Supplementary Information (SI) for Organic Chemistry Frontiers.

Supporting Information

Chiral phosphoric acid catalyzed asymmetric synthesis of C–N axially chiral uracils with antitumor activity through kinetic resolution strategy

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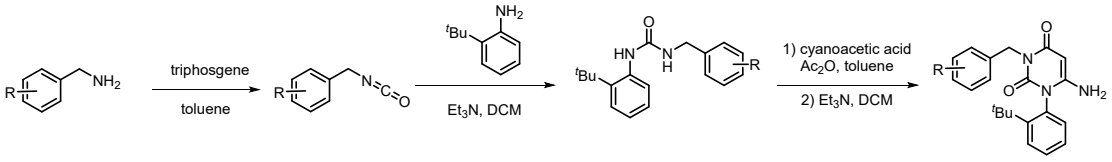
1. General information

Commercially available materials were purchased from Bidepharm, Heowns and Adamas used as received unless otherwise stated. Chiral phosphoric acids were purchased from DAICEL. Anhydrous dichloromethane was purchased from J&K Scientific. ^{1}H, ^{13}C and ^{19}F NMR were recorded on Bruker Avance 400 spectrometer or 600 spectrometer, chemical shifts (δ) were reported in ppm, tetramethylsilane (TMS, δ 0.00 ppm) or chloroform-*d* (δ 7.26 ppm) served as the internal standard for ^{1}H NMR, and chloroform-*d* (δ 77.06 ppm) served as the internal standard for ^{13}C NMR. The following abbreviations were used to designate the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. HPLC analysis was performed using chiralpak columns purchased. Mass spectra were obtained using electrospray ionization (ESI) mass spectrometer.

2. General synthesis of Starting Materials

General synthesis of uracils[1]

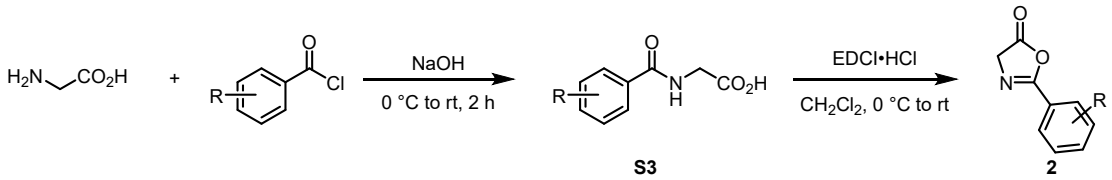


To a solution of benzylamine (1.0 equiv.) in toluene (20 mL) was added triphosgene (0.5 equiv., dissolved in 5 mL toluene) at rt. After stirring at 120 °C for 4 h, The solvent was subsequently removed in vacuo to afforded the desired product **S1** as yellow oil without purification.

Dissolve **S1** (1.1 equiv.) in 20 mL of dichloromethane then added 1.0 equiv. of 2-*tert*-butylaniline and 1.2 equiv. of Et_3N. After stirring at rt for 4 h, added a large amount of petroleum ether and recrystallized to obtain **S2** as a solid.

Cyanoacetic acid (2.5 equiv.) and **S2** (1.0 equiv.) was suspended with toluene (20 mL) and the mixture was warmed to 84 °C. Ac_2O (2 mL) was added and the mixture was stirred at 84 °C for 4 h. After cooled to rt, the mixture was washed three times with water, extracted three times with EtOAc. The organic layers were combined, dried with Na_2SO_4 and concentrated in vacuo. The obtained oil was dissolved in 15 mL CH_2Cl_2, then added 1 mL Et_3N and stirred overnight at rt. After monitored by TLC, the solvent was subsequently removed in vacuo, the obtained oil was purified by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 2:1-1:2) to afford racemic uracil **1** as solid.

General synthesis of azlactones[2]

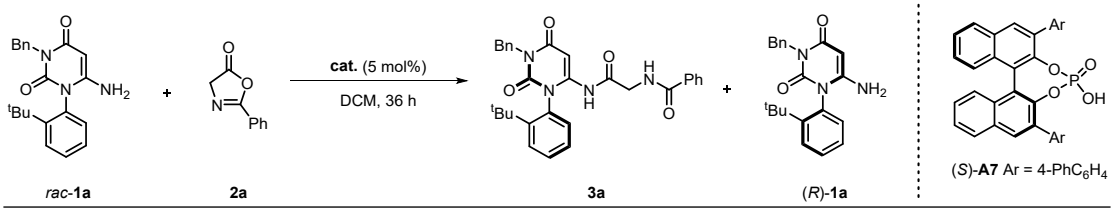


Into a round bottomed flask, the glycine (1.0 equiv.), NaOH (2.0 equiv.) were dissolved in H_2O (1.0 M). Then, the mixture was cooled to 0 °C and the acyl chloride was added dropwise. The reaction was stirred at room temperature for 2 h. Then the reaction was washed with EtOAc twice, separated, and adjusted the pH of aqueous phase to 2~3 with 3 M HCl. The precipitation was filtered and dried to obtain **S3**. The products were used for next step without purification.

To a round bottom flask was charged with **S3** (1.0 equiv.) and CH_2Cl_2 (0.2 M), the mixture was stirred and cooled to 0 °C. Then EDCI•HCl (1.1 equiv.) was added portion. The reaction was stirred at rt for 2 h. The reaction mixture was quenched with water, separated, the organic phase was washed with water and brine, then dried over Na_2SO_4 and concentrated under reduced pressure. The crude products were purified by flash chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 5:1 or dichloromethane/ ethyl acetate = 10:1) to afford azlactone **2** as solid.

3.Optimization of reaction conditions

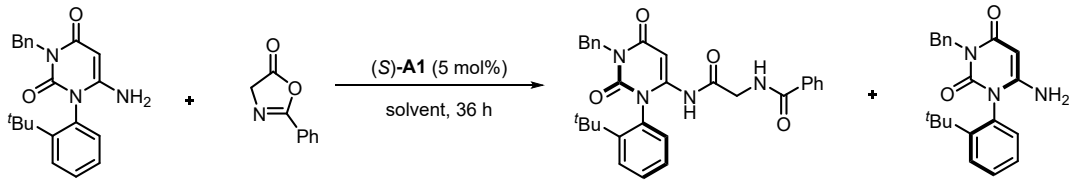
Table S1: Other CPA investigation.[a]



entry	cat.	3a		(*R*)-1a		*s*
		yield (%)	er	yield (%)	er	
1	(*S*)-**A7**	13	57:43	80	51:49	1

[a]The reactions were conducted with *rac*-**1a** (0.1 mmol), **2a** (0.06 mmol, 0.6 equiv.), **cat.** (5 mol %) in dry CH_2Cl_2 (1.0 mL) at room temperature for 36 h. Isolated yields. The er values were determined by chiral HPLC analysis., the selectivity factor was calculated as $s = \ln[(1-C)(1-ee_{sub})]/\ln[(1-C)(1+ee_{sub})]$, $C = ee_{sub}/(ee_{pro}+ee_{sub})$.

Table S2: Other solvents investigation.[a]

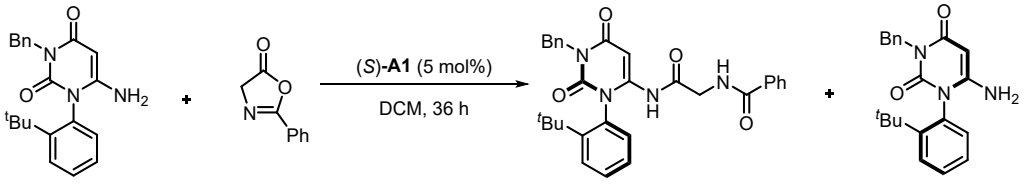


rac-**1a** **2a** **3a** (*R*)-**1a**

entry	solvent	**3a**		(*R*)-**1a**		*s*
		yield (%)	er	yield (%)	er	
1	MeCN	8	95:5	90	51:49	19
2	Et_2O	-	-	-	-	-

[a]The reactions were conducted with *rac*-**1a** (0.1 mmol), **2a** (0.06 mmol, 0.6 equiv.), (*S*)-**A1** (5 mol %) in solvent (1.0 mL) at room temperature for 36 h. Isolated yields. The er values were determined by chiral HPLC analysis., the selectivity factor was calculated as $s = \ln[(1-C)(1-ee_{sub})]/\ln[(1-C)(1+ee_{sub})]$, $C = ee_{sub}/(ee_{pro}+ee_{sub})$.

Table S3: Other material ratios investigation.[a]

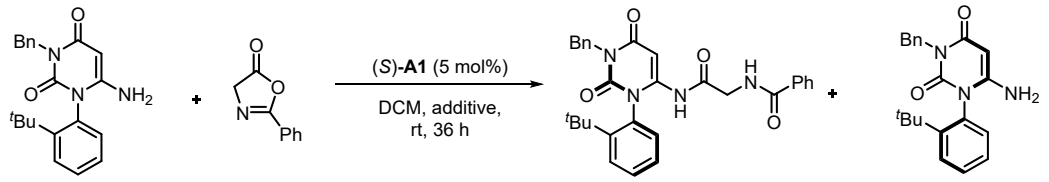


rac-**1a** **2a** **3a** (*R*)-**1a**

entry	equiv. of **2a**	**3a**		(*R*)-**1a**		*s*
		yield (%)	er	yield (%)	er	
1	0.75	55	90:10	43	>99.5:0.5	46
2	1.0	55	82:18	40	>99.5:0.5	22

[a]The reactions were conducted with *rac*-**1a** (0.1 mmol), **2a**, (*S*)-**A1** (5 mol %) in CH_2Cl_2 (1.0 mL) at room temperature for 36 h. Isolated yields. The er values were determined by chiral HPLC analysis., the selectivity factor was calculated as $s = \ln[(1-C)(1-ee_{sub})]/\ln[(1-C)(1+ee_{sub})]$, $C = ee_{sub}/(ee_{pro}+ee_{sub})$.

Table S4: Other additives investigation.[a]

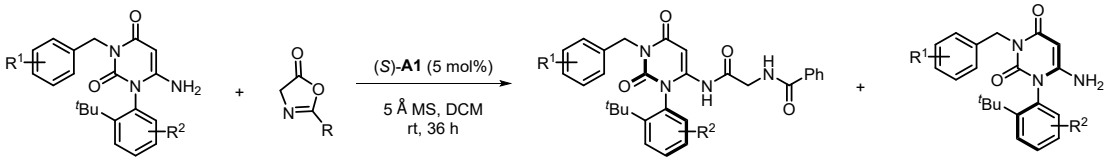


rac-**1a** **2a** **3a** (*R*)-**1a**

entry	additive	**3a**		(*R*)-**1a**		*s*
		yield (%)	er	yield (%)	er	
1	4 Å MS	48	94:6	45	99:1	71
2	$MgSO_4$	44	93:7	47	98:2	52

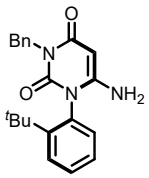
[a]The reactions were conducted with *rac*-**1a** (0.1 mmol), **2a** (0.05 equiv.), (*S*)-**A1** (5 mol %) and additive (50.0 mg) in CH_2Cl_2 (1.0 mL) at room temperature for 36 h. Isolated yields. The er values were determined by chiral HPLC analysis., the selectivity factor was calculated as $s = \ln[(1-C)(1-ee_{sub})]/\ln[(1-C)(1+ee_{sub})]$, $C = ee_{sub}/(ee_{pro}+ee_{sub})$.

4.General Procedure for the kinetic resolution.

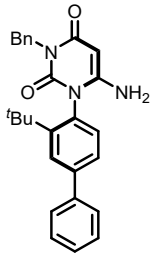


A 5 mL vial containing a magnetic stir bar was charged with *rac*-**1** (0.1 mmol, 1.0 equiv.), **2** (0.05 mmol, 0.5 equiv.), (*S*)-**A1** (0.005 mmol, 5 mol%) and 5 Å MS (50.0 mg). Subsequently, dry CH_2Cl_2 (1 mL) was added. After stirring at room temperature for 36 h, the reaction mixture was purified directly by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 2:1 to obtain (*S*)-**3** and petroleum ether/ethyl acetate = 1:2 to obtain (*R*)-**1**.

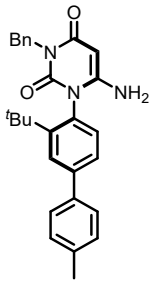
5. Characterization data of (*R*)-1



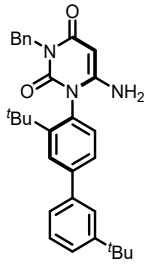
(*R*)-6-amino-3-benzyl-1-(2-(*tert*-butyl)phenyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1a**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 17.12 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-d) δ 7.61 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.45-7.40 (m, 1H), 7.39-7.35 (m, 2H), 7.30 (td, *J* = 7.6, 1.5 Hz, 1H), 7.19 (t, *J* = 7.2 Hz, 2H), 7.15-7.10 (m, 1H), 7.00 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.11 (s, 1H), 5.05 (d, *J* = 20.0 Hz, 2H), 4.72 (s, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.3, 154.1, 151.8, 148.6, 137.5, 131.2, 130.8, 130.42, 130.38, 128.7, 128.1, 128.0, 127.2, 44.0, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{21}H_{24}N_3O_2$ $[M+H]^+$: 350.1863, found: 350.1861; $[\alpha]_D^{25}$ = -57.4 (c = 0.5, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.0 min (minor), 5.7 min (major), 99:1 *er*.



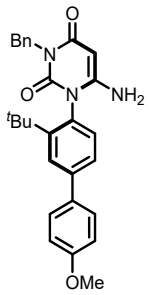
(*R*)-6-amino-3-benzyl-1-(3-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)pyrimidine-2,4(*1H*,*3H*)-dione (**1b**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 18.30 mg, 43% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 (d, J = 2.1 Hz, 1H), 7.64-7.59 (m, 2H), 7.50 (dd, J = 8.1, 2.1 Hz, 1H), 7.40 (dd, J = 8.4, 6.9 Hz, 2H), 7.34- 7.28 (m, 1H), 7.18 (d, J = 3.8 Hz, 4H), 7.14-7.11 (m, 1H), 7.08 (d, J = 8.1 Hz, 1H), 6.25 (s, 2H), 4.83 (d, J = 14.8 Hz, 2H), 4.79 (s, 1H), 1.15 (s, 9H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 161.6, 155.0, 151.7, 148.1, 141.3, 139.7, 138.1, 132.2, 130.9, 129.1, 128.14, 128.08, 127.8, 127.6, 127.0, 126.9, 125.9, 74.7, 42.9, 35.9, 31.1. HRMS (ESI): m/z calcd for $C_{27}H_{28}N_3O_2$ $[M+H]^+$: 426.2176, found: 426.2171; $[\alpha]_D^{25}$ = -4.6 (c = 0.125, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.3 min (minor), 5.0 min (major), 95:5 *er*.



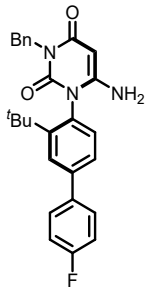
(*R*)-6-amino-3-benzyl-1-(3-(*tert*-butyl)-4'-methyl-[1,1'-biphenyl]-4-yl)pyrimidine-2,4(*1H*,*3H*)-dione (**1c**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 19.34 mg, 44% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, J = 2.1 Hz, 1H), 7.51-7.42 (m, 5H), 7.30-7.17 (m, 5H), 7.08 (d, J = 8.1 Hz, 1H), 5.15 (d, J = 2.4 Hz, 1H), 5.14-5.01 (m, 2H), 4.52 (s, 2H), 2.41 (s, 3H), 1.26 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.7, 151.8, 148.8, 143.4, 138.0, 137.6, 137.3, 131.5, 129.7, 129.2, 129.0, 128.2, 127.3, 127.2, 126.6, 100.0, 77.7, 44.2, 36.4, 31.5, 21.2; HRMS (ESI): m/z calcd for $C_{28}H_{30}N_3O_2$ $[M+H]^+$: 440.2333 found: 440.2333; $[\alpha]_D^{25}$ = 3.2 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.2 min (minor), 5.8 min (major), 96:4 *er*.



(*R*)-6-amino-3-benzyl-1-(3,3'-di-*tert*-butyl-[1,1'-biphenyl]-4-yl)pyrimidine-2,4(*1H*,*3H*)-dione (**1d**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 22.64 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 2.1 Hz, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.50 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.45-7.34 (m, 5H), 7.23 (dd, *J* = 13.7, 6.9 Hz, 2H), 7.17 (d, *J* = 7.1 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 5.17 (s, 1H), 5.13-5.00 (m, 2H), 4.75 (s, 2H), 1.38 (s, 9H), 1.27 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.4, 154.0, 151.9, 151.8, 148.7, 144.1, 140.1, 137.6, 131.5, 129.7, 129.6, 128.9, 128.7, 128.1, 127.2, 127.0, 125.0, 124.5, 44.1, 36.4, 34.8, 31.5, 31.4. HRMS (ESI): m/z calcd for $C_{31}H_{36}N_3O_2$ $[M+H]^+$: 482.2802 found: 482.2801; $[\alpha]_D^{25}$ = 9.0 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 3.8 min (minor), 6.5 min (major), 99:1 *er*.

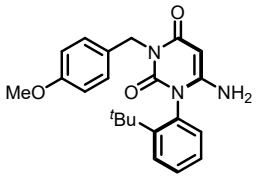


(*R*)-6-amino-3-benzyl-1-(3-(*tert*-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)pyrimidine-2,4(*1H*,*3H*)-dione (**1e**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 22.32 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 2.1 Hz, 1H), 7.52-7.47 (m, 2H), 7.44 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 2H), 7.14-7.07 (m, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 7.01-6.91 (m, 2H), 5.15 (s, 1H), 5.14-4.96 (m, 2H), 4.85 (d, *J* = 8.0 Hz, 2H), 3.84 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.3, 159.6, 154.2, 151.9, 148.6, 142.8, 137.6, 132.6, 131.5, 129.2, 128.8, 128.7, 128.3, 128.1, 127.1, 126.3, 114.4, 77.2, 55.4, 44.1, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{28}H_{30}N_3O_3$ $[M+H]^+$: 456.2282 found: 456.2280; $[\alpha]_D^{25}$ = -7.4 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.2 min (minor), 5.8 min (major), 96:4 *er*.

