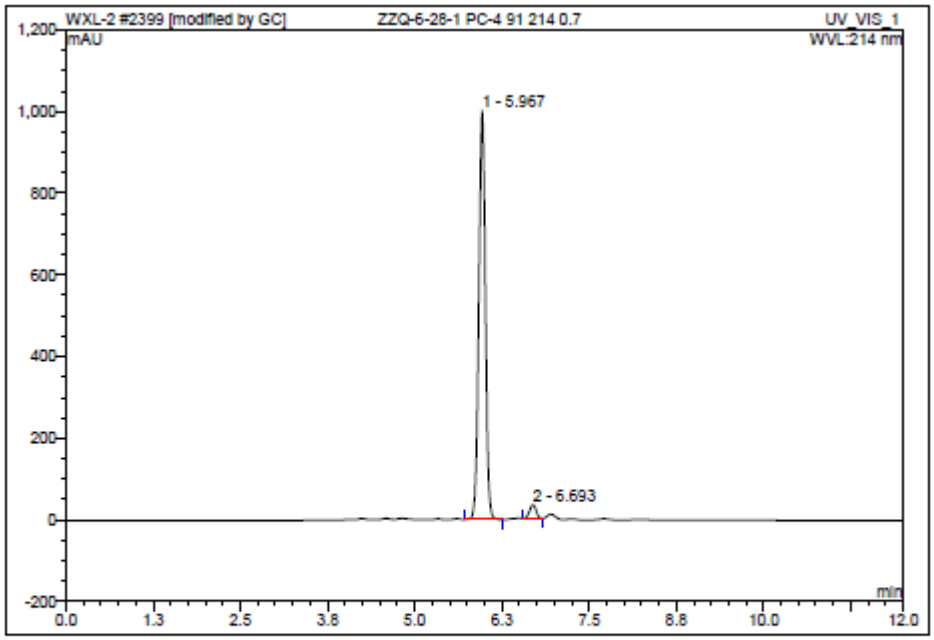


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.91	n.a.	804.581	222.817	87.62	n.a.	BMb*
2	14.83	n.a.	111.409	31.477	12.38	n.a.	bMB*
Total:			915.989	254.294	100.00	0.000	

6m

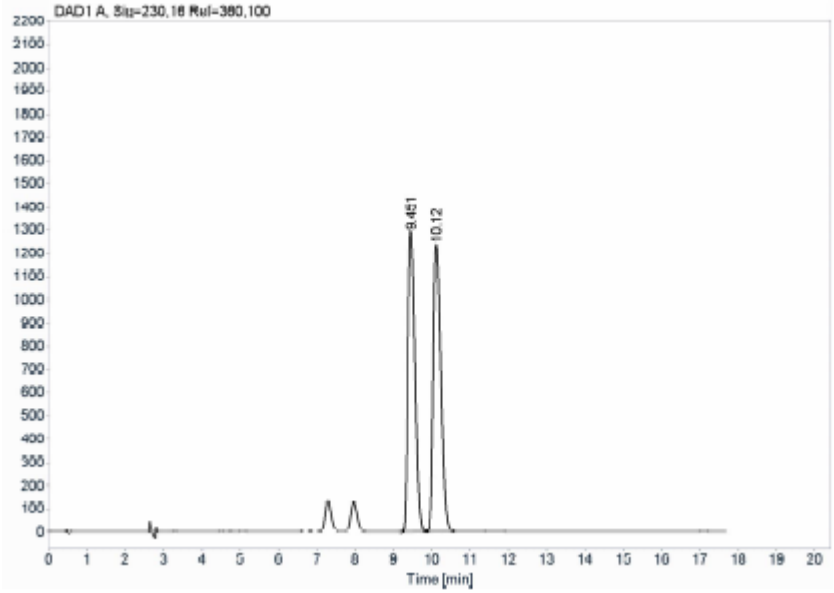


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.03	n.a.	1151.670	122.268	49.68	n.a.	BMB*
2	6.77	n.a.	1008.927	123.858	50.32	n.a.	MB*
Total:			2160.597	246.126	100.00	0.000	



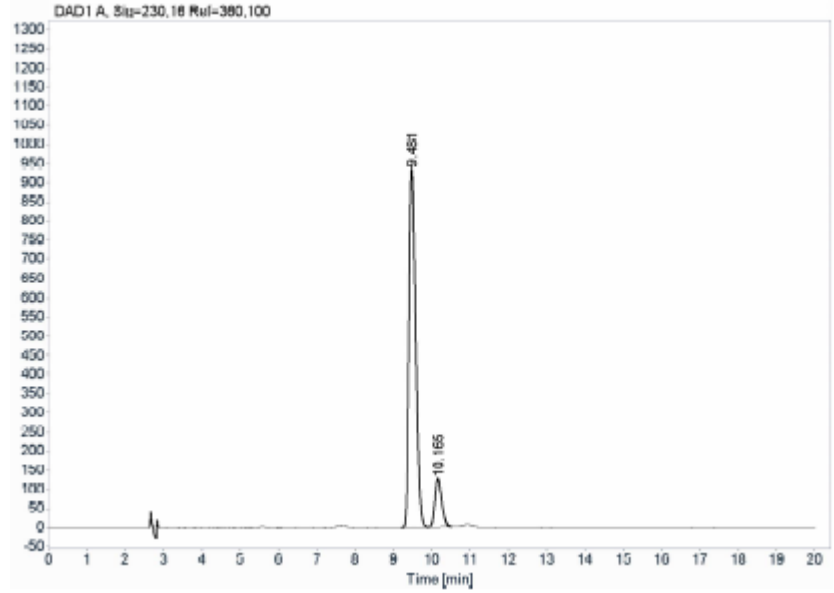
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.97	n.a.	1001.023	108.535	96.66	n.a.	BMB*
2	6.69	n.a.	33.715	3.749	3.34	n.a.	BMB*
Total:			1034.738	112.284	100.00	0.000	

6n



Signal: DAD1 A, Sig=230,16 Ref=360,100

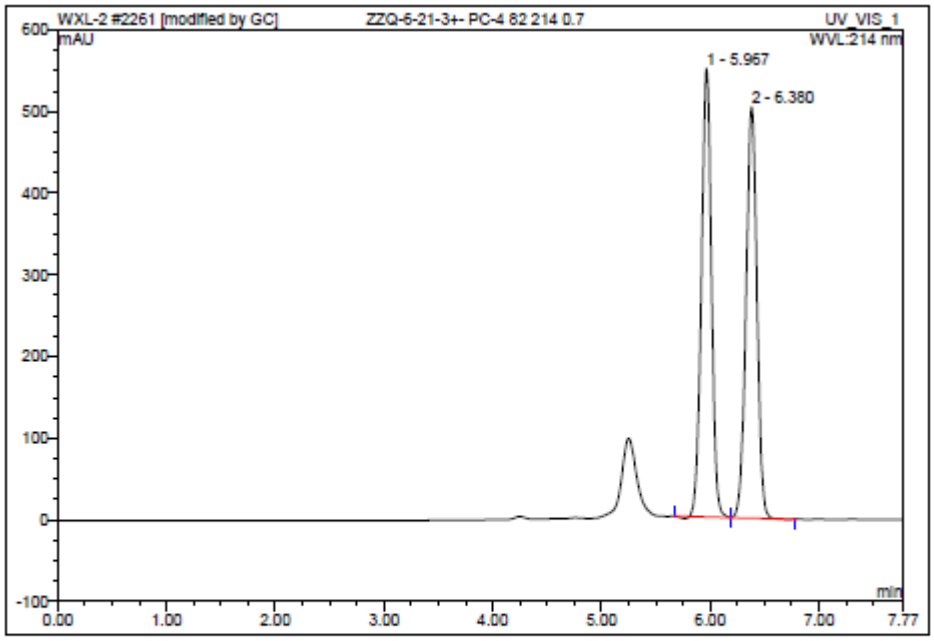
RT [min]	Type	Width [min]	Area	Height	Area%
9.451	BB	0.2050	16707.0605	1291.1135	49.4664
10.120	BV	0.2178	17067.5352	1234.6218	50.5336
		Sum	33774.5957		