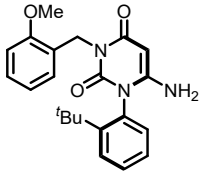


(*R*)-6-amino-3-benzyl-1-(3-(*tert*-butyl)-4'-fluoro-[1,1'-biphenyl]-4-yl)pyrimidine-2,4(*1H*,*3H*)-dione (**1f**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 21.73 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 2.1 Hz, 1H), 7.55-7.48 (m, 2H), 7.45 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.43-7.37 (m, 2H), 7.23-7.18 (m, 2H), 7.17-

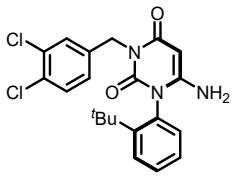
7.14 (m, 2H), 7.12 (s, 1H), 7.08 (d, *J* = 8.1 Hz, 1H), 5.17 (s, 1H), 5.07 (d, *J* = 17.9 Hz, 2H), 4.80 (s, 2H), 1.26 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) *δ* 164.1, 163.3, 161.6, 152.9 (d, *J* = 219.2 Hz), 149.0, 142.4, 137.5, 136.3 (d, *J* = 3.4 Hz), 131.7, 129.9, 129.2, 128.9 (d, *J* = 2.5 Hz), 128.1, 127.2, 126.7, 115.9 (d, *J* = 21.5 Hz), 44.1, 36.4, 31.5; ^{19}F NMR (376 MHz, Chloroform-*d*) *δ* -114.37; HRMS (ESI): m/z calcd for $C_{27}H_{27}FN_3O_2$ $[M+H]^+$: 444.2082 found: 444.2080; $[\alpha]_D^{25}$ = -11.7 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 84:16 hexane/isopropanol, 1 mL/min, t_R = 8.4 min (minor), 11.7 min (major), 96:4 *er*.



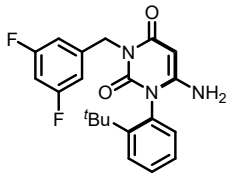
(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(4-methoxybenzyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1g**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 18.59 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.62 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.48-7.36 (m, 3H), 7.31 (d, *J* = 1.4 Hz, 1H), 7.03 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.86-6.66 (m, 2H), 5.10 (s, 1H), 5.01 (d, *J* = 11.7 Hz, 2H), 4.43 (s, 2H), 3.76 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) *δ* 163.2, 158.8, 153.5, 151.8, 148.7, 131.2, 130.8, 130.6, 130.5, 130.4, 129.8, 128.0, 113.5, 77.7, 55.2, 43.5, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{22}H_{26}N_3O_3$ $[M+H]^+$: 380.1969 found: 380.1971; $[\alpha]_D^{25}$ = -52.6 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.2 min (minor), 10.0 min (major), 98:2 *er*.



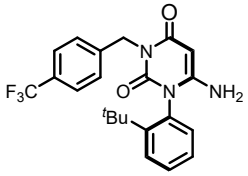
(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(2-methoxybenzyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1h**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 18.59 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.59 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.34-7.22 (m, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 2H), 6.81-6.67 (m, 2H), 5.15 (s, 1H), 5.14-5.00 (m, 2H), 4.72 (s, 2H), 3.76 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) *δ* 156.9, 154.3, 151.7, 148.6, 131.3, 130.9, 130.34, 130.27, 127.9, 127.7, 126.7, 125.5, 120.1, 110.1, 77.1, 55.4, 39.4, 36.2, 31.5; HRMS (ESI): m/z calcd for $C_{22}H_{26}N_3O_3$ $[M+H]^+$: 380.1969 found: 380.1962; $[\alpha]_D^{25}$ = -45.6 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 5.4 min (minor), 6.0 min (major), 98:2 *er*.



(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(3,4-dichlorobenzyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1i**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 20.08 mg, 48% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67-7.62 (m, 1H), 7.56 (d, *J* = 1.4 Hz, 1H), 7.46 (td, *J* = 8.2, 7.7, 1.5 Hz, 1H), 7.37-7.30 (m, 3H), 7.06 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.11 (s, 1H), 5.02 (d, *J* = 15.3 Hz, 2H), 4.43 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.8, 153.6, 151.7, 148.7, 137.7, 132.2, 131.4, 131.2, 131.1, 130.7, 130.60, 130.55, 130.2, 128.7, 128.1, 77.6, 43.0, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{21}H_{22}Cl_2N_3O_2$ $[M+H]^+$: 418.1084 found: 418.1082; $[\alpha]_D^{25}$ = -26.4 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.2 min (minor), 5.7 min (major), 93:7 *er*.

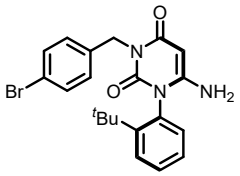


(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(3,5-difluorobenzyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1j**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 18.88 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.48-7.41 (m, 1H), 7.33 (td, *J* = 7.5, 1.5 Hz, 1H), 7.05 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.93 (h, *J* = 4.3 Hz, 2H), 6.64 (tt, *J* = 9.0, 2.4 Hz, 1H), 5.12 (s, 1H), 5.10-4.92 (m, 2H), 4.68 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.9, 162.8 (d, *J* = 248.1 Hz), 154.0, 151.7, 148.6, 141.2 (d, *J* = 9.2 Hz), 131.1, 130.62, 130.56, 130.5, 128.1, 111.6 (d, *J* = 25.4 Hz), 102.8 (d, *J* = 25.3 Hz), 77.2, 43.4, 36.2, 31.4; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.55; HRMS (ESI): m/z calcd for $C_{21}H_{22}F_2N_3O_2$ $[M+H]^+$: 386.1675 found: 386.1673; $[\alpha]_D^{25}$ = -32.8 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.1 min (minor), 6.3 min (major), 96:4 *er*.

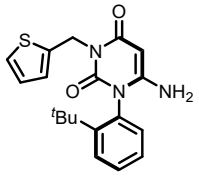


(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(4-(trifluoromethyl)benzyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1k**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 16.70 mg, 40% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.50 (t, *J* = 5.6 Hz, 4H), 7.44-7.38 (m, 1H), 7.30 (td, *J* = 7.5, 1.5 Hz, 1H), 7.00 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.15 (d, *J* = 14.0 Hz, 2H), 5.05 (d, *J* = 14.1 Hz, 1H), 4.86 (s, 2H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.0, 154.2, 151.7, 148.5, 141.4, 131.1, 130.5, 129.4 (d, *J* = 32.2 Hz), 128.5 (d, *J* =

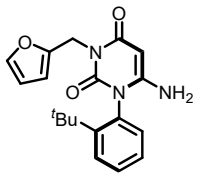
98.3 Hz), 125.1 (d, *J* = 3.7 Hz), 124.1 (q, *J* = 272.0 Hz), 77.0, 43.6, 36.1, 31.3; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.48; HRMS (ESI): m/z calcd for $C_{22}H_{23}F_3N_3O_2$ $[M+H]^+$: 418.1737 found: 418.1736; $[\alpha]_D^{25}$ = -35.2 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 3.7 min (minor), 4.7 min (major), 98:2 *er*.



(*R*)-6-amino-3-(4-bromobenzyl)-1-(2-(*tert*-butyl)phenyl)pyrimidine-2,4(*1H,3H*)-dione (**1l**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 20.99 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-d) δ 7.62 (d, J = 1.5 Hz, 1H), 7.48-7.38 (m, 1H), 7.38-7.26 (m, 4H), 7.14 (s, 1H), 7.02 (dd, J = 7.8, 1.5 Hz, 1H), 5.06 (s, 1H), 5.00 (d, J = 17.5 Hz, 2H), 4.59 (s, 2H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.1, 153.8, 151.8, 148.6, 136.4, 131.9, 131.3, 131.1, 130.8, 130.6, 130.5, 128.1, 121.3, 100.0, 43.4, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{21}H_{23}BrN_3O_2$ $[M+H]^+$: 428.0968 found: 428.0961; $[\alpha]_D^{25}$ = -4.5 (c = 0.125, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.4 min (minor), 6.4 min (major), 99:1 *er*.

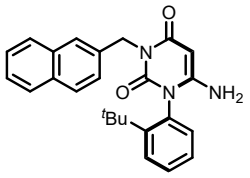


(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(thiophen-2-ylmethyl)pyrimidine-2,4(*1H,3H*)-dione (**1m**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as yellow solid, 16.71 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.43 (td, *J* = 7.7, 1.5 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.14-7.07 (m, 2H), 7.03 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.83 (dd, *J* = 5.1, 3.5 Hz, 1H), 5.21 (d, *J* = 3.4 Hz, 2H), 5.10 (s, 1H), 4.74 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.7, 154.0, 151.5, 148.7, 139.0, 131.2, 130.7, 130.5, 130.4, 128.0, 126.2, 125.4, 77.3, 38.5, 36.2, 31.5; HRMS (ESI): m/z calcd for $C_{19}H_{22}N_3O_2S$ $[M+H]^+$: 356.1427 found: 356.1421; $[\alpha]_D^{25}$ = -42.6 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.1 min (minor), 5.3 min (major), 90:10 *er*.

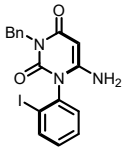


(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(furan-2-ylmethyl)pyrimidine-2,4(*1H,3H*)-dione (**1n**) The

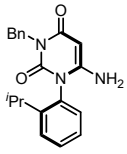
product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 15.95 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.44 (ddd, *J* = 8.3, 7.3, 1.6 Hz, 1H), 7.39-7.30 (m, 1H), 7.24 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.06 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.28 (d, *J* = 3.2 Hz, 1H), 6.23 (dd, *J* = 3.2, 1.9 Hz, 1H), 5.18-5.09 (m, 2H), 5.04 (d, *J* = 14.8 Hz, 1H), 4.62 (s, 2H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.8, 153.9, 151.5, 150.6, 148.7, 141.7, 131.2, 130.7, 130.49, 130.47, 128.0, 110.2, 108.8, 37.0, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{19}H_{22}N_3O_3$ $[M+H]^+$: 340.1656 found: 340.1656; $[\alpha]_D^{25}$ = -54.6 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.3 min (minor), 6.6 min (major), 98:2 *er*.



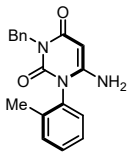
(*R*)-6-amino-1-(2-(*tert*-butyl)phenyl)-3-(naphthalen-2-ylmethyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1o**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 18.78 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 1.6 Hz, 1H), 7.71 (s, 3H), 7.63-7.52 (m, 2H), 7.45-7.35 (m, 3H), 7.30-7.20 (m, 1H), 6.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.23 (d, *J* = 4.9 Hz, 2H), 5.15 (s, 1H), 4.55 (s, 2H), 1.18 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 153.8, 151.8, 148.6, 135.0, 133.3, 132.7, 131.2, 130.8, 130.4, 128.0, 127.9, 127.79, 127.76, 127.5, 127.0, 125.8, 125.6, 77.6, 44.2, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{25}H_{26}N_3O_2$ $[M+H]^+$: 400.2020 found: 400.2018; $[\alpha]_D^{25}$ = -45.5 (c = 0.5, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 5.4 min (minor), 12.9 min (major), 98:2 *er*.



(*R*)-6-amino-3-benzyl-1-(2-iodophenyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1p**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 20.54 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 3H), 7.14 (d, *J* = 7.3 Hz, 1H), 5.11 (s, 1H), 5.07 (d, *J* = 11.5 Hz, 2H), 4.59 (s, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 152.6, 150.6, 140.6, 137.5, 136.7, 131.7, 130.4, 130.2, 128.4, 128.2, 127.2, 99.9, 77.5, 44.2; HRMS (ESI): m/z calcd for $C_{17}H_{15}IN_3O_2$ $[M+H]^+$: 420.0204 found: 420.0201; $[\alpha]_D^{25}$ = -94.2 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 5.3 min (minor), 7.1 min (major), 92:8 *er*.

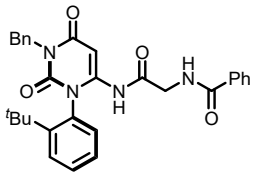


(*R*)-6-amino-3-benzyl-1-(2-isopropylphenyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1q**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 14.42 mg, 43% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49-7.45 (m, 2H), 7.42-7.36 (m, 2H), 7.32 (d, *J* = 3.0 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 2H), 7.14 (dd, *J* = 7.3, 3.5 Hz, 2H), 5.09 (s, 1H), 5.07 (s, 2H), 4.51 (s, 2H), 2.67 (q, *J* = 6.8 Hz, 1H), 1.17 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 153.4, 151.4, 147.7, 137.7, 131.0, 130.8, 129.0, 128.6, 128.2, 127.8, 127.6, 127.2, 77.1, 44.0, 28.3, 23.5; HRMS (ESI): m/z calcd for $C_{20}H_{21}N_3O_2$ $[M+H]^+$: 336.1707 found: 336.1709; $[\alpha]_D^{20}$ = -37.9 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.0 min (minor), 4.9 min (major), 90:10 *er*.



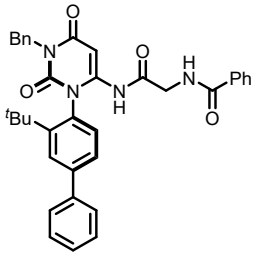
(*R*)-6-amino-3-benzyl-1-(*o*-tolyl)pyrimidine-2,4(*1H*,*3H*)-dione (**1r**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 1:2) as white solid, 14.75 mg, 48% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 (dq, *J* = 14.8, 7.4, 6.9 Hz, 5H), 7.24-7.07 (m, 4H), 5.10 (s, 1H), 5.07 (s, 2H), 4.56 (s, 2H), 2.13 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.2, 153.0, 151.0, 137.7, 137.3, 132.6, 131.9, 130.4, 129.0, 128.5, 128.2, 127.9, 127.2, 44.1, 17.2; HRMS (ESI): m/z calcd for $C_{18}H_{17}N_3O_2$ $[M+H]^+$: 308.1394 found: 308.1307; $[\alpha]_D^{20}$ = -16.3 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.9 min (minor), 6.6 min (major), 65:35 *er*.

6. Characterization data of (*S*)-3

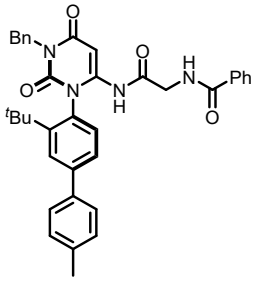


(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropy-rimidin-4-yl)amino)-2-oxoethyl)benzamide (**3a**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 25.02 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.01 (s, 1H), 7.89-7.79 (m, 2H), 7.66 (d, *J* = 1.5 Hz, 1H), 7.49 (td, *J* = 7.7, 1.6 Hz, 4H), 7.46-7.33 (m, 3H), 7.33-7.21 (m, 4H), 7.05 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.21 (s, 1H), 5.18-5.06 (m, 2H), 4.99 (dd, *J* = 12.4, 5.0 Hz, 2H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.1, 161.1, 158.6, 149.9, 148.5, 136.9, 131.3, 131.1, 131.0, 130.9, 129.3, 129.2, 128.6, 128.5, 128.3, 127.6, 127.1, 90.2, 50.5, 44.3, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{30}H_{31}N_4O_4$ $[M+H]^+$: 511.2340 found: 511.2339; $[\alpha]_D^{25}$ = 33.7 (c = 0.5, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol,

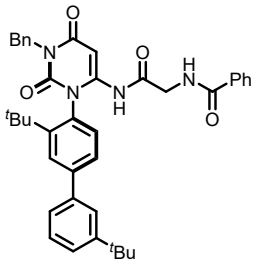
1 mL/min, t_R = 7.2 min (major), 7.9 min (minor), 98:2 *er*.



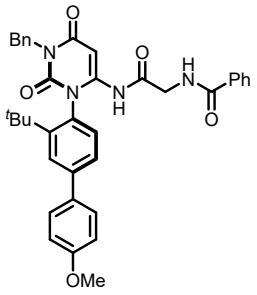
(*S*)-*N*-(2-((1-benzyl-3-(3-(*tert*-butyl)-[1,1'-biphenyl]-4-yl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3b**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 28.75 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.06 (s, 1H), 7.84 (dq, *J* = 4.8, 2.3 Hz, 3H), 7.55 (dt, *J* = 7.2, 2.2 Hz, 3H), 7.53-7.44 (m, 6H), 7.41 (dd, *J* = 6.7, 2.3 Hz, 2H), 7.28 (dtd, *J* = 13.8, 7.4, 6.9, 3.5 Hz, 4H), 7.12 (dd, *J* = 8.1, 2.5 Hz, 1H), 5.25-5.22 (m, 1H), 5.22-5.09 (m, 2H), 5.02 (ddd, *J* = 12.0, 5.1, 2.5 Hz, 2H), 1.26 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.2, 161.1, 158.7, 150.0, 148.8, 144.1, 139.9, 136.9, 134.7, 131.44, 131.37, 129.9, 129.4, 129.0, 128.5, 128.4, 128.3, 128.2, 127.7, 127.4, 127.3, 127.1, 90.2, 50.6, 44.4, 36.4, 31.5; HRMS (ESI): m/z calcd for $C_{36}H_{35}N_4O_4$ $[M+H]^+$: 587.2653 found: 587.2653; $[\alpha]_D^{25}$ = 33.2 (c = 0.1, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.8 min (major), 11.0 min (minor), 97:3 *er*.