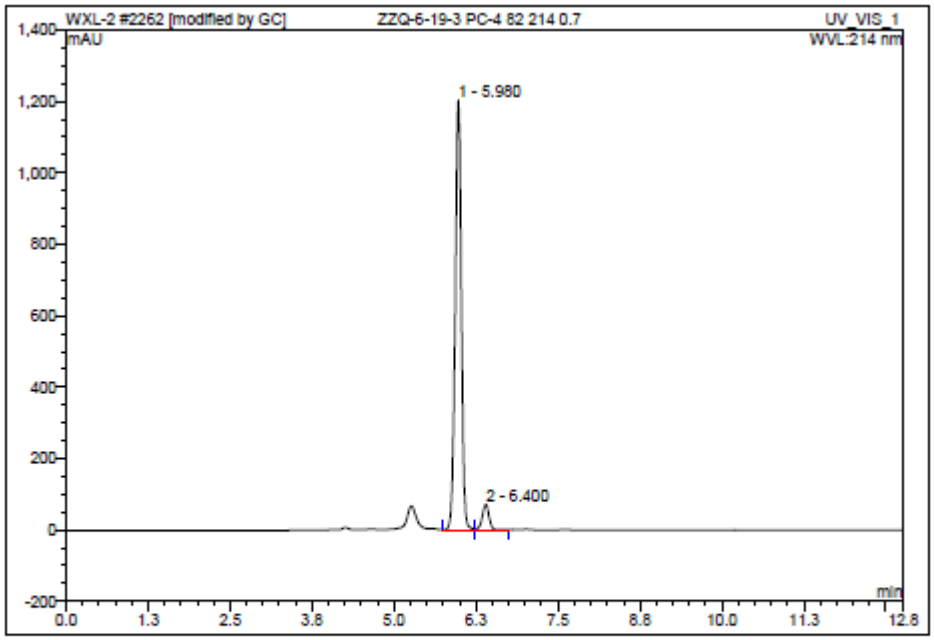
Signal: DAD1 A, Sig=230,16 Ref=360,100

RT [min]	Type	Width [min]	Area	Height	Area%
9.481	BB	0.1862	11376.4307	936.7764	88.1561
10.165	BV	0.1837	1528.4406	127.1735	11.8439
		Sum	12904.8712		

6o

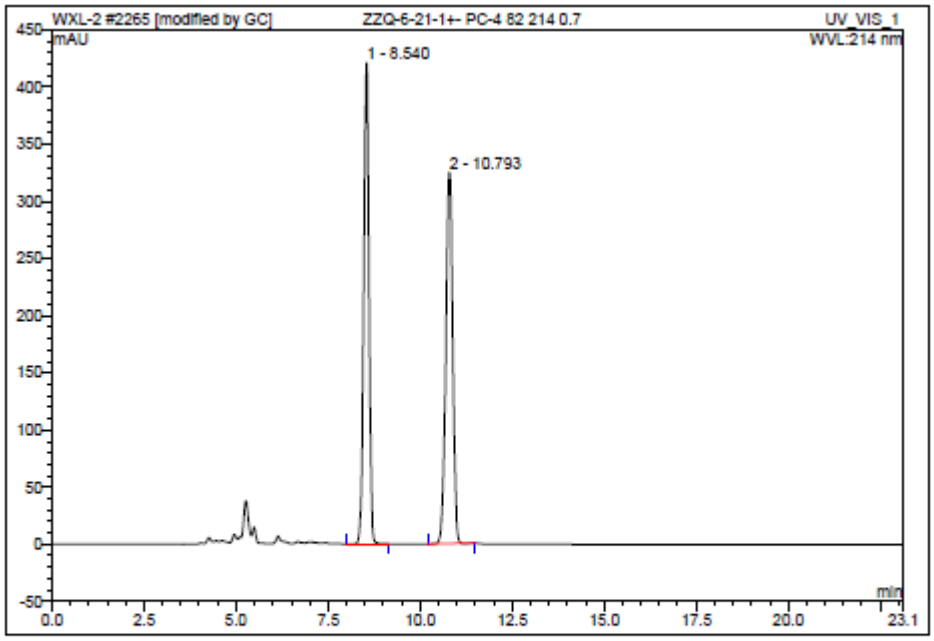


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.97	n.a.	549.255	58.575	50.08	n.a.	BMb*
2	6.38	n.a.	503.524	58.392	49.92	n.a.	bMB*
Total:			1052.779	116.967	100.00	0.000	

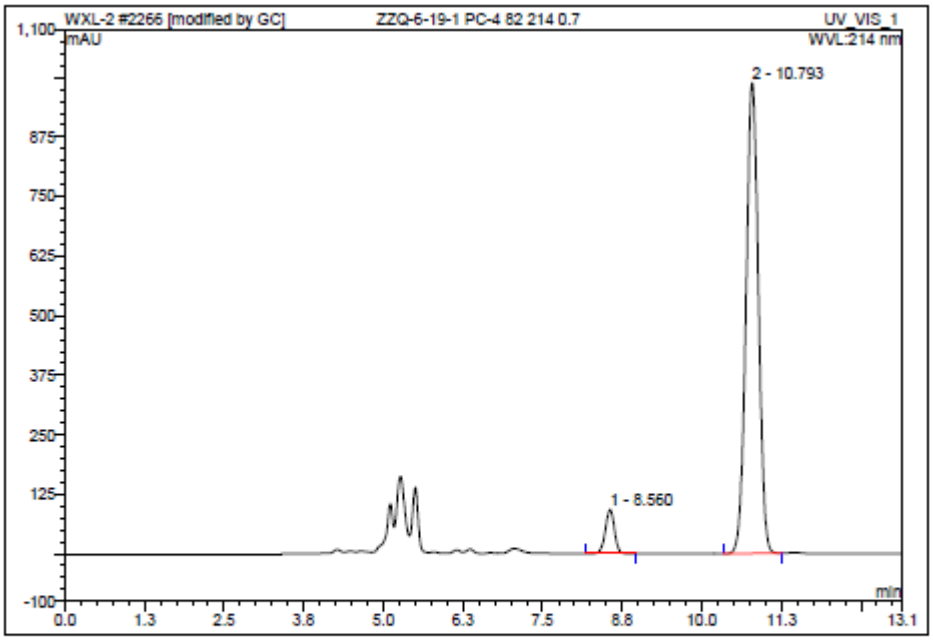


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5.98	n.a.	1202.476	130.377	94.05	n.a.	BM *
2	6.40	n.a.	70.629	8.241	5.95	n.a.	MB*
Total:			1273.104	138.618	100.00	0.000	

6p

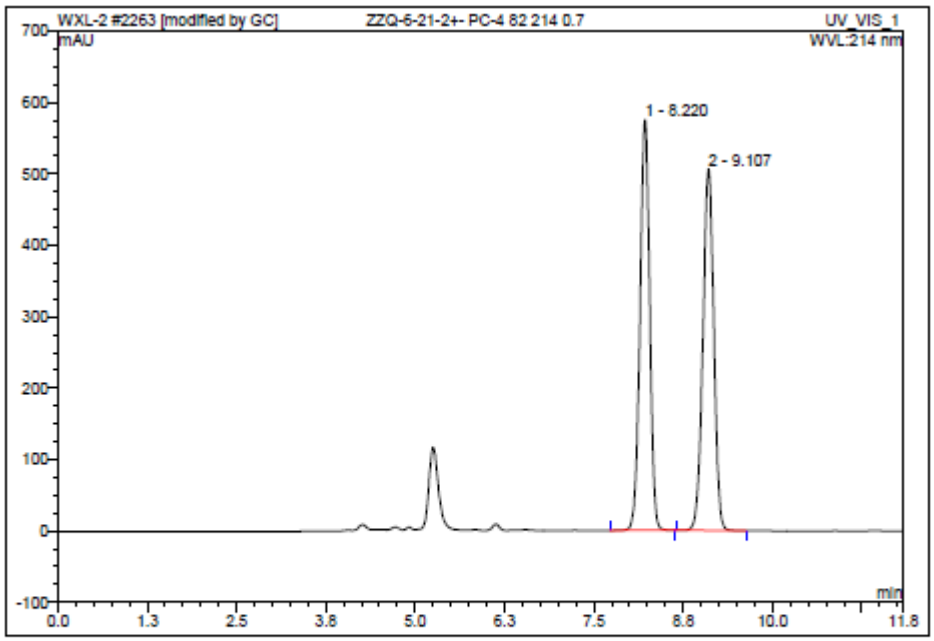


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.54	n.a.	420.760	70.014	49.81	n.a.	BMB*
2	10.79	n.a.	324.880	70.561	50.19	n.a.	BMB*
Total:			745.640	140.575	100.00	0.000	

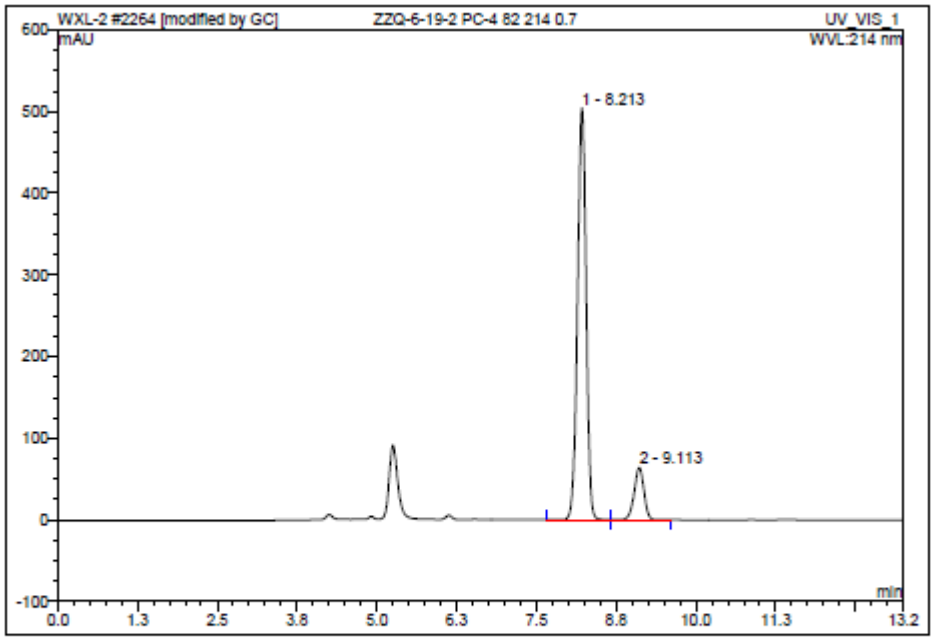


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.56	n.a.	92.356	15.245	6.42	n.a.	BMB*
2	10.79	n.a.	988.128	222.331	93.58	n.a.	BMB*
Total:			1080.483	237.576	100.00	0.000	

6q

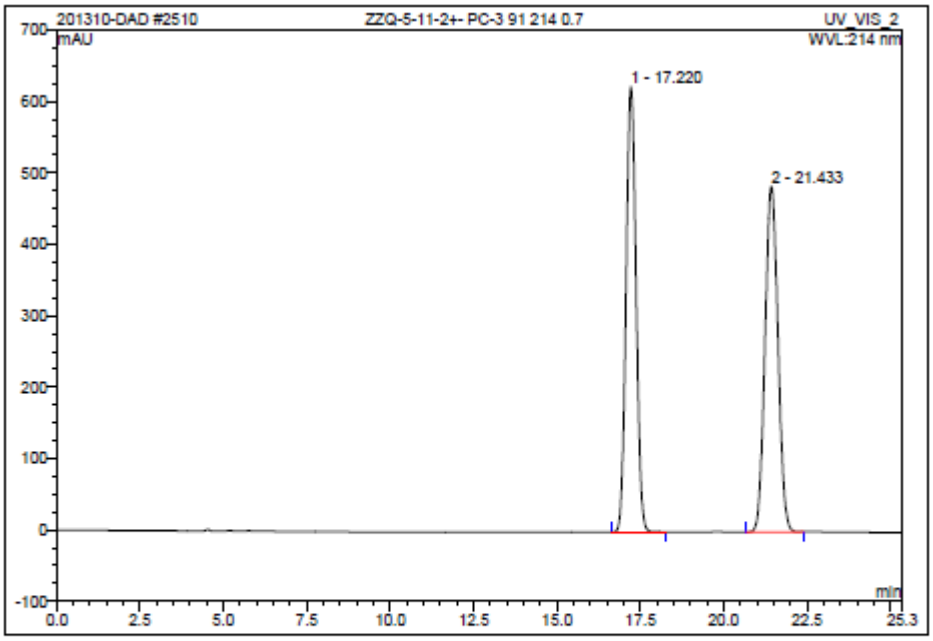


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.22	n.a.	574.314	90.324	50.17	n.a.	BMB*
2	9.11	n.a.	505.875	89.711	49.83	n.a.	BMB*
Total:			1080.189	180.036	100.00	0.000	