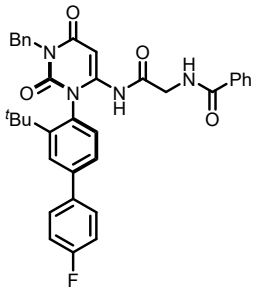
(*S*)-*N*-(2-((1-benzyl-3-(3-(*tert*-butyl)-4'-methyl-[1,1'-biphenyl]-4-yl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3c**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 24.03 mg, 40% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.96 (d, *J* = 4.1 Hz, 1H), 7.84-7.66 (m, 3H), 7.49-7.28 (m, 7H), 7.20 (dd, *J* = 7.9, 2.3 Hz, 7H), 7.03 (s, 1H), 5.15 (s, 1H), 5.13-5.02 (m, 2H), 4.92 (dd, *J* = 10.8, 5.0 Hz, 2H), 2.33 (s, 3H), 1.17 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.5, 167.2, 161.1, 158.7, 150.0, 148.7, 144.0, 138.2, 137.0, 136.9, 134.6, 131.4, 129.8, 129.6, 129.4, 128.5, 128.4, 127.9, 127.7, 127.13, 127.08, 90.2, 50.5, 44.4, 36.4, 31.5, 21.2; HRMS (ESI): m/z calcd for $C_{37}H_{37}N_4O_4$ $[M+H]^+$: 601.2810 found: 601.2814; $[\alpha]_D^{25}$ = 35.7 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.0 min (major), 15.2 min (minor), 97:3 *er*.



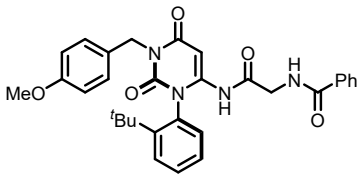
(*S*)-*N*-(2-((1-benzyl-3-(3,3'-di-*tert*-butyl-[1,1'-biphenyl]-4-yl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3d**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 30.21 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.23-10.80 (m, 1H), 7.91-7.85 (m, 2H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.59-7.50 (m, 4H), 7.49-7.39 (m, 5H), 7.37 (s, 1H), 7.33-7.24 (m, 4H), 7.12 (d, *J* = 8.1 Hz, 1H), 5.22 (d, *J* = 13.8 Hz, 1H), 5.14 (d, *J* = 13.8 Hz, 2H), 5.03 (dd, *J* = 12.2, 5.0 Hz, 2H), 1.38 (s, 9H), 1.26 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.2, 161.1, 158.7, 152.0, 150.0, 148.7, 144.9, 139.8, 136.9, 134.7, 131.4, 130.1, 129.5, 128.8, 128.5, 128.4, 128.1, 127.7, 127.6, 127.1, 125.3, 124.6, 100.0, 90.3, 50.6, 44.4, 36.4, 34.9, 31.5, 31.4; HRMS (ESI): m/z calcd for $C_{40}H_{43}N_4O_4$ $[M+H]^+$: 643.3279 found: 643.3279; $[\alpha]_D^{25}$ = 32.6 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 10.0 min (major), 11.5 min (minor), 96:4 *er*.



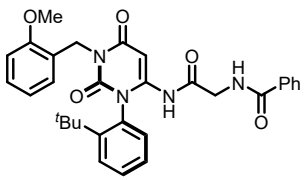
(*S*)-*N*-(2-((1-benzyl-3-(3-(*tert*-butyl)-4'-methoxy-[1,1'-biphenyl]-4-yl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3e**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 29.60 mg, 48% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.04 (d, *J* = 4.1 Hz, 1H), 7.91-7.82 (m, 2H), 7.80 (d, *J* = 2.1 Hz, 1H), 7.58-7.46 (m, 6H), 7.42 (dd, *J* = 8.3, 6.5 Hz, 2H), 7.36-7.22 (m, 4H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.99 (d, *J* = 8.3 Hz, 2H), 5.23 (s, 1H), 5.21-5.08 (m, 2H), 5.01 (dd, *J* = 11.2, 5.0 Hz, 2H), 3.86 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.1, 161.1, 159.8, 158.7, 150.0, 148.6, 143.6, 136.9, 134.6, 132.3, 131.4, 129.4, 129.3, 128.5, 128.4, 128.3, 127.67, 127.63, 127.1, 126.9, 114.4, 90.2, 55.4, 50.5, 44.4, 36.4, 31.5; HRMS (ESI): m/z calcd for $C_{37}H_{37}N_4O_5$ $[M+H]^+$: 617.2759 found: 617.2763; $[\alpha]_D^{25}$ = 40.0 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 13.7 min (major), 22.6 min (minor), 97:3 *er*.



(*S*)-*N*-(2-((1-benzyl-3-(3-(*tert*-butyl)-4'-fluoro-[1,1'-biphenyl]-4-yl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3f**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 25.40 mg, 42% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.99 (d, *J* = 4.1 Hz, 1H), 7.82-7.74 (m, 2H), 7.72 (d, *J* = 2.0 Hz, 1H), 7.47-7.40 (m, 6H), 7.36 (d, *J* = 7.5 Hz, 2H), 7.25-7.17 (m, 4H), 7.13-7.02 (m, 3H), 5.14 (d, *J* = 14.0 Hz, 1H), 5.05 (d, *J* = 13.8 Hz, 2H), 4.94 (dd, *J* = 10.9, 5.0 Hz, 2H), 1.18 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 161.7, 159.8 (d, *J* = 242.0 Hz), 150.0, 149.0, 143.1, 136.8, 136.0 (d, *J* = 3.2 Hz), 134.6, 131.6, 131.4, 129.7, 129.4, 129.0 (d, *J* = 8.1 Hz), 128.5, 128.4, 128.3, 127.7, 127.2, 127.1, 116.0 (d, *J* = 21.4 Hz), 90.2, 50.5, 44.4, 36.4, 31.5; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -113.98; HRMS (ESI): m/z calcd for $C_{36}H_{34}FN_4O_4$ $[M+H]^+$: 605.2557 found: 605.2562; $[\alpha]_D^{25}$ = 16.8 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.7 min (major), 11.2 min (minor), 98:2 *er*.

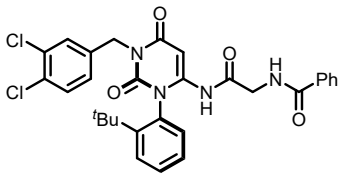


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(4-methoxybenzyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3g**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 21.62 mg, 40% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.94 (s, 1H), 7.78 (dt, *J* = 8.5, 1.7 Hz, 2H), 7.61 (dt, *J* = 8.2, 1.7 Hz, 1H), 7.48-7.32 (m, 6H), 7.29-7.14 (m, 2H), 6.98 (dt, *J* = 7.8, 1.7 Hz, 1H), 6.80-6.65 (m, 2H), 5.03 (d, *J* = 1.6 Hz, 1H), 5.03-4.95 (m, 2H), 4.93 (dd, *J* = 5.0, 1.7 Hz, 2H), 3.71 (d, *J* = 1.7 Hz, 3H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.2, 161.1, 159.2, 158.6, 149.9, 148.6, 131.4, 131.12, 131.09, 131.01, 130.95, 129.3, 129.2, 128.6, 128.5, 127.1, 113.7, 90.3, 55.3, 50.5, 43.8, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{31}H_{33}N_4O_5$ $[M+H]^+$: 541.2446 found: 541.2449; $[\alpha]_D^{25}$ = 31.0 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.9 min (major), 14.8 min (minor), 98.5:1.5 *er*.

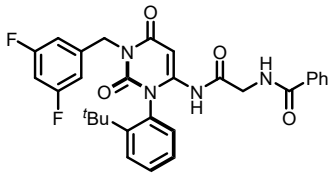


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(2-methoxybenzyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-

4-yl)amino)-2-oxoethyl)benzamide (**3h**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 21.62 mg, 40% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.08-10.89 (m, 1H), 7.80-7.72 (m, 2H), 7.59 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.44-7.38 (m, 2H), 7.34 (dd, *J* = 14.7, 7.8 Hz, 2H), 7.32-7.25 (m, 1H), 7.18-7.10 (m, 2H), 7.05-6.97 (m, 2H), 6.78 (t, *J* = 7.8 Hz, 2H), 5.22 (d, *J* = 15.3 Hz, 1H), 5.13-4.96 (m, 2H), 4.91 (dd, *J* = 10.3, 5.1 Hz, 2H), 3.76 (s, 3H), 1.17 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.8, 167.1, 161.2, 158.8, 157.2, 149.7, 148.6, 134.7, 131.3, 131.1, 131.0, 130.9, 129.3, 128.6, 128.5, 128.2, 127.6, 127.1, 124.7, 120.3, 110.4, 90.2, 55.5, 50.5, 39.9, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{31}H_{33}N_4O_5$ $[M+H]^+$: 541.2446 found: 541.2448; $[\alpha]_D^{25}$ = 40.3 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.0 min (major), 13.3 min (minor), 98:2 *er*.

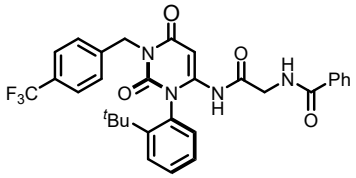


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(3,4-dichlorobenzyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3i**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 28.39 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.99 (d, *J* = 3.9 Hz, 1H), 7.82-7.74 (m, 2H), 7.63 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.53 (d, *J* = 1.2 Hz, 1H), 7.48-7.41 (m, 2H), 7.39-7.32 (m, 3H), 7.29 (d, *J* = 1.2 Hz, 2H), 7.19-7.12 (m, 1H), 6.99 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.05 (d, *J* = 13.9 Hz, 1H), 5.00 (s, 2H), 4.92 (dd, *J* = 10.6, 5.0 Hz, 2H), 1.15 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 160.8, 158.7, 149.9, 148.6, 137.0, 134.6, 132.4, 131.9, 131.44, 131.37, 131.3, 131.03, 130.99, 130.3, 129.0, 128.7, 128.5, 127.1, 90.1, 50.5, 43.3, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{30}H_{29}Cl_2N_4O_4$ $[M+H]^+$: 579.1561 found: 579.1565; $[\alpha]_D^{25}$ = 45.9 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.1 min (major), 10.8 min (minor), 99:1 *er*.

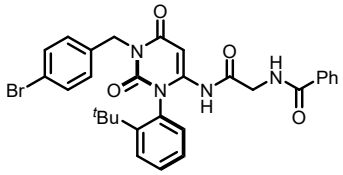


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(3,5-difluorobenzyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3j**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as yellow solid, 26.78 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.19-10.64 (m, 1H), 7.79-7.72 (m, 2H), 7.62 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.46-7.43 (m, 1H), 7.42-7.39 (m, 1H), 7.39-7.29 (m, 3H), 7.15 (t, *J* = 4.6 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.97-6.91 (m, 2H), 6.67-6.59 (m, 1H), 5.08 (d, *J* = 13.9 Hz, 1H), 4.98 (d, *J* = 13.9 Hz, 2H), 4.91 (dd, *J* = 10.7, 5.0 Hz, 2H), 1.15 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.5, 167.2, 162.8 (d, *J* = 248.5 Hz), 160.8, 158.7, 149.9, 148.5, 140.5 (d, *J* = 9.2 Hz), 134.6, 131.4, 131.3, 131.0 , 129.0, 128.7, 128.5, 127.1, 112.1 (d, *J* = 25.4 Hz), 103.2 (d, *J* = 50.5 Hz), 90.0, 50.5, 43.6, 36.3, 31.4; ^{19}F NMR (376 MHz,

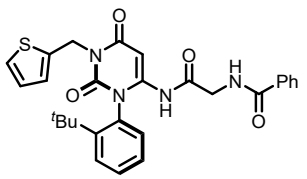
Chloroform-*d*) δ -109.79; HRMS (ESI): m/z calcd for $C_{30}H_{29}F_2N_4O_4$ $[M+H]^+$: 547.2152 found: 547.2157; $[\alpha]_D^{25}$ = 43.4 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.2 min (major), 12.6 min (minor), 98:2 *er*.



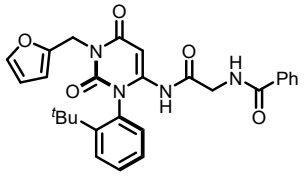
(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1-(4-(trifluoromethyl)benzyl)-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3k**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 27.19 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.06 (s, 1H), 7.89-7.82 (m, 2H), 7.70 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.58-7.48 (m, 4H), 7.47-7.36 (m, 3H), 7.23 (d, *J* = 4.3 Hz, 1H), 7.06 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.29-5.12 (m, 2H), 5.07 (s, 1H), 5.01 (dd, *J* = 11.7, 5.0 Hz, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.4, 167.2, 161.0, 158.7, 149.9, 148.4, 140.7, 134.5, 131.4, 131.2, 130.9 (d, *J* = 2.4 Hz), 129.8 (d, *J* = 32.5 Hz), 129.6, 129.0, 128.6, 128.5, 128.0, 127.0, 125.3 (d, *J* = 3.7 Hz), 124.1 (q, *J* = 272.0 Hz), 90.0, 50.5, 43.8, 36.2, 31.4; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.55; HRMS (ESI): m/z calcd for $C_{31}H_{30}F_3N_4O_4$ $[M+H]^+$: 579.2214 found: 579.2219; $[\alpha]_D^{25}$ = 35.2 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 6.1 min (major), 7.5 min (minor), 97:3 *er*.



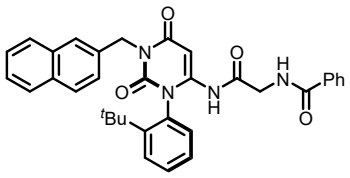
(*S*)-*N*-(2-((1-(4-bromobenzyl)-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3l**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 28.88 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.04 (d, *J* = 4.0 Hz, 1H), 7.89-7.82 (m, 2H), 7.69 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.54-7.47 (m, 2H), 7.46-7.37 (m, 7H), 7.28-7.22 (m, 1H), 7.05 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.14 (d, *J* = 13.8 Hz, 1H), 5.07 (d, *J* = 2.1 Hz, 2H), 5.00 (dd, *J* = 11.3, 5.0 Hz, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 161.0, 158.7, 149.9, 148.6, 135.8, 134.6, 131.5, 131.4, 131.3, 131.2, 131.02, 130.97, 129.1, 128.6, 128.5, 127.1, 121.8, 90.1, 50.5, 43.7, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{30}H_{30}BrN_4O_4$ $[M+H]^+$: 589.1445 found: 589.1448; $[\alpha]_D^{25}$ = 11.8 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 7.1 min (major), 8.4 min (minor), 97:3 *er*.



(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1-(thiophen-2-ylmethyl)-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3m**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as yellow solid, 25.31 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.02 (d, *J* = 4.0 Hz, 1H), 7.87-7.81 (m, 2H), 7.69 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.54-7.46 (m, 2H), 7.45-7.35 (m, 3H), 7.26-7.15 (m, 3H), 7.06 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.92 (dd, *J* = 4.8, 3.7 Hz, 1H), 5.36-5.26 (m, 2H), 5.10 (d, *J* = 3.8 Hz, 1H), 5.00 (dd, *J* = 8.4, 5.0 Hz, 2H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 160.6, 158.7, 149.6, 148.6, 138.1, 134.7, 131.4, 131.2, 131.05, 130.98, 129.1, 128.7, 128.6, 128.5, 127.1, 126.4, 125.9, 90.2, 50.5, 38.8, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{28}H_{29}N_4O_4S$ $[M+H]^+$: 517.1904 found: 517.1910; $[\alpha]_D^{25}$ = 33.4 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.9 min (major), 13.1 min (minor), 98.5:1.5 *er*.

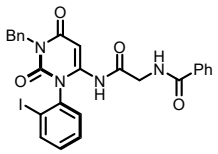


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(furan-2-ylmethyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3n**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 23.02 mg, 46% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.05 (s, 1H), 7.90-7.79 (m, 2H), 7.70 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.54-7.47 (m, 2H), 7.45-7.36 (m, 3H), 7.32 (dd, *J* = 1.9, 0.9 Hz, 1H), 7.26-7.17 (m, 1H), 7.07 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.41-6.35 (m, 1H), 6.30 (dd, *J* = 3.2, 1.8 Hz, 1H), 5.28-5.12 (m, 2H), 5.06 (d, *J* = 4.3 Hz, 1H), 5.00 (dd, *J* = 8.0, 5.0 Hz, 2H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.2, 160.7, 158.8, 150.0, 149.6, 148.7, 142.1, 131.4, 131.2, 131.1, 130.0, 128.6, 128.5, 127.1, 110.4, 109.4, 90.1, 50.5, 37.2, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{28}H_{29}N_4O_5$ $[M+H]^+$: 501.2133 found: 501.2137; $[\alpha]_D^{25}$ = 39.8 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 7.3 min (major), 8.2 min (minor), 97:3 *er*.

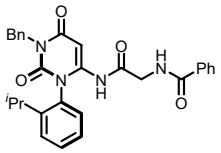


(*S*)-*N*-(2-((3-(2-(*tert*-butyl)phenyl)-1-(naphthalen-2-ylmethyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3o**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 27.47 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-d) δ 11.17-10.92 (m, 1H), 7.97 (s, 1H), 7.88-7.83 (m, 2H), 7.83-7.75 (m, 3H), 7.66 (ddd, *J* = 14.6, 8.3, 1.6 Hz, 2H), 7.53-7.35 (m, 7H), 7.25 (d, *J* = 6.0 Hz, 1H), 7.05 (dd, *J* = 7.9, 1.5 Hz, 1H), 5.32 (d, *J* = 5.3 Hz, 2H), 5.13-5.03 (m, 1H), 5.07-4.98 (m, 2H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 161.1, 158.7, 150.0, 148.6, 134.7, 134.3, 133.3, 132.9, 131.4, 131.2, 131.1, 131.0, 129.2, 128.6, 128.5, 128.1, 127.6, 127.3, 127.1, 126.0, 125.9, 90.2, 50.6, 44.5,

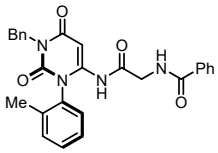
36.3, 31.4; HRMS (ESI): m/z calcd for $C_{34}H_{33}N_4O_4$ $[M+H]^+$: 561.2497 found: 561.2500; [α] = 36.8 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.0 min (major), 10.0 min (minor), 98:2 *er*.