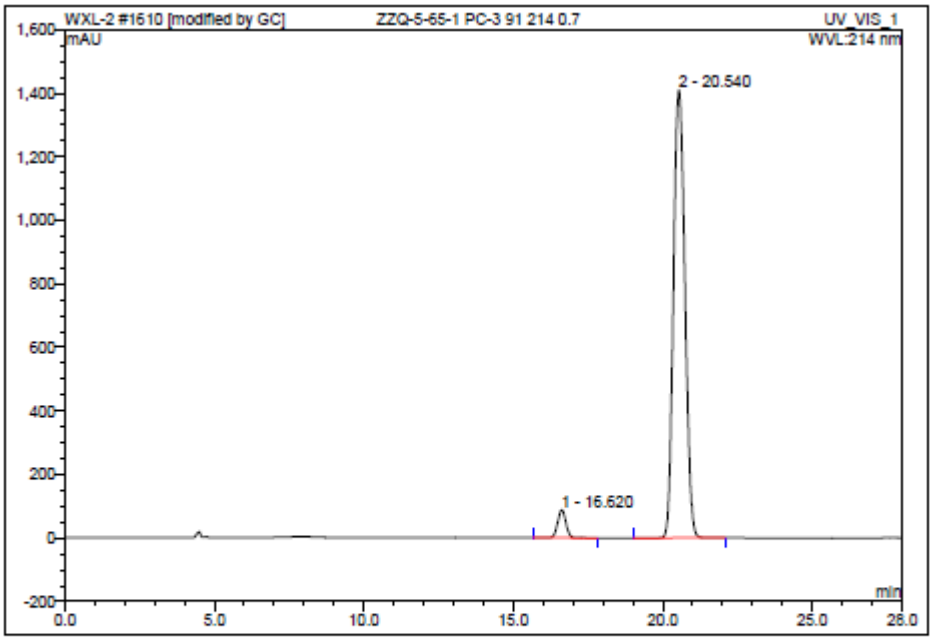


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.21	n.a.	504.288	78.948	87.52	n.a.	BMb*
2	9.11	n.a.	63.962	11.253	12.48	n.a.	bMB*
Total:			568.250	90.202	100.00	0.000	

6r

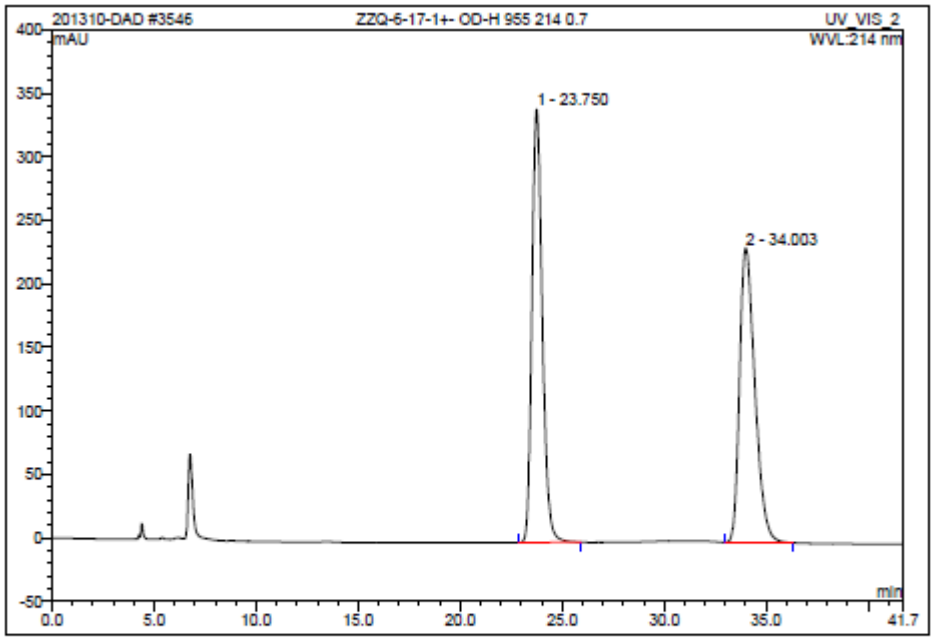


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.22	n.a.	623.245	216.114	49.85	n.a.	BMB
2	21.43	n.a.	483.199	217.448	50.15	n.a.	BMB
Total:			1106.444	433.562	100.00	0.000	

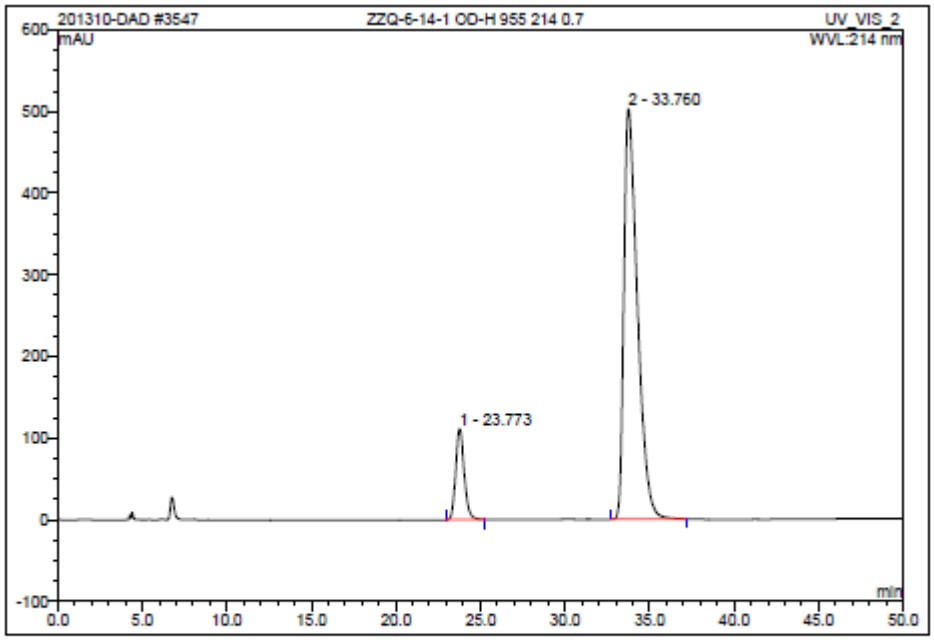


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.62	n.a.	87.347	27.891	4.27	n.a.	BMB*
2	20.54	n.a.	1409.858	624.893	95.73	n.a.	BMB*
Total:			1497.204	652.783	100.00	0.000	

6s

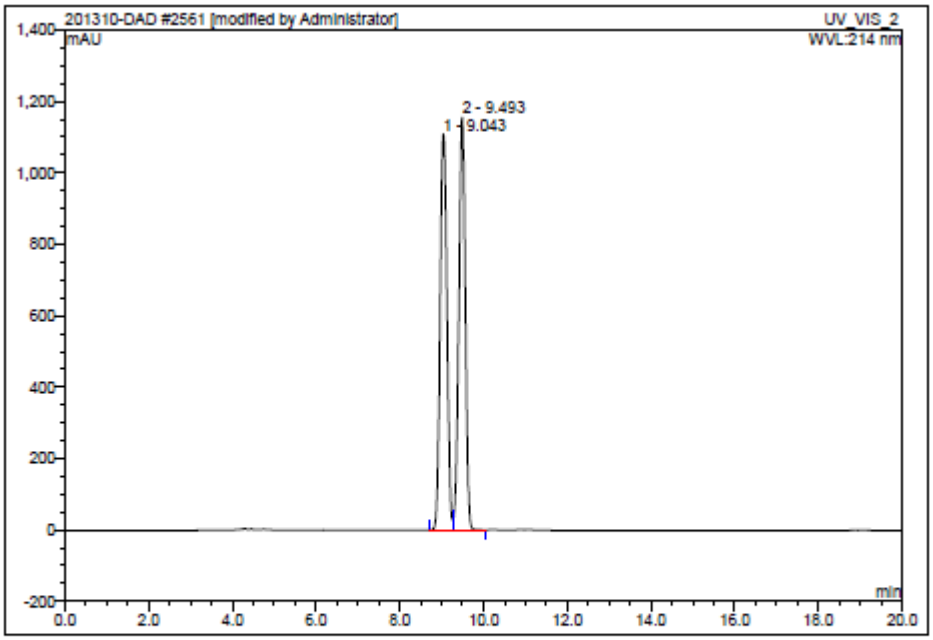


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	23.75	n.a.	341.045	201.277	49.92	n.a.	BMB
2	34.00	n.a.	231.802	201.916	50.08	n.a.	BMB
Total:			572.847	403.193	100.00	0.000	

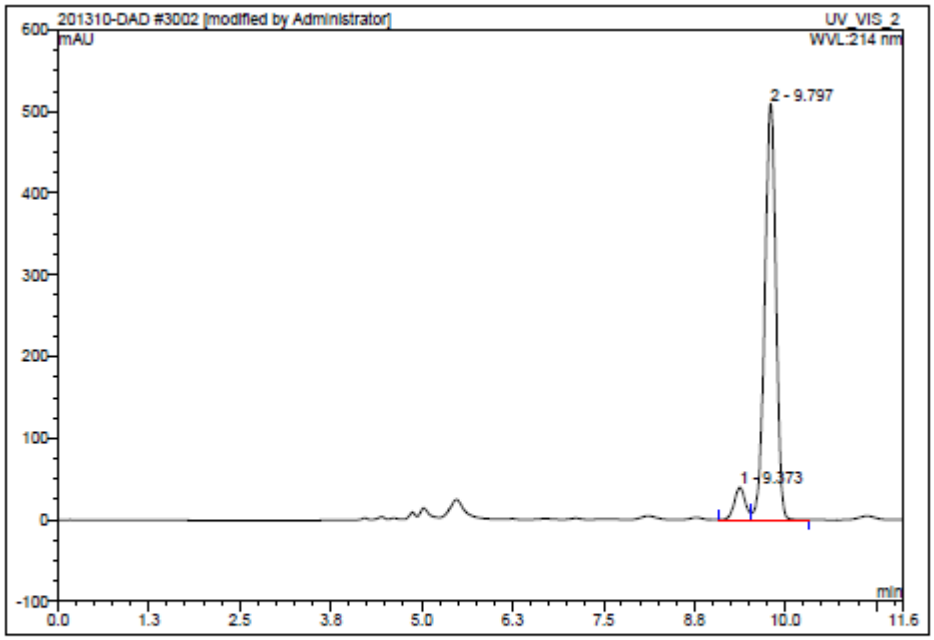


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	23.77	n.a.	111.086	65.063	12.26	n.a.	BMB
2	33.76	n.a.	502.464	465.758	87.74	n.a.	BMB
Total:			613.550	530.821	100.00	0.000	

6t

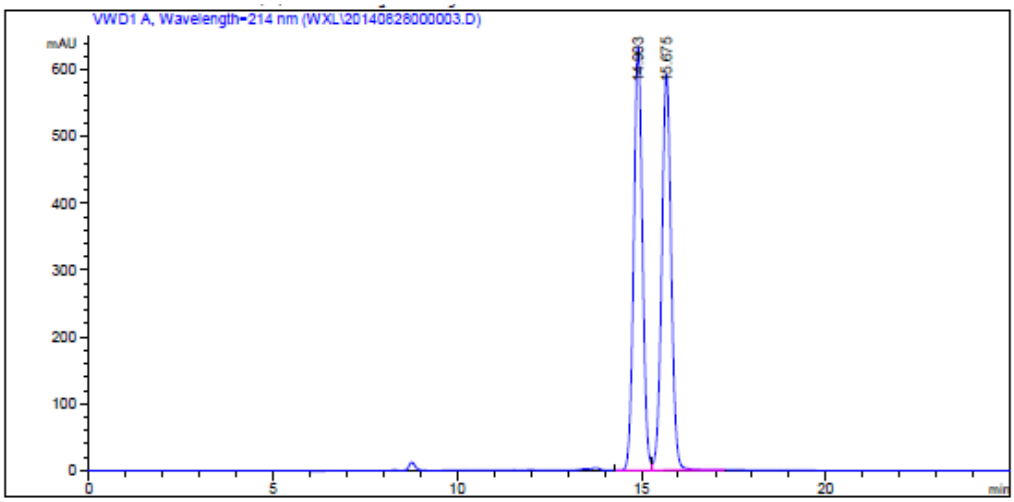


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.04	n.a.	1107.950	208.864	49.99	n.a.	BM *
2	9.49	n.a.	1154.667	208.927	50.01	n.a.	MB*
Total:			2262.616	417.791	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.37	n.a.	39.494	6.952	7.11	n.a.	BM
2	9.80	n.a.	509.244	90.877	92.89	n.a.	MB
Total:			548.738	97.829	100.00	0.000	

6u



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Area Percent Report

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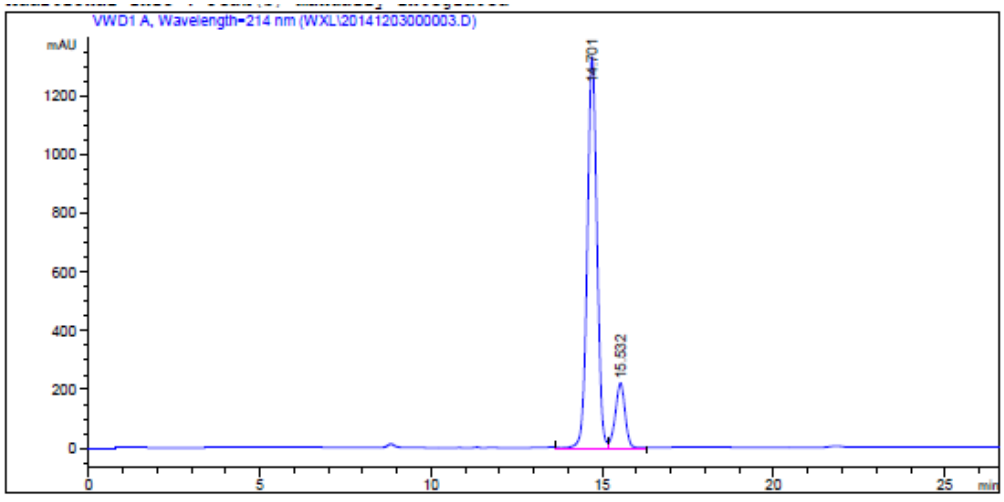
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.903	BV	0.2517	1.03748e4	634.79932	49.5993
2	15.675	VB	0.2735	1.05424e4	592.76959	50.4007
Totals :				2.09173e4	1227.56891	