(*S*)-*N*-(2-((1-benzyl-3-(2-iodophenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3p**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 28.44 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 10.98 (s, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 7.5 Hz, 2H), 7.51 (dt, *J* = 17.6, 8.7 Hz, 4H), 7.45-7.35 (m, 3H), 7.27 (dt, *J* = 22.3, 7.6 Hz, 5H), 5.23 (d, *J* = 10.7 Hz, 1H), 5.21-5.09 (m, 2H), 4.95 (d, *J* = 5.0 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) *δ* 194.6, 167.2, 160.9, 157.3, 148.7, 141.1, 136.8, 135.3, 134.6, 132.3, 131.4, 130.7, 130.4, 129.0, 128.5, 128.4, 127.7, 127.1, 99.5, 90.0, 50.6, 44.4; HRMS (ESI): m/z calcd for $C_{26}H_{22}IN_4O_4$ $[M+H]^+$: 581.0680 found: 580.0684; [α] = 27.5 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 10.9 min (major), 12.1 min (minor), 97:3 *er*.

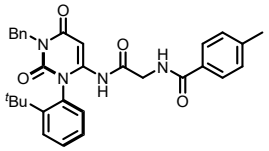


(*S*)-*N*-(2-((1-benzyl-3-(2-isopropylphenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3q**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 24.33 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 10.90 (s, 1H), 7.86-7.68 (m, 2H), 7.52-7.45 (m, 2H), 7.42 (td, *J* = 5.4, 4.9, 2.7 Hz, 3H), 7.36 (dd, *J* = 8.0, 6.4 Hz, 3H), 7.26-7.16 (m, 4H), 7.14-7.08 (m, 1H), 5.09 (s, 2H), 4.97 (d, *J* = 4.7 Hz, 1H), 4.93 (t, *J* = 5.3 Hz, 2H), 2.67-2.49 (m, 1H), 1.11 (d, *J* = 6.8 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) *δ* 194.7, 161.0, 158.2, 149.4, 147.6, 137.0, 134.7, 131.6, 131.4, 129.4, 129.2, 128.9, 128.5, 128.4, 128.3, 128.2, 127.7, 127.1, 112.5, 110.6, 90.0, 50.5, 44.3, 28.4, 23.6; HRMS (ESI): m/z calcd for $C_{29}H_{28}N_4O_4$ $[M+H]^+$: 497.2183 found: 497.2186; [α] = 7.1 (c = 0.5, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 10.4 min (major), 16.2 min (minor), 82:18 *er*.

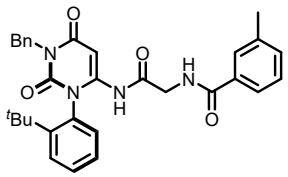


(*S*)-*N*-(2-((1-benzyl-2,6-dioxo-3-(o-tolyl)-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)benzamide (**3r**) The product was isolated by flash chromatography (petroleum

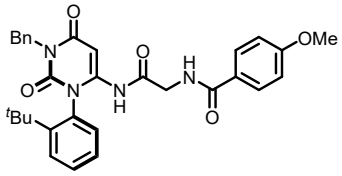
ether/ethyl acetate = 2:1) as white solid, 2295 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.11-10.69 (m, 1H), 7.84-7.66 (m, 2H), 7.41 (dt, *J* = 9.8, 3.4 Hz, 3H), 7.35 (dd, *J* = 6.3, 4.0 Hz, 5H), 7.29-7.07 (m, 6H), 5.11 (d, *J* = 3.4 Hz, 1H), 5.08 (d, *J* = 3.0 Hz, 2H), 4.90 (d, *J* = 5.0 Hz, 2H), 2.06 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 167.2, 161.0, 157.8, 149.1, 137.1, 136.9, 134.6, 132.4, 131.4, 131.14, 131.07, 129.1, 128.9, 128.50, 128.47, 127.7, 127.1, 89.9, 50.5, 44.4, 17.2; HRMS (ESI): m/z calcd for $C_{27}H_{24}N_4O_4$ $[M+H]^+$: 469.1870 found: 469.1871; $[\alpha]_D^{20}$ = 8.6 (c = 0.5, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 15.1 min (major), 19.7 min (minor), 71:29 *er*.



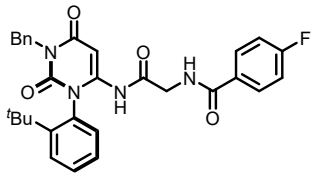
(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-4-methylbenzamide (**3s**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 24.66 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.94 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 1H), 7.42 (d, *J* = 7.2 Hz, 3H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.17 (dq, *J* = 16.6, 8.5, 7.6 Hz, 6H), 6.97 (d, *J* = 7.8 Hz, 1H), 5.12 (d, *J* = 13.8 Hz, 1H), 5.07-4.97 (m, 2H), 4.91 (dd, *J* = 12.7, 4.8 Hz, 2H), 2.31 (s, 3H), 1.13 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.1, 161.1, 158.6, 149.9, 148.5, 141.7, 136.9, 131.8, 131.08, 131.05, 130.88, 129.33, 129.26, 129.1, 128.6, 128.3, 127.6, 127.1, 90.2, 50.5, 44.3, 36.2, 31.4, 21.5; HRMS (ESI): m/z calcd for $C_{31}H_{33}N_4O_4$ $[M+H]^+$: 525.2497 found: 525.2495; $[\alpha]_D^{25}$ = 45.6 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 15.9 min (major), 19.4 min (minor), 97:3 *er*.



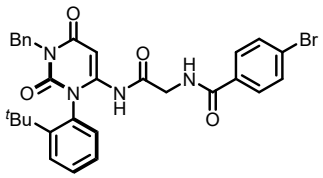
(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-3-methylbenzamide (**3t**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 25.71 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.95 (s, 1H), 7.65-7.58 (m, 2H), 7.55 (d, *J* = 6.1 Hz, 1H), 7.43 (dd, *J* = 7.4, 5.1 Hz, 3H), 7.31 (t, *J* = 7.5 Hz, 1H), 7.25-7.17 (m, 5H), 7.13 (s, 1H), 6.98 (d, *J* = 7.9 Hz, 1H), 5.13 (d, *J* = 13.8 Hz, 1H), 5.08-4.96 (m, 2H), 4.95-4.85 (m, 2H), 2.32 (s, 3H), 1.13 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.4, 161.1, 158.6, 149.9, 148.6, 138.3, 136.8, 134.6, 132.1, 131.12, 131.06, 130.9, 129.4, 129.2, 128.6, 128.37, 128.35, 127.9, 127.7, 90.2, 50.5, 44.3, 36.3, 31.4, 21.4; HRMS (ESI): m/z calcd for $C_{31}H_{33}N_4O_4$ $[M+H]^+$: 525.2497 found: 525.2495; $[\alpha]_D^{25}$ = 48.5 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.3 min (major), 15.1 min (minor), 99:1 *er*.



(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-4-methoxybenzamide (**3u**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 26.49 mg, 49% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.95 (s, 1H), 7.73 (d, *J* = 8.7 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.46-7.36 (m, 3H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.25-7.13 (m, 3H), 7.08 (d, *J* = 5.0 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 2H), 5.12 (d, *J* = 13.8 Hz, 1H), 5.06-4.95 (m, 2H), 4.90 (dd, *J* = 12.2, 4.9 Hz, 2H), 3.76 (s, 3H), 1.13 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.8, 166.7, 162.1, 161.1, 158.6, 149.9, 148.6, 136.9, 131.1, 130.9, 129.32, 129.27, 128.9, 128.6, 128.3, 127.6, 127.0, 113.7, 90.2, 55.4, 50.5, 44.3, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{31}H_{33}N_4O_5$ $[M+H]^+$: 541.2446 found: 541.2446; $[\alpha]_D^{25}$ = 45.3 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 10.0 min (major), 12.4 min (minor), 96:4 *er*.

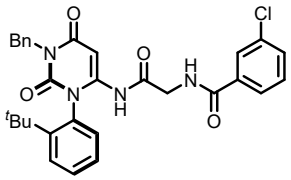


(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-4-fluorobenzamide (**3v**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 24.84 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.02 (s, 1H), 7.85 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.49 (d, *J* = 6.7 Hz, 3H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.28 (p, *J* = 5.4, 4.5 Hz, 3H), 7.20 (d, *J* = 4.7 Hz, 1H), 7.15-7.00 (m, 3H), 5.18 (s, 1H), 5.09 (d, *J* = 30.2 Hz, 2H), 4.99 (dd, *J* = 13.4, 4.9 Hz, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.5, 166.1, 164.7 (d, *J* = 251.2 Hz), 163.2, 161.1, 158.7, 149.9, 148.6, 136.8, 131.14, 131.06, 131.0, 129.5, 129.4 (d, *J* = 3.9 Hz), 129.2, 128.6, 128.4, 127.7, 115.5 (d, *J* = 21.6 Hz), 90.2, 50.5, 44.4, 36.3, 31.4; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.57; HRMS (ESI): m/z calcd for $C_{30}H_{30}FN_4O_4$ $[M+H]^+$: 529.2446 found: 529.2449; $[\alpha]_D^{25}$ = 42.4 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 6.9 min (major), 8.6 min (minor), 96:4 *er*.

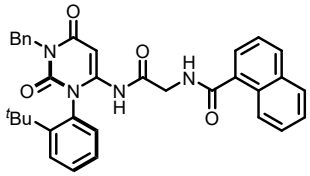


(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-4-bromobenzamide (**3w**) The product was isolated by flash chromatography

(petroleum ether/ethyl acetate = 2:1) as brown solid, 25.94 mg, 44% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.93 (s, 1H), 7.64 (tt, *J* = 5.9, 2.0 Hz, 2H), 7.60 (d, *J* = 1.8 Hz, 1H), 7.53-7.46 (m, 2H), 7.42 (dt, *J* = 7.7, 1.9 Hz, 3H), 7.31 (tt, *J* = 7.5, 1.8 Hz, 1H), 7.25-7.13 (m, 4H), 6.98 (dt, *J* = 7.9, 1.8 Hz, 1H), 5.13 (dd, *J* = 13.8, 1.9 Hz, 1H), 5.04 (dd, *J* = 13.8, 1.9 Hz, 2H), 4.93-4.82 (m, 2H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.4, 166.2, 161.1, 158.7, 149.9, 148.6, 136.8, 133.5, 131.7, 131.2, 131.05, 130.97 , 129.4, 129.2, 128.8, 128.6, 128.4, 127.7, 126.0, 90.2, 50.5, 44.4, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{30}H_{30}BrN_4O_4$ $[M+H]^+$: 589.1445 found: 589.1453; $[\alpha]_D^{25}$ = 37.8 (c = 0.125, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 16.8 min (major), 24.0 min (minor), 97:3 *er*.

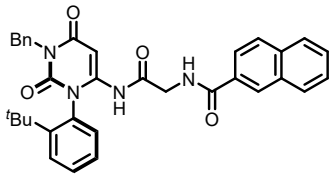


(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-3-chlorobenzamide (**3x**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 25.62 mg, 47% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.93 (s, 1H), 7.76 (t, *J* = 1.9 Hz, 1H), 7.68-7.57 (m, 2H), 7.48-7.36 (m, 4H), 7.34-7.26 (m, 2H), 7.24-7.12 (m, 4H), 6.98 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.13 (d, *J* = 13.8 Hz, 1H), 5.08-4.97 (m, 2H), 4.96-4.82 (m, 2H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.3, 165.8, 161.1, 158.7, 149.9, 148.6, 136.8, 136.5, 134.7, 131.4, 131.2, 131.05, 130.95, 129.8, 129.4, 129.2, 128.6, 128.4, 127.7, 127.5, 125.2, 90.2, 50.5, 44.4, 36.3, 31.4; HRMS (ESI): m/z calcd for $C_{30}H_{30}ClN_4O_4$ $[M+H]^+$: 545.1950 found: 545.1954; $[\alpha]_D^{25}$ = 38.6 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 7.0 min (major), 10.9 min (minor), 98:2 *er*.

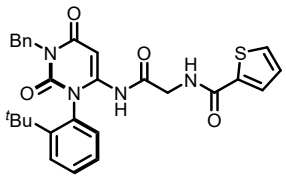


(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-1-naphthamide (**3y**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 19.06 mg, 34% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.98 (s, 1H), 8.36 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 8.3 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.69-7.58 (m, 2H), 7.45 (d, *J* = 7.8 Hz, 6H), 7.27-7.12 (m, 4H), 6.98 (d, *J* = 7.8 Hz, 1H), 6.92-6.81 (m, 1H), 5.13 (s, 1H), 5.11-5.04 (m, 2H), 4.90 (s, 2H), 1.15 (s, 9H).; ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 169.5, 161.1, 160.0, 158.7, 150.0, 148.6, 136.9, 134.8, 133.7, 131.2, 131.1, 131.0, 130.5, 129.4, 128.6, 128.4, 128.2, 127.7, 127.1, 126.4, 125.8, 125.2, 124.8, 90.3, 50.6, 44.4, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{34}H_{33}N_4O_4$ $[M+H]^+$: 561.2497 found: 561.2503; $[\alpha]_D^{25}$ = 48.3 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 7.5 min (major), 12.9 min

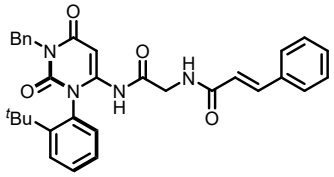
(minor), 99:1 *er*.



(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)-2-naphthamide (**3z**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 24.67 mg, 44% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.19-10.85 (m, 1H), 8.38 (s, 1H), 7.90 (td, *J* = 16.1, 14.9, 7.3 Hz, 4H), 7.69 (s, 1H), 7.53 (dd, *J* = 15.3, 6.9 Hz, 4H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.34-7.23 (m, 4H), 7.06 (d, *J* = 7.8 Hz, 1H), 5.22 (d, *J* = 13.8 Hz, 1H), 5.16 -5.07 (m, 2H), 5.07-4.97 (m, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.7, 167.2, 161.1, 158.7, 149.9, 148.6, 136.9, 134.8, 132.7, 131.9, 131.14, 131.08, 131.0, 129.4, 129.2, 129.0, 128.6, 128.4, 127.8, 127.7, 127.60, 127.55, 126.6, 123.8, 90.3, 50.7, 44.4, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{34}H_{33}N_4O_4$ $[M+H]^+$: 561.2497 found: 561.2502; $[\alpha]_D^{25}$ = 23.5 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 9.4 min (major), 11.6 min (minor), 96:4 *er*.



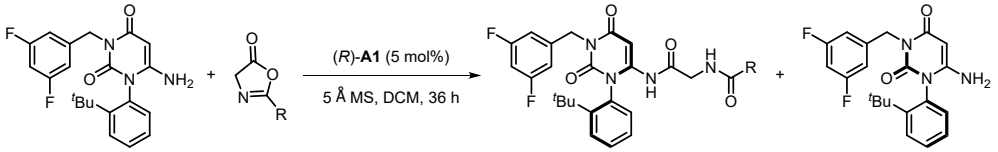
(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-2-oxoethyl)thiophene-2-carboxamide (**3aa**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 23.25 mg, 45% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.01 (s, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 3.7 Hz, 1H), 7.47 (dd, *J* = 15.0, 6.1 Hz, 4H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.32-7.22 (m, 3H), 7.07 (td, *J* = 7.8, 6.7, 3.6 Hz, 3H), 5.20 (d, *J* = 13.8 Hz, 1H), 5.14-5.01 (m, 2H), 5.02-4.90 (m, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.4, 161.7, 161.1, 158.7, 149.9, 148.6, 139.1, 136.8, 131.13, 131.06, 130.9, 129.7, 129.3, 129.2, 128.6, 128.4, 128.2, 127.7, 127.6, 90.2, 50.4, 44.4, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{28}H_{29}N_4O_4S$ $[M+H]^+$: 517.1904 found: 517.1906; $[\alpha]_D^{25}$ = 46.9 (c = 0.25, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 12.5 min (major), 19.0 min (minor), 99:1 *er*.



(*S*)-*N*-(2-((1-benzyl-3-(2-(*tert*-butyl)phenyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)amino)-

2-oxoethyl)cinnamamide (**3ab**) The product was isolated by flash chromatography (petroleum ether/ethyl acetate = 2:1) as white solid, 14.49 mg, 27% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.95 (s, 1H), 7.67-7.53 (m, 2H), 7.51-7.37 (m, 5H), 7.36-7.25 (m, 4H), 7.24-7.14 (m, 3H), 6.98 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.57 (t, *J* = 5.2 Hz, 1H), 6.43 (d, *J* = 15.6 Hz, 1H), 5.12 (d, *J* = 13.8 Hz, 1H), 5.03 (d, *J* = 13.8 Hz, 2H), 4.87 (dd, *J* = 9.0, 5.1 Hz, 2H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.6, 165.8, 161.1, 158.6, 149.9, 148.6, 141.0, 136.8, 135.0, 131.12, 131.06, 130.9, 129.6, 129.4, 129.2, 128.8, 128.6, 128.4, 127.8, 127.7, 120.8, 90.2, 50.3, 44.4, 36.3, 31.5; HRMS (ESI): m/z calcd for $C_{32}H_{33}N_4O_4$ $[M+H]^+$: 537.2497 found: 537.2493; $[\alpha]_D^{25}$ = 43.4 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 8.5 min (major), 11.1 min (minor), 99:1 *er*.

7. Kinetic resolution of *rac*-1j catalyzed by (*R*)-A1

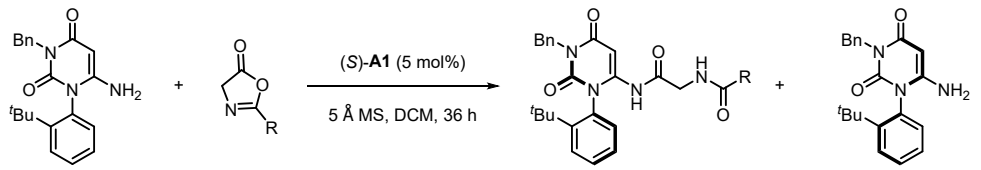


rac-**1j** **2a** (*R*)-**3j** (*S*)-**1j**

A 5 mL vial containing a magnetic stir bar, was added *rac*-**1j** (0.1 mmol, 1.0 equiv.), **2a** (0.05 mmol, 0.5 equiv.), CPA (*R*)-**A1** (0.005 mmol, 5 mol%) and 5 Å MS (50.0 mg), add 1.0 mL dry CH_2Cl_2. After stirring at room temperature for 36 h, the reaction mixture was directly purified by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 2:1 to obtain (*R*)-**3j** and petroleum ether/ethyl acetate = 1:2 to obtain (*S*)-**1j**.

8. Synthetic applications

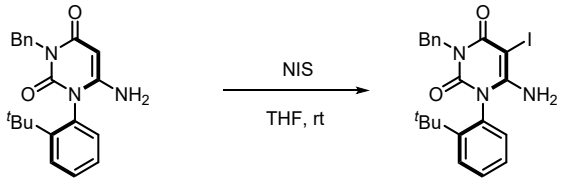
Large-scale synthesis of C–N axially chiral uracils



rac-**1a** **2a** (*S*)-**3a** (*R*)-**1a**

A 25 mL vial containing a magnetic stir bar charged with *rac*-**1a** (524.0 mg, 1.5 mmol, 1.0 equiv.), **2a** (120.9 mg, 0.75 mmol, 0.5 equiv.), CPA (*S*)-**A1** (56.5 mg, 0.075 mmol, 5 mol%) and 5Å MS (750.0 mg). Subsequently, dry CH_2Cl_2 (15 mL) was added. After stirring at rt for 36 h, the reaction mixture was purified directly by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 2:1 to 1:2) to afford the products (*S*)-**3a** as white solid (360.0 mg, 49% yield, 97:3 er) and recovered (*R*)-**1a** (259.0 mg, 49% yield, 99:1 er).

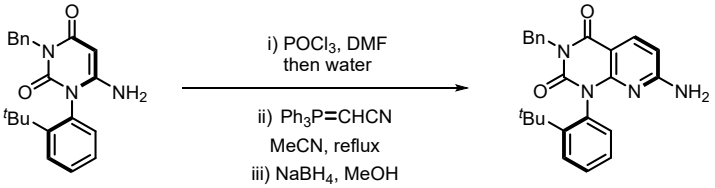
Transformations of (*R*)-1a



(*R*)-**1a**, 98:2 er

(*R*)-**4**
90% yield, 97:3 er

To a solution of (*R*)-**1a** (0.1 mmol, 1.0 equiv.) in THF (1 mL), *N*-Iodosuccinimide (0.11 mmol, 1.1 equiv.) was added in batch. After stirring at rt for 6 h, the reaction mixture was quenched with water and then extracted with DCM, washed by saturated sodium sulfate solution. After that, the mixture was concentrated to give a residue, which was purified by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 1:2) to afford (*R*)-**4** as pink solid, 42.78 mg, 90% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68-7.59 (m, 1H), 7.53-7.40 (m, 3H), 7.33 (td, *J* = 7.5, 1.5 Hz, 1H), 7.27-7.19 (m, 3H), 7.03 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.28-5.02 (m, 2H), 4.80 (s, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.8, 152.0, 151.0, 148.3, 137.0, 131.6, 131.0, 130.8, 130.6, 129.4, 128.2, 127.5, 46.0, 45.4, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{21}H_{23}IN_3O_2$ [M+H]$^{+}$: 476.0830 found: 476.0833; [α] $^{25}_{D}$ = -26.2 (c = 0.5, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 5.7 min (major), 6.5 min (minor), 97:3 *er*.



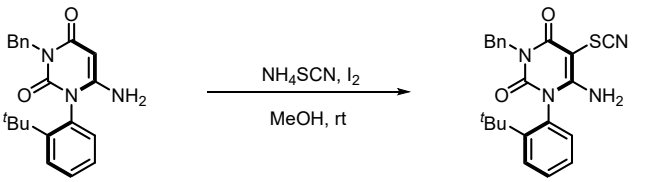
(*R*)-**1a**, 98:2 er

(*R*)-**5**
60% yield, 98:2 er

To a solution of compound (*R*)-**1a** (0.1 mmol, 1.0 equiv.) in DMF (3 mL), $POCl_3$ (0.11 mmol, 1.1 equiv.) was added at 0 °C. The mixture was stirred at rt for 2 h. Water was then added and the mixture was stirred at rt for 1 h before being filtered. The resulting cake was washed with water and dried under vacuo at 60 °C for 1 h to give a white solid without purification.

A mixture of the white solid and (triphenylphosphoranylidene)acetonitrile (0.2 mmol, 2 equiv.) in CH_3CN (3 mL) was stirred at 100 °C for 1.5 h. (triphenylphos-phoranylidene)acetonitrile (0.8 mmol, 0.8 equiv.) was then added, and the mixture was further stirred at 100 °C for another 1.5 h. Afterward, the mixture was cooled to rt and concentrated. The resulting residue was suspended in MeOH (3 mL). $NaBH_4$ (0.6 mmol, 0.6 equiv.) was added, and the mixture was stirred at rt for 0.5 h. Water was then added and the mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 1:2) to afford (*R*)-**5** as white solid, 24.03 mg, 60% yield over two steps; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.12 (d, *J* = 8.6 Hz, 1H), 7.59 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.49 (dt, *J* = 6.0, 1.6 Hz, 3H), 7.42-7.35 (m, 1H), 7.29-7.21 (m, 3H), 6.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.13 (d, *J* = 8.6 Hz, 1H), 5.29-5.15 (m, 2H), 4.90 (s, 2H), 1.11 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.5, 161.2, 153.2, 151.9, 147.7, 138.6, 137.1, 134.1, 131.6, 129.4, 129.1, 128.8, 128.3, 127.5, 127.1, 104.6, 100.9, 44.7, 36.0, 31.5; HRMS

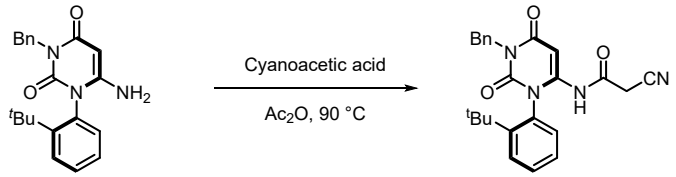
(ESI): m/z calcd for $C_{24}H_{25}N_4O_2$ $[M+H]^+$: 401.1972 found: 401.1973; $[\alpha]_D^{25}$ = -86.4 (c = 0.10, $CHCl_3$); HPLC: Chiralcel OD-H column, 60:40 hexane/isopropanol, 1 mL/min, t_R = 4.2 min (minor), 4.9 min (major), 98:2 *er.*



(*R*)-**1a,** 98:2 er

(*R*)-**6**
95% yield, 97.5:2.5 er

To a solution of compound (*R*)-**1a** (0.1 mmol, 1.0 equiv.) in MeOH (3 mL), NH_4SCN (0.3 mmol, 3.0 equiv.) and iodine (0.1 mmol, 1.0 equiv.) were added at rt. The mixture was stirred at rt for 4 h. After the reaction completed, it was quenched with saturated $Na_2S_2O_3$ solution, extract with EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (300~400 mesh silica gel, petroleum ether/ethyl acetate = 1:2) to afford (*R*)-**6** as white solid, 38.62 mg, 95% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.52-7.48 (m, 1H), 7.47-7.42 (m, 2H), 7.36 (td, *J* = 7.6, 1.5 Hz, 1H), 7.30-7.21 (m, 3H), 7.06 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.41 (s, 2H), 5.20-5.02 (m, 2H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.6, 156.7, 150.3, 148.3, 136.5, 131.2, 130.9, 130.3, 129.3, 128.5, 128.3, 127.7, 110.5, 69.9, 45.4, 36.2, 31.4; HRMS (ESI): m/z calcd for $C_{22}H_{23}N_4O_2S$ $[M+H]^+$: 407.1536 found: 407.1540; $[\alpha]_D^{25}$ = -43.8 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 84:16 hexane/isopropanol, 1 mL/min, t_R = 6.5 min (major), 7.2 min (minor), 97.5:2.5 *er*.



(*R*)-**1a,** 98:2 er

(*R*)-**7**
95% yield, 98:2 er

(*R*)-**1a** (0.1 mol, 1.0 equiv.) was added to a mixture of cyanoacetic acid (0.2 mol, 2.0 equiv.) and Ac_2O (100 μL) and heated at 90 °C for 1 h. The mixture was allowed to cool and poured into ice. The resulting precipitate was collected and dried. (*R*)-**7** was obtained as a white solid, 39.56 mg, 95% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.53 (s, 1H), 7.70 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.52 (td, *J* = 8.1, 7.7, 1.7 Hz, 1H), 7.44-7.23 (m, 8H), 5.17-4.88 (m, 2H), 4.48 (d, *J* = 3.7 Hz, 2H), 1.17 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 187.2, 161.2, 158.6, 149.6, 147.3, 137.1, 131.4, 130.4, 130.2, 130.1, 128.2, 128.1, 127.7, 127.2, 116.4, 89.5, 43.7, 35.7, 33.5, 31.1; HRMS (ESI): m/z calcd for $C_{24}H_{25}N_4O_3$ $[M+H]^+$: 417.1921 found: 417.1923; $[\alpha]_D^{25}$ = -64.2 (c = 0.25, $CHCl_3$); HPLC: Chiralpak AD-H column, 75:25 hexane/isopropanol, 1 mL/min, t_R = 7.4 min (major), 15.5 min (minor), 98:2 *er*.

Biological evaluation of selected C–N Axially Chiral Uracils

We performed a preliminary investigation on the cytotoxicity of different products against various kinds of tumor cells, including renal cancer cell ACHN, colorectal cancer cell HCT116, cervical cancer cell HeLa, myeloma cell U266, liver cancer HepG2, as well as prostate cancer cells LNCaP and PC3. (*S*)-**1j** and (*S*)-**1i** exhibited better cytotoxicity with an IC_{50} value of 7.17±1.69 - 34.13±5.96 μM and 13.61±2.64 - 81.15±5.23 respectively against different cancer cells, compared to their racemic products.

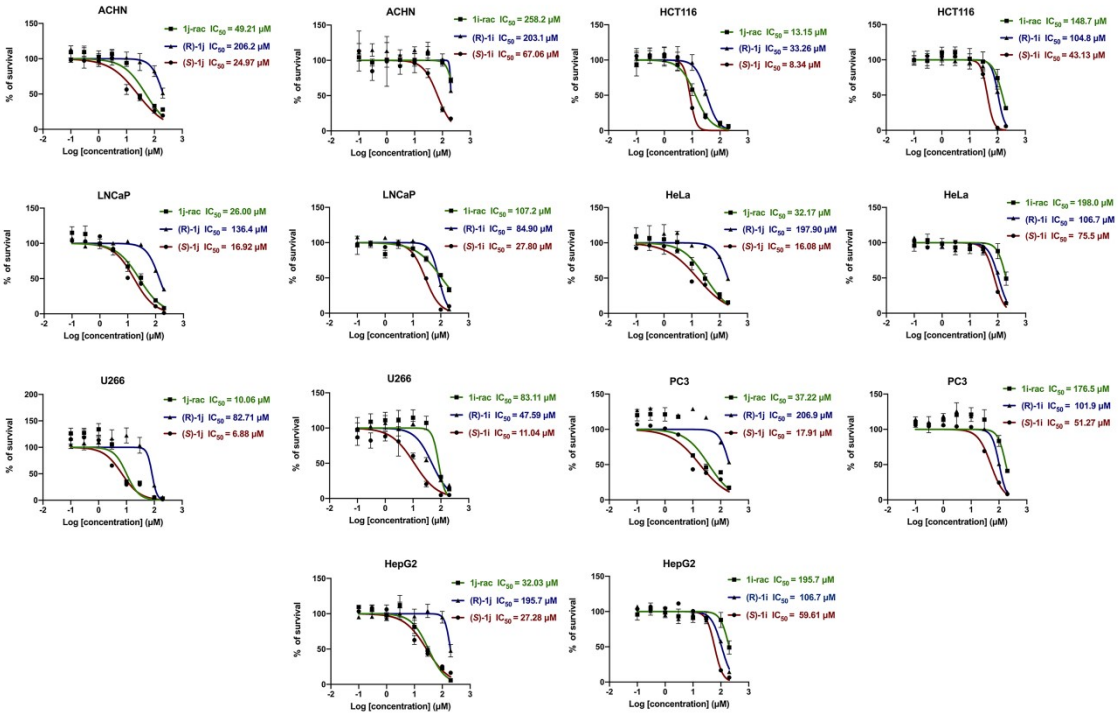


Table S5 Cytotoxicity of different products on 7 types of tumor cells, including renal cancer cell ACHN, colorectal cancer cell HCT116, cervical cancer cell HeLa, myeloma cell U266, liver cancer cell HepG2, as well as prostate cancer cells LNCaP and PC3. The IC_{50} value corresponded to the compound concentration causing 50% mortality in cancer cells.

Procedure for determination of U266 and LNCaP viability by CCK-8 asssay:

Renal cancer cell ACHN, colorectal cancer cell HCT116, cervical cancer cell HeLa, liver cancer HepG2, and prostate cancer cell PC3 were seeded in 96-well plates at the density of 4,000 cells per well with 100 μL of complete culture medium. Myeloma U266 cells were seeded 8,000 cells per well and prostate cancer LNCaP cells were seeded 10,000 cells per well. After 24 hours, selected different products were added to the medium with eight concentrations ranging from 0.1 μM to 200 μM. The cells were then cultured for another 48 h. Cells without product exposure were used as control, and the wells to which only culture medium was added served as blank. At the end of stimulation, 10 μL SuperKine™ Cell-Counting-Kit-8 (BMU 106-CN, Abbkine, USA) was added to the medium, and the cells were cultured for 1-3 h at 37 °C. Then, the culture plates were shaken for 10 seconds, and the optical density (OD) values were read at wave-length of 450 nm in microplate reader (Thermo Scientific™ Multiskan™ FC, USA).

Note: N = 6 for each experimental group, and measurements were taken from 3 distinct samples.

Data analysis

Data are represented as means ± SD, and IC_{50} was performed using Prism 9.0 software (Graphpad Prism).

9. X-Ray crystallographic data

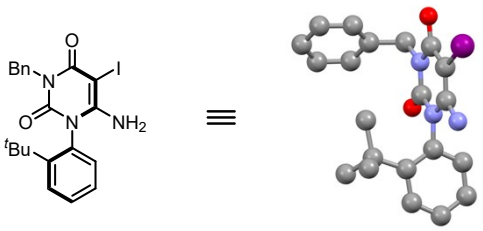


Table S6 Crystal data and structure refinement for R20240527a_auto.

Identification code	R20240527a_auto
Empirical formula	$C_{21}H_{22}N_3O_2I$
Formula weight	475.31
Temperature/K	294.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.08226(8)
b/Å	11.95569(19)
c/Å	28.8869(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2100.59(5)
Z	4
ρ_{calc}g/cm^3	1.503
μ/mm^{-1}	1.544
F(000)	952.0
Crystal size/mm^3	0.42 × 0.14 × 0.08
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.432 to 56.554
Index ranges	-8 ≤ h ≤ 7, -11 ≤ k ≤ 15, -38 ≤ l ≤ 38
Reflections collected	28525
Independent reflections	5195 [R_{int} = 0.0366, R_{sigma} = 0.0244]
Data/restraints/parameters	5195/66/260
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0325, wR_2 = 0.0734
Final R indexes [all data]	R_1 = 0.0356, wR_2 = 0.0757
Largest diff. peak/hole / e Å^{-3}	0.75/-0.59
Flack parameter	-0.050(6)

10. Computational details

Computational details of racemic energy barrier

All density functional theory (DFT) calculations were performed using Gaussian 16.[3] Geometry optimizations and frequencies were calculated at the B3LYP/def2-SVP level of theory.[4-7]Frequency calculations confirmed that optimized structures are minima (no imaginary frequency) or transition structures (one imaginary frequency). To obtain more accurate electronic energies, single-point energy calculations were performed at the M06-2X-D3/6-311+G(d,p)-SMD(DCM)[8-13] and M06-2X-D3/Lanl2DZ(I)-SMD(DCM)[14] level of theory with the optimized structures. Structures were generated using CYLview.[15]

The Calculated Cartesian Coordinates and energies of structures.