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Area Percent Report

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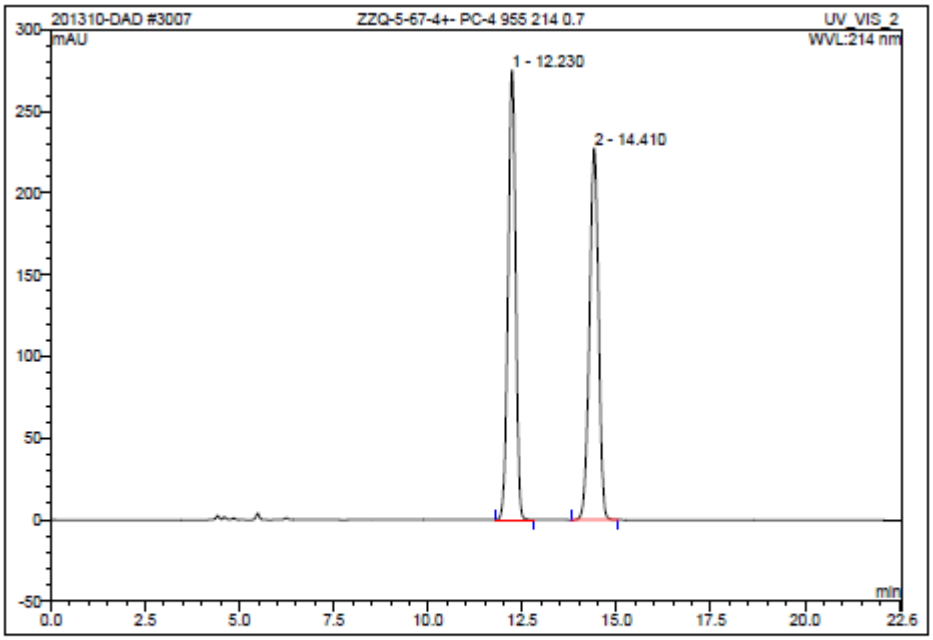
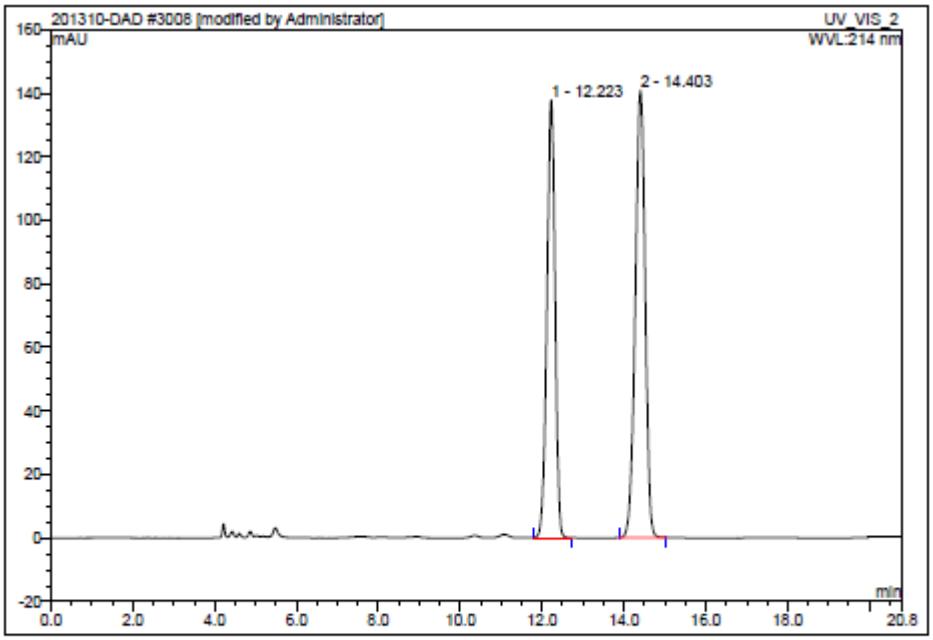
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.701	MF	0.3270	2.61334e4	1331.85266	85.5312
2	15.532	FM	0.3336	4420.82324	220.88565	14.4688
Totals :				3.05542e4	1552.73831	

6v

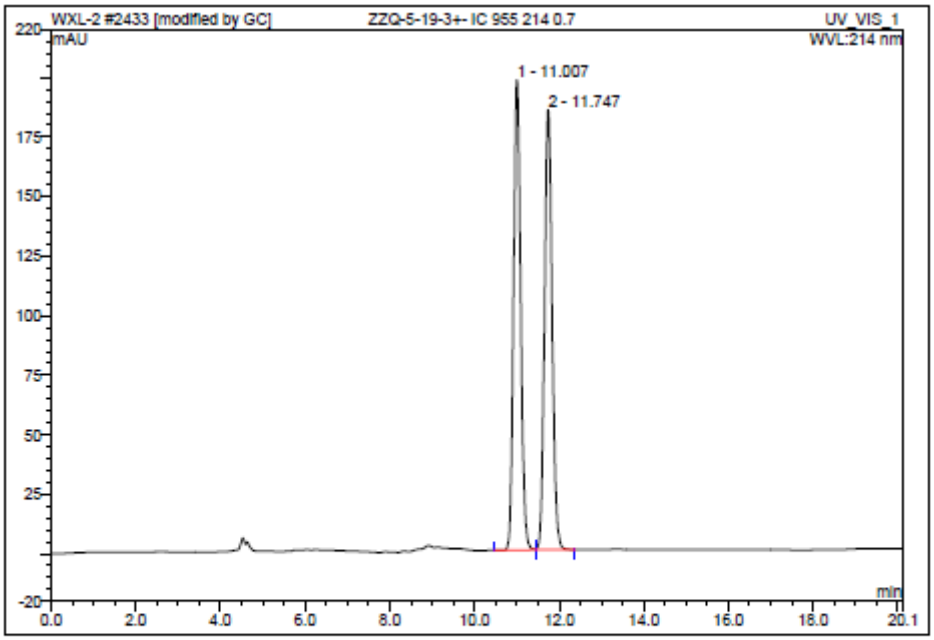


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.23	n.a.	275.223	63.764	49.99	n.a.	BMB
2	14.41	n.a.	227.511	63.777	50.01	n.a.	BMB
Total:			502.733	127.542	100.00	0.000	