(*S*)-1a

C	-2.638713	-0.871720	0.083436
C	-3.878235	-1.348766	-0.394973
C	-4.675226	-0.647834	-1.298898
C	-4.258363	0.592499	-1.781538
C	-3.038142	1.095318	-1.341818
C	-2.238756	0.387787	-0.428593
N	-1.4313	1.050525	-0.062692
C	-0.990277	2.039772	0.913076
C	0.167458	2.722692	1.187144
C	1.389801	2.448431	0.484663
N	1.286490	1.440290	-0.522925
C	0.134138	0.750953	-0.840747
O	0.0736	-0.078237	-1.730534
O	2.460740	3.3472	0.679910
N	-2.153920	2.244096	1.594045
C	3.291583	-0.042741	-0.765264
C	3.169638	-1.319279	-1.334983
C	3.910138	-2.394924	-0.834647
C	4.778258	-2.207474	0.244781
C	4.902948	-0.938882	0.821256
C	4.165905	0.137122	0.3202
C	2.494856	1.127777	-1.309858
C	-1.814969	-1.788886	1.027951
C	-0.979268	-2.745933	0.142348
C	-2.753242	-2.635540	1.922555
C	-0.869850	-1.034738	1.990744
H	-4.237550	-2.317812	-0.052445
H	-5.624342	-1.079287	-1.626811
H	-4.864685	1.154720	-2.495257
H	-2.669881	2.055327	-1.711015
H	0.195818	3.490777	1.958166
H	-3.024058	1.884398	1.223696
H	-2.203738	3.042650	2.211369
H	2.482765	-1.466450	-2.171855
H	3.808145	-3.383379	-1.290766
H	5.358694	-3.047762	0.635234
H	5.582522	-0.785145	1.663918
H	4.257080	1.129922	0.767416
H	3.103994	2.039069	-1.290984
H	2.170371	0.920635	-2.336492
H	-0.371466	-3.413406	0.775368
H	-1.632903	-3.372815	-0.484947
H	-0.308375	-2.187711	-0.525207
H	-2.146976	-3.224460	2.627492
H	-3.359828	-3.3551	1.354443
H	-3.434944	-2.1986	2.512964
H	-1.398231	-0.249222	2.551773
H	-0.465076	-1.750670	2.722609
H	-0.7946	-0.582443	1.487528

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1128.718079 Hartree

Corrected Gibbs Free Energy = -1128.365999 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 19.84 cm^{-1}

(*R*)-1a

C	2.638703	-0.871729	0.083446
C	3.878222	-1.348790	-0.394956
C	4.675216	-0.647878	-1.298894
C	4.258358	0.592449	-1.781556
C	3.038142	1.095284	-1.341841
C	2.238753	0.387774	-0.428602
N	1.4318	1.050526	-0.062703
C	0.990295	2.039780	0.913058
C	-0.167438	2.722702	1.187137
C	-1.389788	2.448439	0.484672
N	-1.286487	1.440301	-0.522921
C	-0.134139	0.750964	-0.840755
O	-0.073609	-0.078226	-1.730543
O	-2.460723	3.3486	0.679923
N	2.153947	2.244120	1.5940
C	-3.291579	-0.042735	-0.765259
C	-4.165883	0.137109	0.3225
C	-4.902917	-0.938904	0.821271
C	-4.778237	-2.207486	0.244771
C	-3.910135	-2.394917	-0.834675
C	-3.169643	-1.319262	-1.3354
C	-2.494859	1.127793	-1.309846
C	1.814946	-1.788875	1.027969
C	0.869894	-1.034695	1.990803
C	2.753206	-2.635592	1.922527
C	0.979175	-2.745868	0.142374
H	4.237533	-2.317832	-0.052411
H	5.624329	-1.079341	-1.626801
H	4.864682	1.154653	-2.495287
H	2.669887	2.055290	-1.711051

H	-0.195788	3.490794	1.958154
H	3.024075	1.884348	1.223704
H	2.203771	3.042640	2.211363
H	-4.257049	1.129901	0.767458
H	-5.582476	-0.785183	1.663948
H	-5.358666	-3.047781	0.635219
H	-3.808149	-3.383364	-1.290813
H	-2.482784	-1.466418	-2.171890
H	-2.170381	0.920661	-2.336485
H	-3.1040	2.039082	-1.290960
H	0.7996	-0.582350	1.487620
H	0.465107	-1.750617	2.722672
H	1.398329	-0.249212	2.551827
H	2.146932	-3.224497	2.627471
H	3.434958	-2.2085	2.512929
H	3.359737	-3.355072	1.354381
H	0.371359	-3.413322	0.775401
H	0.308289	-2.187606	-0.525156
H	1.632764	-3.372770	-0.484948

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1128.718079 Hartree

Corrected Gibbs Free Energy = -1128.365999 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 19.84 cm^{-1}

2

N	-1.256042	1.437533	-0.61
C	-0.643984	0.317078	0.25
O	-1.435274	-0.820751	0.0255
C	-2.755842	-0.392862	0.0428
C	-2.670465	1.1359	-0.0382
O	-3.682061	-1.140667	0.02
C	0.807965	0.099384	-0.03
C	1.667206	1.212913	0.0206
C	3.047824	1.026245	0.0132
C	3.582401	-0.268562	-0.41
C	2.730951	-1.377277	-0.0183
C	1.345973	-1.198235	-0.0153
H	-3.186849	1.544556	0.883384
H	-3.186154	1.543662	-0.884992
H	1.230414	2.213259	0.0312
H	3.713402	1.892916	0.0210
H	4.665994	-0.411887	-0.55
H	3.146804	-2.387729	-0.0328
H	0.675180	-2.058622	-0.0328

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -552.324163 Hartree

Corrected Gibbs Free Energy = -552.215259 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 55.60 cm^{-1}

(*S*)-3a

C	-0.374229	-1.870511	0.1979
C	-1.373491	-2.8010	-0.161386
C	-2.192527	-2.654371	-1.276597
C	-2.049351	-1.540491	-2.105964
C	-1.061392	-0.613424	-1.8284
C	-0.231952	-0.7705	-0.676324
N	0.790925	0.247449	-0.536460
C	0.510974	1.516895	-0.030710
C	1.431391	2.519096	-0.125239
C	2.724935	2.293441	-0.729124
N	2.948961	0.973296	-1.202606
C	2.028383	-0.056117	-1.140489
O	2.249778	-1.169327	-1.580333
O	3.597779	3.139929	-0.837079
N	-0.733813	1.643025	0.585998
C	-1.279697	2.803436	1.1175
C	-2.628417	2.6751	1.823087
O	-0.761086	3.898733	1.067995
N	-3.705884	2.077082	1.0658
C	-3.874364	0.734796	0.832549
O	-3.041829	-0.059109	1.269882
C	5.274767	0.110398	-0.853588
C	5.497556	-1.272853	-0.772270
C	6.442652	-1.789156	0.119667
C	7.173376	-0.928514	0.943986
C	6.954794	0.451297	0.871990
C	6.012589	0.968557	-0.020850
C	4.253756	0.673831	-1.824014
C	0.470922	-2.1985	1.459214
C	1.450486	-3.3322	1.095918
C	-0.467409	-2.649755	2.604362
C	1.292706	-1.012223	2.0254
C	-5.109186	0.278161	0.114163
C	-5.514515	-1.052132	0.3073

C	-6.659453	-1.538536	-0.324225
C	-7.401596	-0.707235	-1.170326
C	-6.992875	0.612590	-1.384981
C	-5.853168	1.1043	-0.744753
H	-1.513986	-3.685423	0.459754
H	-2.946791	-3.414106	-1.496497
H	-2.683460	-1.405562	-2.985052
H	-0.897634	0.253636	-2.444579
H	1.222292	3.504962	0.272465
H	-1.290194	0.791232	0.718271
H	-2.473889	1.919208	2.676604
H	-2.912133	3.589598	2.202663
H	-4.4349	2.716010	0.699789
H	4.918065	-1.944512	-1.4118
H	6.608793	-2.868673	0.1732
H	7.913615	-1.331768	1.640315
H	7.524614	1.129934	1.512475
H	5.834696	2.045136	-0.078179
H	4.610642	1.624442	-2.237263
H	4.069298	-0.037896	-2.637141
H	2.116945	-3.023172	0.277439
H	2.066503	-3.598299	1.970872
H	0.912166	-4.237117	0.773245
H	-1.233403	-1.887722	2.818097
H	0.121546	-2.815912	3.5248
H	-0.984608	-3.594043	2.382650
H	0.666791	-0.134250	2.244202
H	1.746778	-1.329836	2.976558
H	2.117571	-0.704499	1.371983
H	-4.913045	-1.687874	0.958723
H	-6.973903	-2.572073	-0.159515
H	-8.295882	-1.089889	-1.668607
H	-7.559175	1.260292	-2.058517
H	-5.534604	2.129722	-0.950418

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1681.077554 Hartree

Corrected Gibbs Free Energy = -1680.594407 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 7.54 cm^{-1}

TS1-major

P	1.343174	-0.521875	-0.478760
O	2.459177	-0.175487	0.667201
O	1.786921	-2.029155	-0.934239
C	3.807408	-0.3937	0.433620
C	4.652924	0.755796	0.366810
C	5.997230	0.545220	0.130665
H	6.674044	1.402418	0.105780
C	6.529626	-0.749287	-0.107388
C	7.899634	-0.930439	-0.449187
H	8.544892	-0.049289	-0.501956
C	8.401693	-2.183187	-0.727108
H	9.453125	-2.309212	-0.997121
C	7.543646	-3.308752	-0.679866
H	7.934422	-4.298830	-0.927940
C	6.216253	-3.167725	-0.329586
H	5.570895	-4.045541	-0.308295
C	5.667401	-1.891161	-0.014501
C	4.285379	-1.697351	0.351713
C	3.392428	-2.862274	0.628483
C	3.749791	-3.865796	1.6403
C	4.843220	-3.721822	2.502242
H	5.438210	-2.808884	2.476969
C	5.151156	-4.708698	3.416681
H	5.989341	-4.566484	4.103586
C	4.388617	-5.9471	3.476598
H	4.647761	-6.678711	4.198756
C	3.311278	-6.064502	2.633063
H	2.701178	-6.970587	2.681755
C	2.954214	-5.055810	1.693957
C	1.811904	-5.198398	0.862130
H	1.232260	-6.122893	0.921636
C	1.388241	-4.192922	0.015169
C	2.192431	-3.014383	-0.058036
O	-0.017471	-0.461450	0.184808
O	1.520818	0.337763	-1.728232
H	0.392565	0.501599	-2.382975
C	4.1346	2.142990	0.607769
C	3.989071	3.054513	-0.467182
C	3.844294	2.562919	1.932309
C	3.587924	4.370177	-0.185914
C	3.438332	3.884815	2.153485
C	3.311358	4.811166	1.111723
H	3.495871	5.081997	-1.011058
H	3.228749	4.203283	3.178108
C	0.138032	-4.327372	-0.801699
C	-1.129630	-4.314898	-0.167352

C	0.218937	-4.475921	-2.210827	H	6.034845	2.272083	3.620141
C	-2.282847	-4.424131	-0.959546	H	4.781437	3.1405	4.572070
C	-0.964267	-4.592498	-2.9556	C	4.282834	2.660924	-1.915823
C	-2.229029	-4.559994	-2.349978	C	5.632983	3.230935	-2.389874
H	-3.264440	-4.388028	-0.481179	C	3.156863	3.060715	-2.883081
H	-0.893177	-4.713479	-4.034054	H	4.350407	1.564213	-1.951459
C	1.554276	-4.557016	-2.951801	H	5.853249	2.903202	-3.419234
C	1.705218	-3.452987	-4.012734	H	5.622992	4.333838	-2.384235
C	1.770326	-5.954294	-3.562550	H	6.465018	2.904771	-1.747342
H	2.358897	-4.407967	-2.217884	H	2.192641	2.651029	-2.553392
H	1.593098	-2.455763	-3.563388	H	3.063343	4.154767	-2.983216
H	2.701675	-3.504974	-4.482085	H	3.365205	2.660709	-3.888760
H	0.957637	-3.555020	-4.816634	C	2.908788	6.256884	1.378890
H	2.763016	-6.021259	-4.038044	C	3.973379	7.3526	2.202063
H	1.707172	-6.7428	-2.795044	C	1.521608	6.368119	2.034127
H	1.016232	-6.180529	-4.334263	H	2.849264	6.7569	0.395312
C	-1.298748	-4.183670	1.347719	H	4.081074	6.565472	3.207962
C	-1.916435	-5.454465	1.958922	H	4.959087	6.960254	1.713168
C	-2.099625	-2.930494	1.737970	H	3.7392	8.064406	2.328390
H	-0.3569	-4.065066	1.790470	H	0.748791	5.871084	1.426961
H	-1.975428	-5.368830	3.056740	H	1.511722	5.903911	3.034021
H	-2.938195	-5.627753	1.583238	H	1.231154	7.424662	2.158035
H	-1.320979	-6.350265	1.719946	C	-1.614937	3.725804	-2.855556
H	-2.158276	-2.840433	2.835626	C	-1.370754	1.528383	-2.472524
H	-1.613140	-2.026393	1.343801	C	-2.639399	1.832559	-3.287485
H	-3.132333	-2.968692	1.355101	H	-2.5233	1.359266	-4.2764
C	-3.509966	-4.695325	-3.164989	H	-3.562036	1.424803	-2.849768
C	-3.689017	-6.129713	-3.694186	O	-0.617295	0.563399	-2.856825
C	-3.596852	-3.668099	-4.304911	O	-0.763422	2.788528	-2.293595
H	-4.343645	-4.479898	-2.477899	N	-2.677648	3.276689	-3.398793
H	-3.674858	-6.863490	-2.872880	C	-1.194473	5.130103	-2.770138
H	-4.648373	-6.234738	-4.227979	C	-1.990553	6.114439	-3.384383
H	-2.883641	-6.401628	-4.397059	C	-0.018643	5.502096	-2.098379
H	-2.801851	-3.815210	-5.054614	C	-1.615549	7.454750	-3.3203
H	-4.563439	-3.752208	-4.828529	H	-2.895740	5.805209	-3.910121
H	-3.511707	-2.640936	-3.918222	C	0.350379	6.848388	-2.039476
C	3.992285	1.631108	3.135629	H	0.605885	4.739468	-1.631087
C	2.647766	1.387478	3.842929	C	-0.444399	7.824702	-2.646607
C	5.062998	2.135023	4.120205	H	-2.234918	8.216121	-3.8722
H	4.339433	0.656058	2.766180	H	1.266075	7.134290	-1.517137
H	1.904393	0.979375	3.142332	H	-0.1536	8.876235	-2.599420
H	2.770595	0.666870	4.668373	N	-1.827851	1.189859	-0.766904
H	2.241213	2.317574	4.274081	C	-2.829916	1.866318	3.043852
H	5.202861	1.413682	4.942182	C	-5.372706	0.999959	0.312438

C	-3.112053	0.629270	-0.519773
C	-3.127203	2.932172	1.951370
C	-3.414565	-0.621704	-0.946710
C	-3.689629	2.731191	0.665914
C	-3.9461	3.805908	-0.202779
C	-4.749731	-1.161774	-0.756542
C	-3.012186	5.335096	1.383138
C	-3.617127	5.110435	0.145575
C	-2.779954	4.269297	2.248581
H	-1.055819	0.501889	-0.410678
H	-2.668556	-1.245398	-1.435976
H	-3.817528	5.932505	-0.543956
H	-2.310439	4.487211	3.207267
H	-1.709132	2.075528	-0.266067
C	-3.569431	0.523258	2.873778
H	-3.364410	-0.101662	3.756149
H	-4.658772	0.661668	2.820588
H	-3.231822	-0.056093	2.6236
C	-1.305875	1.595250	3.071137
H	-0.949103	1.121011	2.143740
H	-0.729810	2.520908	3.224741
H	-1.060935	0.907510	3.896546
C	-3.268491	2.418217	4.425330
H	-4.334075	2.696312	4.422290
H	-3.123304	1.6444	5.190280
H	-2.6873	3.293623	4.747359
H	-2.722033	6.345204	1.6822
H	-4.401938	3.596357	-1.171795
N	-4.036709	1.423062	0.140314
O	-6.191290	1.721257	0.842457
N	-5.670884	-0.273255	-0.153889
C	-7.065118	-0.738113	0.023013
H	-7.709813	0.138769	-0.106917
H	-7.247353	-1.451988	-0.788391
C	-7.329375	-1.392043	1.366298
C	-7.079454	-2.761768	1.551813
C	-7.833425	-0.640868	2.440118
C	-7.329431	-3.366922	2.786439
H	-6.683485	-3.347993	0.719494
C	-8.084367	-1.247983	3.674226
H	-8.020682	0.426537	2.303272
C	-7.832790	-2.611880	3.850485
H	-7.133630	-4.434501	2.916787
H	-8.480575	-0.652617	4.501132
H	-8.031335	-3.086721	4.814969
O	-5.098458	-2.280917	-1.095575

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -4262.820721 Hartree

Corrected Gibbs Free Energy = -4261.454835 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -299.63 cm^{-1}

TS1-minor

P	-1.387802	-0.448551	0.320113
O	-2.897372	-0.185515	-0.261871
O	-1.402235	-2.064953	0.567546
C	-3.985039	-0.612812	0.488801
C	-4.829198	0.383703	1.067602
C	-5.899441	-0.055983	1.823632
H	-6.586086	0.679687	2.247487
C	-6.125503	-1.430152	2.0970
C	-7.169654	-1.847924	2.9755
H	-7.815443	-1.085444	3.413995
C	-7.353181	-3.180688	3.268034
H	-8.1516	-3.489373	3.947403
C	-6.489879	-4.151804	2.704190
H	-6.618015	-5.205937	2.962793
C	-5.484105	-3.779529	1.835769
H	-4.824624	-4.540408	1.418263
C	-5.277783	-2.413029	1.4974
C	-4.239522	-1.977543	0.590287
C	-3.4735	-2.955789	-0.236280
C	-4.159306	-3.889458	-1.095960
C	-5.561353	-3.837349	-1.346877
H	-6.156710	-3.046784	-0.891191
C	-6.176467	-4.760317	-2.168023
H	-7.252070	-4.689587	-2.348724
C	-5.427861	-5.793820	-2.782229
H	-5.928506	-6.524831	-3.421971
C	-4.066068	-5.858606	-2.583897
H	-3.4707	-6.635524	-3.070410
C	-3.399145	-4.907022	-1.760922
C	-1.987863	-4.922287	-1.618744
H	-1.418695	-5.701576	-2.131506
C	-1.305441	-3.954648	-0.905989
C	-2.082136	-2.975322	-0.215528