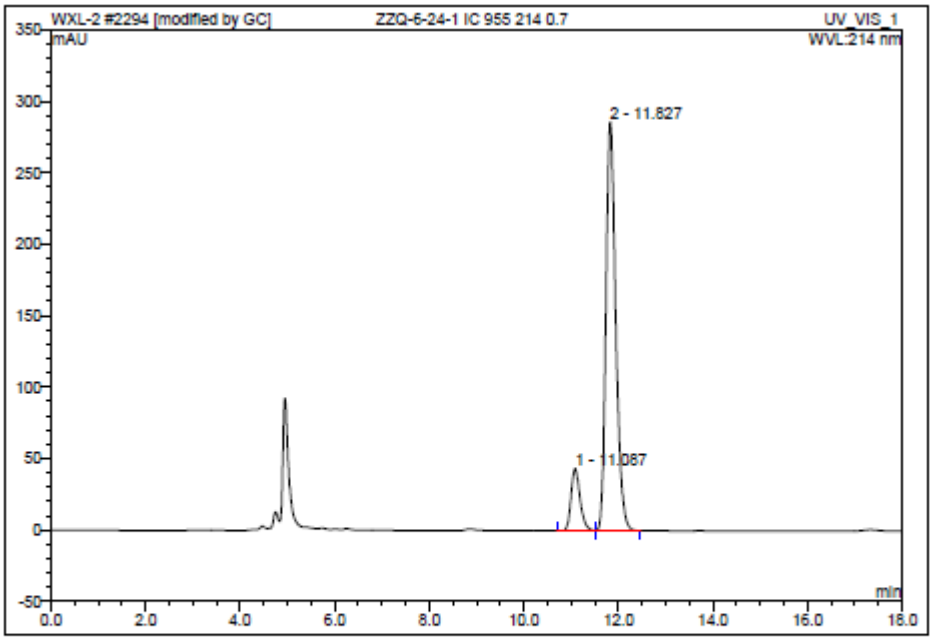


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.22	n.a.	137.808	31.854	44.74	n.a.	BMB
2	14.40	n.a.	140.789	39.341	55.26	n.a.	BMB
Total:			278.597	71.195	100.00	0.000	

6w

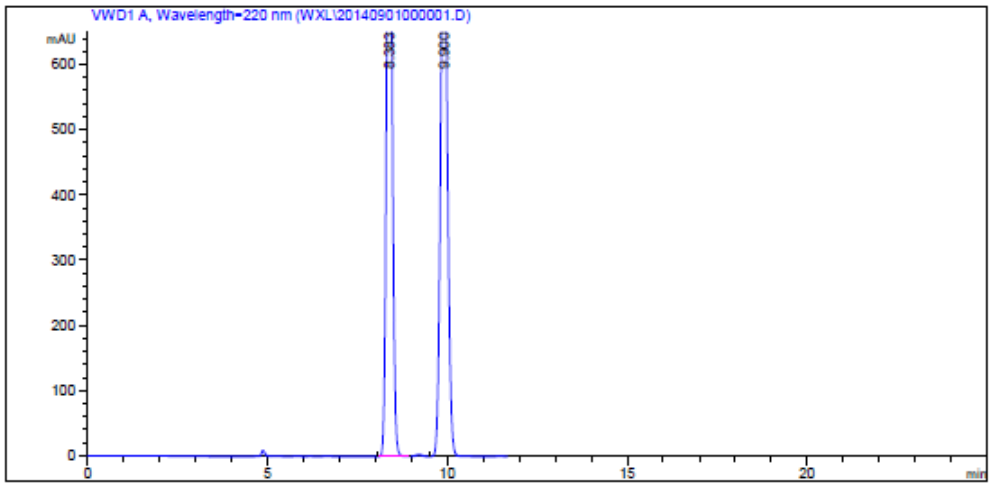


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.01	n.a.	197.454	38.408	49.93	n.a.	BM *
2	11.75	n.a.	184.675	38.518	50.07	n.a.	MB*
Total:			382.129	76.927	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.09	n.a.	43.509	9.537	12.22	n.a.	BMb*
2	11.83	n.a.	286.027	68.539	87.78	n.a.	bMB*
Total:			329.537	78.076	100.00	0.000	

6x



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Area Percent Report

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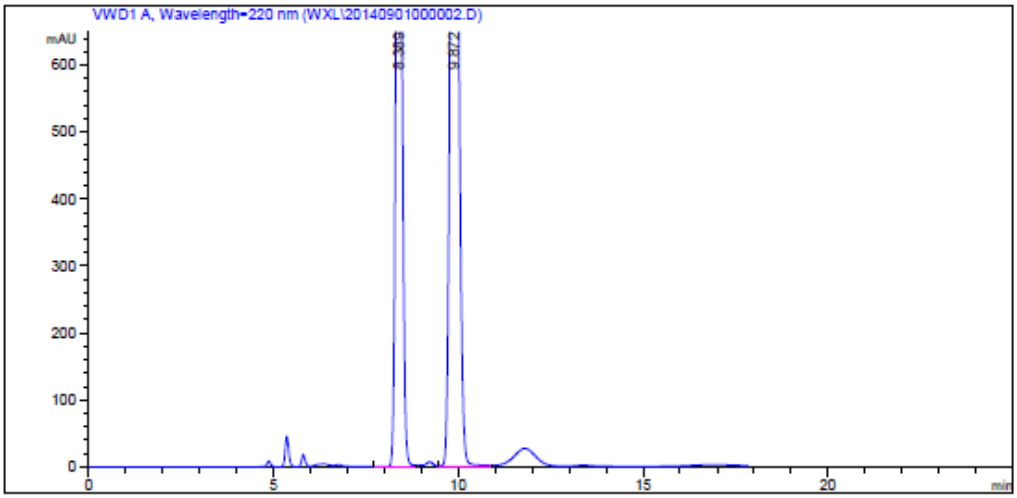
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.383	BV	0.1584	1.17899e4	1152.44873	49.7920
2	9.900	VV	0.1942	1.18884e4	942.44446	50.2080

Totals : 2.36783e4 2094.89319



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Area Percent Report

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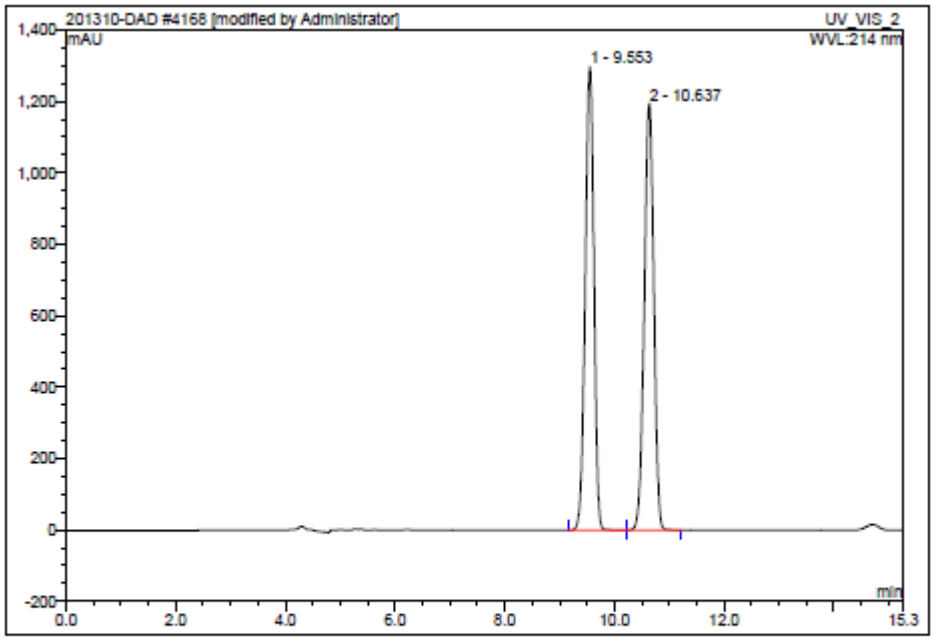
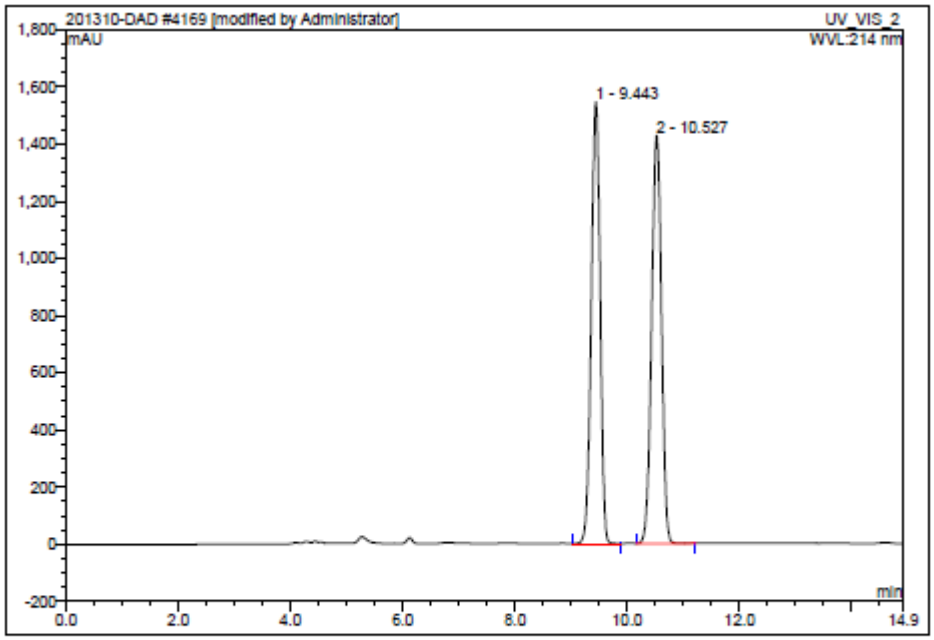
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.389	BV	0.1594	1.48449e4	1438.25928	37.8181
2	9.872	VV	0.2040	2.44086e4	1836.74048	62.1819