O	-0.389589	-0.017327	-0.729943	H	5.095580	-2.523965	-2.118844
O	-1.228642	0.153602	1.716662	H	6.354118	-3.773602	-2.106770
H	-0.367818	1.041261	1.915484	H	4.432822	-6.2994	-2.178680
C	-4.631133	1.853575	0.831554	H	5.906577	-6.095029	-1.193221
C	-4.238983	2.706363	1.897313	H	4.348812	-6.473660	-0.412319
C	-4.927698	2.408239	-0.438683	C	-5.383896	1.555043	-1.623070
C	-4.176494	4.0882	1.669902	C	-4.389881	1.614771	-2.796037
C	-4.838088	3.797054	-0.6110	C	-6.808767	1.922769	-2.075675
C	-4.476120	4.6602	0.428601	H	-5.421412	0.508136	-1.291715
H	-3.885058	4.739316	2.497019	H	-4.318719	2.633136	-3.213860
H	-5.075921	4.227773	-1.587051	H	-3.386248	1.297463	-2.476316
C	0.194653	-3.946558	-0.911602	H	-4.713389	0.947049	-3.611653
C	0.878975	-3.630557	-2.112682	H	-7.145379	1.248735	-2.880728
C	0.931919	-4.325445	0.239281	H	-7.526284	1.842554	-1.243832
C	2.278380	-3.741280	-2.149338	H	-6.861828	2.953502	-2.463048
C	2.327074	-4.406158	0.148962	C	-3.896933	2.176682	3.292097
C	3.024559	-4.146312	-1.038603	C	-5.033824	2.446789	4.296219
H	2.793336	-3.515549	-3.085109	C	-2.571422	2.738258	3.833170
H	2.894987	-4.707343	1.034219	H	-3.768301	1.087875	3.210675
C	0.257188	-4.7191	1.559336	H	-5.988612	2.7577	3.970505
C	0.618121	-3.726996	2.695878	H	-4.788011	2.023279	5.284039
C	0.557952	-6.158316	1.953589	H	-5.196522	3.529681	4.427297
H	-0.8303	-4.633907	1.410139	H	-1.747807	2.584714	3.123911
H	0.124790	-4.034216	3.632918	H	-2.638867	3.816418	4.053950
H	1.702608	-3.689514	2.885720	H	-2.303037	2.231304	4.774234
H	0.279455	-2.708141	2.460344	C	-4.453403	6.169166	0.214826
H	1.626757	-6.309309	2.176745	C	-3.120857	6.813334	0.6297
H	-0.8971	-6.437117	2.856993	C	-5.641527	6.849652	0.919341
H	0.281590	-6.858807	1.149331	H	-4.575024	6.337169	-0.869644
C	0.154630	-3.167520	-3.379818	H	-3.119790	7.889599	0.390255
C	0.351654	-4.145925	-4.551136	H	-2.943339	6.718601	1.712860
C	0.553167	-1.735090	-3.775597	H	-2.271485	6.348338	0.106165
H	-0.921233	-3.139547	-3.1627	H	-5.656873	7.931990	0.708511
H	-0.231045	-3.822025	-5.429292	H	-6.601277	6.423318	0.587745
H	1.408447	-4.206643	-4.859321	H	-5.580644	6.722110	2.012888
H	0.026151	-5.164487	-4.286775	C	0.659687	4.208983	-0.209811
H	0.350167	-1.033873	-2.951973	C	0.963630	2.465401	1.159247
H	1.621829	-1.673441	-4.0421	C	1.960512	3.592624	1.443461
H	-0.024372	-1.405507	-4.655502	H	1.709901	4.0217	2.429266
C	4.530578	-4.390514	-1.094803	H	3.2679	3.251473	1.496436
C	5.2683	-3.608462	-2.188676	O	0.476771	1.795716	2.135726
C	4.821821	-5.899514	-1.223632	O	0.055404	3.054110	0.245254
H	4.938492	-4.065413	-0.120875	N	1.738596	4.558759	0.381315
H	4.968878	-3.939286	-3.196810	C	0.2024	4.886144	-1.334287

C	0.472932	6.144486	-1.751379
C	-1.076120	4.283020	-2.3767
C	-0.128916	6.789208	-2.829774
H	1.308589	6.598997	-1.216303
C	-1.669984	4.934550	-3.087014
H	-1.439962	3.308231	-1.675821
C	-1.2224	6.184616	-3.5342
H	0.235769	7.767995	-3.150822
H	-2.504921	4.460899	-3.608024
H	-1.669885	6.691852	-4.347076
N	1.725018	1.363381	0.032075
C	5.744751	3.225629	-0.839181
C	5.075837	-0.251788	0.048684
C	2.815818	0.552832	0.484191
C	4.805395	2.441826	-1.797619
C	2.698795	-0.225216	1.585969
C	4.050290	1.270889	-1.547628
C	3.294879	0.652921	-2.562949
C	3.807921	-1.049491	2.034402
C	3.958357	2.342777	-4.120394
C	3.231368	1.183481	-3.845419
C	4.720896	2.936406	-3.119116
H	0.874347	0.756238	-0.287615
H	1.784729	-0.243144	2.172064
H	2.630934	0.692628	-4.613881
H	5.286359	3.832310	-3.376103
H	2.5673	1.907870	-0.789903
C	5.792168	2.746988	0.625501
H	4.802565	2.705058	1.097964
H	6.279047	1.770879	0.732740
H	6.393525	3.463675	1.2055
C	7.186976	3.104801	-1.393576
H	7.283966	3.534821	-2.401630
H	7.888214	3.640506	-0.733354
H	7.491823	2.048533	-1.439274
C	5.311511	4.714044	-0.816646
H	4.282497	4.830602	-0.440804
H	5.983661	5.284280	-0.155793
H	5.358735	5.183883	-1.809718
H	3.938141	2.786489	-5.118756
H	2.751249	-0.263616	-2.323989
N	3.991282	0.596763	-0.262210
O	6.051844	-0.303935	-0.673828
N	4.958577	-0.995976	1.2117
C	6.117430	-1.831826	1.593598
H	5.702614	-2.675611	2.156833
H	6.571752	-2.195294	0.665361
C	7.143980	-1.093533	2.431070
C	8.2995	-0.561527	1.837943
C	6.952898	-0.934075	3.813957
C	9.2477	0.115138	2.611615
H	8.450147	-0.677933	0.7625
C	7.899686	-0.255259	4.585251
H	6.053420	-1.345622	4.2782
C	9.049477	0.270536	3.986555
H	10.145764	0.520536	2.137966
H	7.741358	-0.140734	5.660864
H	9.791582	0.797539	4.592094
O	3.785582	-1.752737	3.029139

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -4262.819075 Hartree

Corrected Gibbs Free Energy = -4261.451959 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -384.47 cm^{-1}

TS1R (Rotating intermediate)

C	-3.154223	0.448368	-0.138106
C	-3.902231	1.482635	-0.742680
C	-3.501232	2.809105	-0.852926
C	-2.289515	3.167295	-0.280113
C	-1.488143	2.180664	0.280742
C	-1.825829	0.805726	0.302020
N	-0.717403	-0.059630	0.7586
C	-0.591144	-1.465248	0.578492
C	0.194733	-1.940339	-0.431970
C	1.038884	-1.040232	-1.196742
N	1.262527	0.216713	-0.551437
C	0.6691	0.558574	0.608892
O	1.028271	1.351438	1.413717
O	1.648133	-1.324148	-2.209953
N	-1.225777	-2.259739	1.477548
C	3.762136	0.521168	-0.3758
C	4.550763	-0.411875	-1.068555
C	5.768220	-0.846679	-0.536817
C	6.213788	-0.354724	0.693565
C	5.434507	0.573874	1.390705

C	4.2179	1.8706	0.8602
C	2.444864	0.999797	-0.961213
C	-3.927511	-0.885957	0.092908
C	-5.419863	-0.803202	-0.326057
C	-3.986617	-1.145725	1.627825
C	-3.375929	-2.055646	-0.762033
H	-4.882570	1.235056	-1.139582
H	-4.147535	3.542495	-1.340150
H	-1.946486	4.204677	-0.266667
H	-0.556567	2.501699	0.733070
H	0.330434	-3.7917	-0.606961
H	-1.532386	-1.860534	2.3521
H	-1.067143	-3.258023	1.445984
H	4.196586	-0.802883	-2.024906
H	6.372606	-1.571694	-1.088523
H	7.167570	-0.692565	1.107701
H	5.777174	0.964207	2.352779
H	3.602352	1.724884	1.409744
H	2.252933	2.039392	-0.667880
H	2.475817	0.937294	-2.055968
H	-5.552203	-0.671234	-1.410148
H	-5.902039	-1.756796	-0.057635
H	-5.965064	-0.2693	0.194743
H	-4.152557	-2.211052	1.852994
H	-4.825031	-0.577712	2.0651
H	-3.095509	-0.804416	2.164158
H	-3.832805	-3.8505	-0.4472
H	-3.651833	-1.889552	-1.815458
H	-2.292550	-2.171559	-0.745315

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1128.643789 Hartree

Corrected Gibbs Free Energy = -1128.290364 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -45.97 cm^{-1}

TS1IR (Rotating intermediate)

C	2.738314	0.754602	-0.033825
C	3.643129	1.790392	0.265690
C	3.234687	3.107341	0.429592
C	1.878669	3.393952	0.291927
C	0.977382	2.378422	0.6203
C	1.348446	1.019153	-0.170734
N	0.281840	0.089686	-0.460992
C	0.241022	-1.255705	0.021227
C	-0.503260	-1.525831	1.132581
C	-1.507963	-0.577940	1.576320
N	-1.806194	0.454761	0.622608
C	-1.044174	0.688292	-0.5056
O	-1.388013	1.397499	-1.4162
O	-2.183854	-0.680523	2.5828
N	0.827063	-2.189667	-0.7654
C	-4.273217	0.453087	0.145428
C	-5.038317	-0.446892	0.904816
C	-6.129806	-1.107568	0.333869
C	-6.4719	-0.877655	-1.2630
C	-5.712233	0.015537	-1.766481
C	-4.620609	0.676452	-1.196715
C	-3.088890	1.170153	0.767504
H	4.701231	1.547143	0.366418
H	3.965752	3.885834	0.656687
H	1.505281	4.413680	0.410634
H	-0.064538	2.663075	-0.105766
H	-0.548939	-2.522710	1.572085
H	1.493795	-1.897361	-1.467369
H	0.938054	-3.129177	-0.403306
H	-4.765531	-0.631705	1.946465
H	-6.718765	-1.803479	0.937277
H	-7.325624	-1.392301	-1.447979
H	-5.973266	0.2717	-2.811869
H	-4.021451	1.366387	-1.795492
H	-2.958773	2.157532	0.307439
H	-3.243043	1.290178	1.846492
I	3.819487	-1.1035	-0.232912

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -982.17625 Hartree

Corrected Gibbs Free Energy = -981.943784 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -36.54 cm^{-1}

(*R*)-**1p**

C	-2.6062	0.886390	-0.030478
C	-3.536242	1.929664	-0.108658
C	-3.256883	3.158722	0.493316
C	-2.052329	3.351990	1.175230

C	-1.128329	2.310991	1.252846
C	-1.392457	1.071293	0.654818
N	-0.412974	0.026996	0.758234
C	-0.4307	-0.881158	1.812870
C	0.533125	-1.851327	1.893731
C	1.591320	-1.950554	0.924603
N	1.547638	-0.973348	-0.116021
C	0.5947	0.014268	-0.237815
O	0.580442	0.839817	-1.129277
O	2.484078	-2.783928	0.936348
N	-1.411170	-0.712829	2.748434
C	3.797985	-0.115277	-0.802839
C	4.828910	-0.586692	0.026928
C	5.920158	0.230154	0.334784
C	5.995655	1.527913	-0.181544
C	4.972246	2.5672	-1.5578
C	3.879303	1.189799	-1.313176
C	2.614205	-1.4445	-1.135485
H	-4.475251	1.782604	-0.644527
H	-3.987483	3.968305	0.423411
H	-1.829737	4.313704	1.642518
H	-0.178105	2.443523	1.773982
H	0.532546	-2.575032	2.707038
H	-2.244162	-0.190716	2.506726
H	-1.535178	-1.461459	3.417235
H	4.760118	-1.598117	0.434494
H	6.717628	-0.149920	0.979085
H	6.851628	2.165072	0.056881
H	5.024843	3.019112	-1.412744
H	3.071668	1.565693	-1.945601
H	2.161733	-0.696426	-2.085520
H	2.934033	-2.050802	-1.2639
I	-3.062784	-0.964015	-0.969146

M062X-D3/6-311+G(d,p) and Lanl2DZ(I)-SMD(CCl4): E = -982.235594 Hartree

Corrected Gibbs Free Energy = -982.004627 Hartree

Computational details of the enantioselectivity

All density functional theory (DFT) calculations were performed using Gaussian 16.[3] Geometry optimizations and frequencies were calculated at the B3LYP/def2-SVP level of theory.[4-7] Frequency calculations confirmed that optimized structures are minima (no imaginary frequency) or transition structures (one imaginary frequency). To obtain more accurate electronic energies, single-point energy calculations were performed at the M06-2X-D3/6-311+G(d,p)-SMD(DCM)[8-13] level of theory with the optimized structures. Structures were generated using CYLview.[15]

The calculated Cartesian coordinates and energies of structures.

(*S*)-1

C	-2.638713	-0.871720	0.083436
C	-3.878235	-1.348766	-0.394973
C	-4.675226	-0.647834	-1.298898
C	-4.258363	0.592499	-1.781538
C	-3.038142	1.095318	-1.341818
C	-2.238756	0.387787	-0.428593
N	-1.4313	1.050525	-0.062692
C	-0.990277	2.039772	0.913076
C	0.167458	2.722692	1.187144
C	1.389801	2.448431	0.484663
N	1.286490	1.440290	-0.522925
C	0.134138	0.750953	-0.840747
O	0.0736	-0.078237	-1.730534
O	2.460740	3.3472	0.679910
N	-2.153920	2.244096	1.594045
C	3.291583	-0.042741	-0.765264
C	3.169638	-1.319279	-1.334983
C	3.910138	-2.394924	-0.834647
C	4.778258	-2.207474	0.244781
C	4.902948	-0.938882	0.821256
C	4.165905	0.137122	0.3202
C	2.494856	1.127777	-1.309858
C	-1.814969	-1.788886	1.027951
C	-0.979268	-2.745933	0.142348
C	-2.753242	-2.635540	1.922555
C	-0.869850	-1.034738	1.990744
H	-4.237550	-2.317812	-0.052445
H	-5.624342	-1.079287	-1.626811
H	-4.864685	1.154720	-2.495257
H	-2.669881	2.055327	-1.711015
H	0.195818	3.490777	1.958166

H	-3.024058	1.884398	1.223696
H	-2.203738	3.042650	2.211369
H	2.482765	-1.466450	-2.171855
H	3.808145	-3.383379	-1.290766
H	5.358694	-3.047762	0.635234
H	5.582522	-0.785145	1.663918
H	4.257080	1.129922	0.767416
H	3.103994	2.039069	-1.290984
H	2.170371	0.920635	-2.336492
H	-0.371466	-3.413406	0.775368
H	-1.632903	-3.372815	-0.484947
H	-0.308375	-2.187711	-0.525207
H	-2.146976	-3.224460	2.627492
H	-3.359828	-3.3551	1.354443
H	-3.434944	-2.1986	2.512964
H	-1.398231	-0.249222	2.551773
H	-0.465076	-1.750670	2.722609
H	-0.7946	-0.582443	1.487528

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1128.718079 Hartree

Corrected Gibbs Free Energy = -1128.365999 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 19.84 cm^{-1}

(*R*)-1

C	2.638703	-0.871729	0.083446
C	3.878222	-1.348790	-0.394956
C	4.675216	-0.647878	-1.298894
C	4.258358	0.592449	-1.781556
C	3.038142	1.095284	-1.341841
C	2.238753	0.387774	-0.428602
N	1.4318	1.050526	-0.062703
C	0.990295	2.039780	0.913058
C	-0.167438	2.722702	1.187137
C	-1.389788	2.448439	0.484672
N	-1.286487	1.440301	-0.522921
C	-0.134139	0.750964	-0.840755
O	-0.073609	-0.078226	-1.730543
O	-2.460723	3.3486	0.679923
N	2.153947	2.244120	1.5940
C	-3.291579	-0.042735	-0.765259
C	-4.165883	0.137109	0.3225
C	-4.902917	-0.938904	0.821271
C	-4.778237	-2.207486	0.244771
C	-3.910135	-2.394917	-0.834675
C	-3.169643	-1.319262	-1.3354
C	-2.494859	1.127793	-1.309846
C	1.814946	-1.788875	1.027969
C	0.869894	-1.034695	1.990803
C	2.753206	-2.635592	1.922527
C	0.979175	-2.745868	0.142374
H	4.237533	-2.317832	-0.052411
H	5.624329	-1.079341	-1.626801
H	4.864682	1.154653	-2.495287
H	2.669887	2.055290	-1.711051
H	-0.195788	3.490794	1.958154
H	3.024075	1.884348	1.223704
H	2.203771	3.042640	2.211363
H	-4.257049	1.129901	0.767458
H	-5.582476	-0.785183	1.663948
H	-5.358666	-3.047781	0.635219
H	-3.808149	-3.383364	-1.290813
H	-2.482784	-1.466418	-2.171890
H	-2.170381	0.920661	-2.336485
H	-3.1040	2.039082	-1.290960
H	0.7996	-0.582350	1.487620
H	0.465107	-1.750617	2.722672
H	1.398329	-0.249212	2.551827
H	2.146932	-3.224497	2.627471
H	3.434958	-2.2085	2.512929
H	3.359737	-3.355072	1.354381
H	0.371359	-3.413322	0.775401
H	0.308289	-2.187606	-0.525156
H	1.632764	-3.372770	-0.484948

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1128.718079 Hartree

Corrected Gibbs Free Energy = -1128.365999 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 19.84 cm^{-1}

2

N	-1.256042	1.437533	-0.61
C	-0.643984	0.317078	0.25
O	-1.435274	-0.820751	0.0255
C	-2.755842	-0.392862	0.0428
C	-2.670465	1.1359	-0.0382

O	-3.682061	-1.140667	0.02
C	0.807965	0.099384	-0.03
C	1.667206	1.212913	0.0206
C	3.047824	1.026245	0.0132
C	3.582401	-0.268562	-0.41
C	2.730951	-1.377277	-0.0183
C	1.345973	-1.198235	-0.0153
H	-3.186849	1.544556	0.883384
H	-3.186154	1.543662	-0.884992
H	1.230414	2.213259	0.0312
H	3.713402	1.892916	0.0210
H	4.665994	-0.411887	-0.55
H	3.146804	-2.387729	-0.0328
H	0.675180	-2.058622	-0.0328