Totals : 3.92535e4 3274.99976

6y



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.55	n.a.	1296.085	238.518	49.80	n.a.	BM *
2	10.64	n.a.	1193.930	240.432	50.20	n.a.	M *
Total:			2490.016	478.950	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9.44	n.a.	1545.676	283.797	49.42	n.a.	BM *
2	10.53	n.a.	1427.641	290.510	50.58	n.a.	BMB
Total:			2973.317	574.307	100.00	0.000	

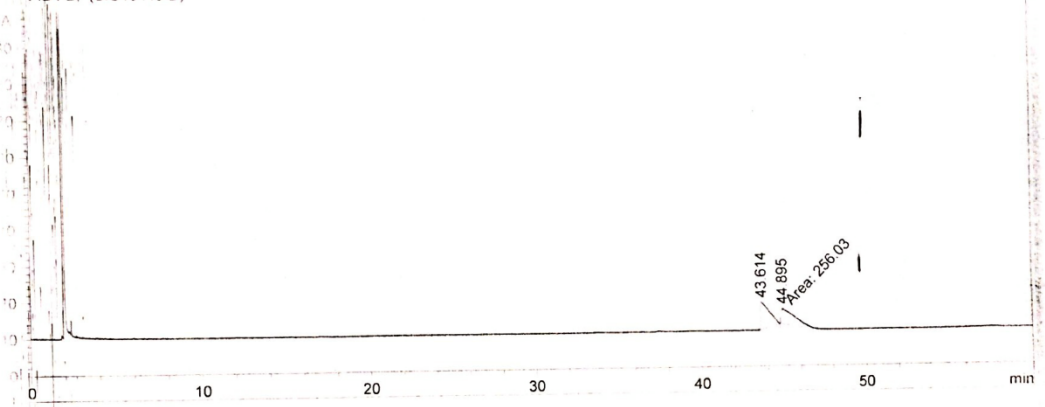
6z

C:\HPCHEM\1\DATA\SIG10419.D Sample Name: 22q-6-94-1(+/-)

on Date : 2/4/2015 4:17:00 AM
Name : 22q-6-94-1(+/-) Location : Vial 1
erator : LXL Inj : 1
Inj Volume : Manually

thod : C:\HPCHEM\1\METHODS\DEF_GC1.M
anged : 2/4/2015 5:20:14 AM by LXL
(modified after loading)
is Method : C:\HPCHEM\1\METHODS\DEF_GC1.M
anged : 2/4/2015 7:00:11 AM by LXL
(modified after loading)

FID1 B, (SIG10419 D)



Area Percent Report

By : Signal
lier : 1.0000
n : 1.0000
tiplier & Dilution Factor with ISTDs

1: FID1 B,

tTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
3.614	BB	0.4456	286.82013	7.86291	52.83593
4.895	MM	0.9496	256.03043	4.49357	47.16407
			542.85056	12.35648	

s obtained with enhanced integrator!

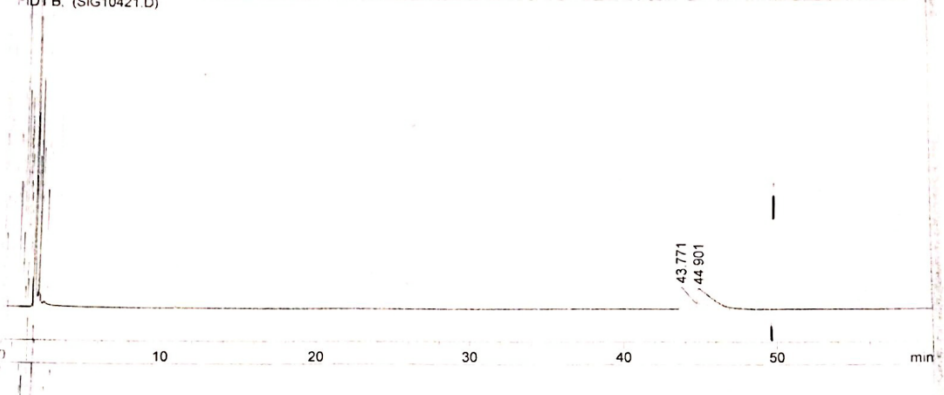
*** End of Report ***

:\HPCHEM\1\DATA\SIG10421.D Sample Name: 22q-6-93-1

on Date : 2/4/2015 3:24:41 PM
lame : 22q-6-93-1 Location : Vial 1
rator : LXL Inj : 1
Inj Volume : Manually

thod : C:\HPCHEM\1\METHODS\DEF_GC1.M
nged : 2/4/2015 5:20:14 AM by LXL
(modified after loading)
Method : C:\HPCHEM\1\METHODS\DEF_GC1.M
nged : 2/4/2015 4:54:41 PM by LXL
(modified after loading)

FID1 B, (SIG10421.D)



Area Percent Report

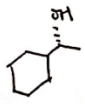
ed by : Signal
ip ier : 1.0000
n : 1.0000
tiplier & Dilution Factor with ISTDs

nal 1: FID1 B,

k	R Time [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	43.771	BB	0.3996	211.07878	6.55679	45.25019
2	44.901	BB	0.6270	255.39168	4.78283	54.74981
als :				466.47046	11.33962	

esul s obtained with enhanced integrator!

*** End of Report ***



9.49%

Pri 1 2/4/2015 4:54:49 PM LXL Page 1 of 1