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -552.324163 Hartree

Corrected Gibbs Free Energy = -552.215259 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 55.60 cm^{-1}

(*S*)-3

C	-0.374229	-1.870511	0.1979
C	-1.373491	-2.8010	-0.161386
C	-2.192527	-2.654371	-1.276597
C	-2.049351	-1.540491	-2.105964
C	-1.061392	-0.613424	-1.8284
C	-0.231952	-0.7705	-0.676324
N	0.790925	0.247449	-0.536460
C	0.510974	1.516895	-0.030710
C	1.431391	2.519096	-0.125239
C	2.724935	2.293441	-0.729124
N	2.948961	0.973296	-1.202606
C	2.028383	-0.056117	-1.140489
O	2.249778	-1.169327	-1.580333
O	3.597779	3.139929	-0.837079
N	-0.733813	1.643025	0.585998
C	-1.279697	2.803436	1.1175
C	-2.628417	2.6751	1.823087
O	-0.761086	3.898733	1.067995
N	-3.705884	2.077082	1.0658
C	-3.874364	0.734796	0.832549
O	-3.041829	-0.059109	1.269882
C	5.274767	0.110398	-0.853588
C	5.497556	-1.272853	-0.772270
C	6.442652	-1.789156	0.119667
C	7.173376	-0.928514	0.943986
C	6.954794	0.451297	0.871990
C	6.012589	0.968557	-0.020850
C	4.253756	0.673831	-1.824014
C	0.470922	-2.1985	1.459214
C	1.450486	-3.3322	1.095918
C	-0.467409	-2.649755	2.604362
C	1.292706	-1.012223	2.0254
C	-5.109186	0.278161	0.114163
C	-5.514515	-1.052132	0.3073
C	-6.659453	-1.538536	-0.324225
C	-7.401596	-0.707235	-1.170326
C	-6.992875	0.612590	-1.384981
C	-5.853168	1.1043	-0.744753
H	-1.513986	-3.685423	0.459754
H	-2.946791	-3.414106	-1.496497
H	-2.683460	-1.405562	-2.985052
H	-0.897634	0.253636	-2.444579
H	1.222292	3.504962	0.272465
H	-1.290194	0.791232	0.718271
H	-2.473889	1.919208	2.676604
H	-2.912133	3.589598	2.202663
H	-4.4349	2.716010	0.699789
H	4.918065	-1.944512	-1.4118
H	6.608793	-2.868673	0.1732
H	7.913615	-1.331768	1.640315
H	7.524614	1.129934	1.512475
H	5.834696	2.045136	-0.078179
H	4.610642	1.624442	-2.237263
H	4.069298	-0.037896	-2.637141
H	2.116945	-3.023172	0.277439
H	2.066503	-3.598299	1.970872
H	0.912166	-4.237117	0.773245
H	-1.233403	-1.887722	2.818097
H	0.121546	-2.815912	3.5248
H	-0.984608	-3.594043	2.382650
H	0.666791	-0.134250	2.244202
H	1.746778	-1.329836	2.976558
H	2.117571	-0.704499	1.371983
H	-4.913045	-1.687874	0.958723
H	-6.973903	-2.572073	-0.159515
H	-8.295882	-1.089889	-1.668607

H	-7.559175	1.260292	-2.058517
H	-5.534604	2.129722	-0.950418

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -1681.077554 Hartree

Corrected Gibbs Free Energy = -1680.594407 Hartree

Number of imaginary frequencies: 0

Wavenumber of lowest frequency: 7.54 cm^{-1}

TS1-major

P	1.343174	-0.521875	-0.478760
O	2.459177	-0.175487	0.667201
O	1.786921	-2.029155	-0.934239
C	3.807408	-0.3937	0.433620
C	4.652924	0.755796	0.366810
C	5.997230	0.545220	0.130665
H	6.674044	1.402418	0.105780
C	6.529626	-0.749287	-0.107388
C	7.899634	-0.930439	-0.449187
H	8.544892	-0.049289	-0.501956
C	8.401693	-2.183187	-0.727108
H	9.453125	-2.309212	-0.997121
C	7.543646	-3.308752	-0.679866
H	7.934422	-4.298830	-0.927940
C	6.216253	-3.167725	-0.329586
H	5.570895	-4.045541	-0.308295
C	5.667401	-1.891161	-0.014501
C	4.285379	-1.697351	0.351713
C	3.392428	-2.862274	0.628483
C	3.749791	-3.865796	1.6403
C	4.843220	-3.721822	2.502242
H	5.438210	-2.808884	2.476969
C	5.151156	-4.708698	3.416681
H	5.989341	-4.566484	4.103586
C	4.388617	-5.9471	3.476598
H	4.647761	-6.678711	4.198756
C	3.311278	-6.064502	2.633063
H	2.701178	-6.970587	2.681755
C	2.954214	-5.055810	1.693957
C	1.811904	-5.198398	0.862130
H	1.232260	-6.122893	0.921636
C	1.388241	-4.192922	0.015169
C	2.192431	-3.014383	-0.058036
O	-0.017471	-0.461450	0.184808
O	1.520818	0.337763	-1.728232
H	0.392565	0.501599	-2.382975
C	4.1346	2.142990	0.607769
C	3.989071	3.054513	-0.467182
C	3.844294	2.562919	1.932309
C	3.587924	4.370177	-0.185914
C	3.438332	3.884815	2.153485
C	3.311358	4.811166	1.111723
H	3.495871	5.081997	-1.011058
H	3.228749	4.203283	3.178108
C	0.138032	-4.327372	-0.801699
C	-1.129630	-4.314898	-0.167352
C	0.218937	-4.475921	-2.210827
C	-2.282847	-4.424131	-0.959546
C	-0.964267	-4.592498	-2.9556
C	-2.229029	-4.559994	-2.349978
H	-3.264440	-4.388028	-0.481179
H	-0.893177	-4.713479	-4.034054
C	1.554276	-4.557016	-2.951801
C	1.705218	-3.452987	-4.012734
C	1.770326	-5.954294	-3.562550
H	2.358897	-4.407967	-2.217884
H	1.593098	-2.455763	-3.563388
H	2.701675	-3.504974	-4.482085
H	0.957637	-3.555020	-4.816634
H	2.763016	-6.021259	-4.038044
H	1.707172	-6.7428	-2.795044
H	1.016232	-6.180529	-4.334263
C	-1.298748	-4.183670	1.347719
C	-1.916435	-5.454465	1.958922
C	-2.099625	-2.930494	1.737970
H	-0.3569	-4.065066	1.790470
H	-1.975428	-5.368830	3.056740
H	-2.938195	-5.627753	1.583238
H	-1.320979	-6.350265	1.719946
H	-2.158276	-2.840433	2.835626
H	-1.613140	-2.026393	1.343801
H	-3.132333	-2.968692	1.355101
C	-3.509966	-4.695325	-3.164989
C	-3.689017	-6.129713	-3.694186
C	-3.596852	-3.668099	-4.304911
H	-4.343645	-4.479898	-2.477899
H	-3.674858	-6.863490	-2.872880
H	-4.648373	-6.234738	-4.227979

H	-2.883641	-6.401628	-4.397059	C	-0.018643	5.502096	-2.098379
H	-2.801851	-3.815210	-5.054614	C	-1.615549	7.454750	-3.3203
H	-4.563439	-3.752208	-4.828529	H	-2.895740	5.805209	-3.910121
H	-3.511707	-2.640936	-3.918222	C	0.350379	6.848388	-2.039476
C	3.992285	1.631108	3.135629	H	0.605885	4.739468	-1.631087
C	2.647766	1.387478	3.842929	C	-0.444399	7.824702	-2.646607
C	5.062998	2.135023	4.120205	H	-2.234918	8.216121	-3.8722
H	4.339433	0.656058	2.766180	H	1.266075	7.134290	-1.517137
H	1.904393	0.979375	3.142332	H	-0.1536	8.876235	-2.599420
H	2.770595	0.666870	4.668373	N	-1.827851	1.189859	-0.766904
H	2.241213	2.317574	4.274081	C	-2.829916	1.866318	3.043852
H	5.202861	1.413682	4.942182	C	-5.372706	0.999959	0.312438
H	6.034845	2.272083	3.620141	C	-3.112053	0.629270	-0.519773
H	4.781437	3.1405	4.572070	C	-3.127203	2.932172	1.951370
C	4.282834	2.660924	-1.915823	C	-3.414565	-0.621704	-0.946710
C	5.632983	3.230935	-2.389874	C	-3.689629	2.731191	0.665914
C	3.156863	3.060715	-2.883081	C	-3.9461	3.805908	-0.202779
H	4.350407	1.564213	-1.951459	C	-4.749731	-1.161774	-0.756542
H	5.853249	2.903202	-3.419234	C	-3.012186	5.335096	1.383138
H	5.622992	4.333838	-2.384235	C	-3.617127	5.110435	0.145575
H	6.465018	2.904771	-1.747342	C	-2.779954	4.269297	2.248581
H	2.192641	2.651029	-2.553392	H	-1.055819	0.501889	-0.410678
H	3.063343	4.154767	-2.983216	H	-2.668556	-1.245398	-1.435976
H	3.365205	2.660709	-3.888760	H	-3.817528	5.932505	-0.543956
C	2.908788	6.256884	1.378890	H	-2.310439	4.487211	3.207267
C	3.973379	7.3526	2.202063	H	-1.709132	2.075528	-0.266067
C	1.521608	6.368119	2.034127	C	-3.569431	0.523258	2.873778
H	2.849264	6.7569	0.395312	H	-3.364410	-0.101662	3.756149
H	4.081074	6.565472	3.207962	H	-4.658772	0.661668	2.820588
H	4.959087	6.960254	1.713168	H	-3.231822	-0.056093	2.6236
H	3.7392	8.064406	2.328390	C	-1.305875	1.595250	3.071137
H	0.748791	5.871084	1.426961	H	-0.949103	1.121011	2.143740
H	1.511722	5.903911	3.034021	H	-0.729810	2.520908	3.224741
H	1.231154	7.424662	2.158035	H	-1.060935	0.907510	3.896546
C	-1.614937	3.725804	-2.855556	C	-3.268491	2.418217	4.425330
C	-1.370754	1.528383	-2.472524	H	-4.334075	2.696312	4.422290
C	-2.639399	1.832559	-3.287485	H	-3.123304	1.6444	5.190280
H	-2.5233	1.359266	-4.2764	H	-2.6873	3.293623	4.747359
H	-3.562036	1.424803	-2.849768	H	-2.722033	6.345204	1.6822
O	-0.617295	0.563399	-2.856825	H	-4.401938	3.596357	-1.171795
O	-0.763422	2.788528	-2.293595	N	-4.036709	1.423062	0.140314
N	-2.677648	3.276689	-3.398793	O	-6.191290	1.721257	0.842457
C	-1.194473	5.130103	-2.770138	N	-5.670884	-0.273255	-0.153889
C	-1.990553	6.114439	-3.384383	C	-7.065118	-0.738113	0.023013

H	-7.709813	0.138769	-0.106917
H	-7.247353	-1.451988	-0.788391
C	-7.329375	-1.392043	1.366298
C	-7.079454	-2.761768	1.551813
C	-7.833425	-0.640868	2.440118
C	-7.329431	-3.366922	2.786439
H	-6.683485	-3.347993	0.719494
C	-8.084367	-1.247983	3.674226
H	-8.020682	0.426537	2.303272
C	-7.832790	-2.611880	3.850485
H	-7.133630	-4.434501	2.916787
H	-8.480575	-0.652617	4.501132
H	-8.031335	-3.086721	4.814969
O	-5.098458	-2.280917	-1.095575

M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -4262.820721 Hartree

Corrected Gibbs Free Energy = -4261.454835 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -299.63 cm^{-1}

TS1-minor

P	-1.387802	-0.448551	0.320113
O	-2.897372	-0.185515	-0.261871
O	-1.402235	-2.064953	0.567546
C	-3.985039	-0.612812	0.488801
C	-4.829198	0.383703	1.067602
C	-5.899441	-0.055983	1.823632
H	-6.586086	0.679687	2.247487
C	-6.125503	-1.430152	2.0970
C	-7.169654	-1.847924	2.9755
H	-7.815443	-1.085444	3.413995
C	-7.353181	-3.180688	3.268034
H	-8.1516	-3.489373	3.947403
C	-6.489879	-4.151804	2.704190
H	-6.618015	-5.205937	2.962793
C	-5.484105	-3.779529	1.835769
H	-4.824624	-4.540408	1.418263
C	-5.277783	-2.413029	1.4974
C	-4.239522	-1.977543	0.590287
C	-3.4735	-2.955789	-0.236280
C	-4.159306	-3.889458	-1.095960
C	-5.561353	-3.837349	-1.346877
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H	-7.252070	-4.689587	-2.348724
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M062X-D3/6-311+G(d,p)-SMD(CCl4): E = -4262.819075 Hartree

Corrected Gibbs Free Energy = -4261.451959 Hartree

Number of imaginary frequencies: 1

Wavenumber of lowest frequency: -384.47 cm^{-1}

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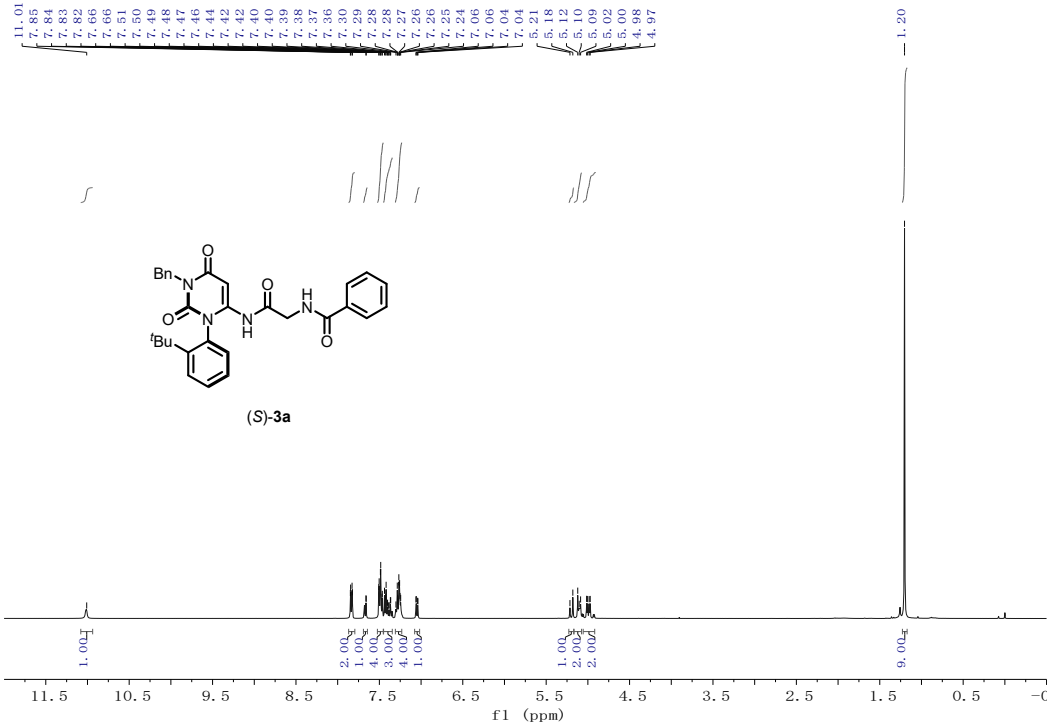
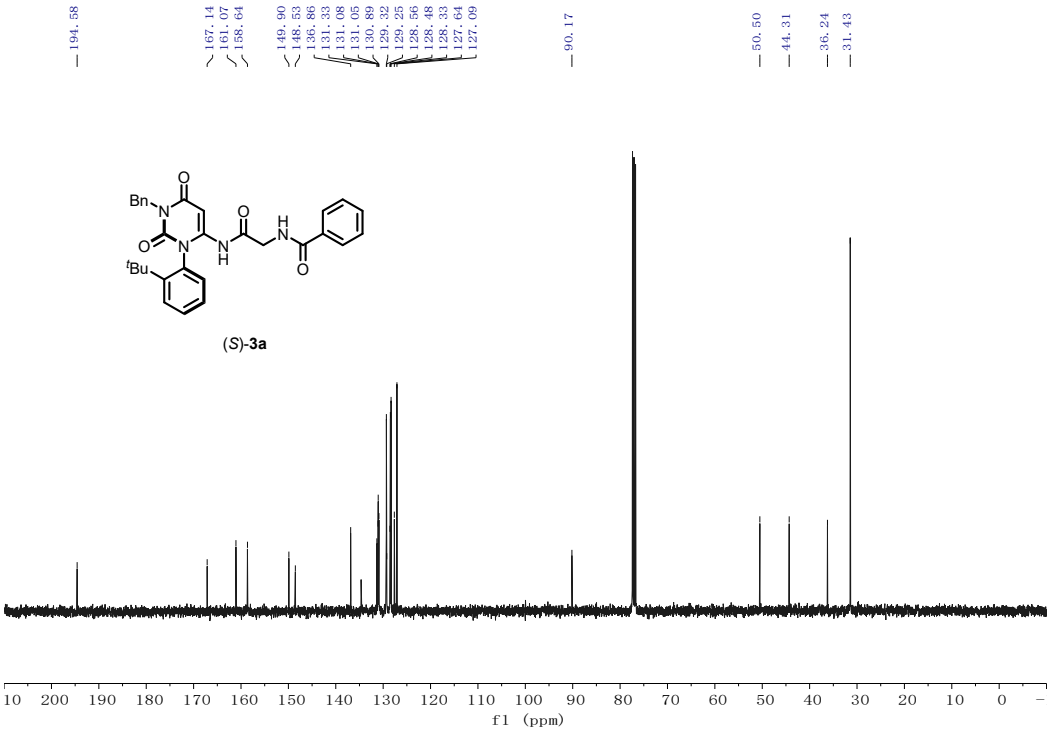
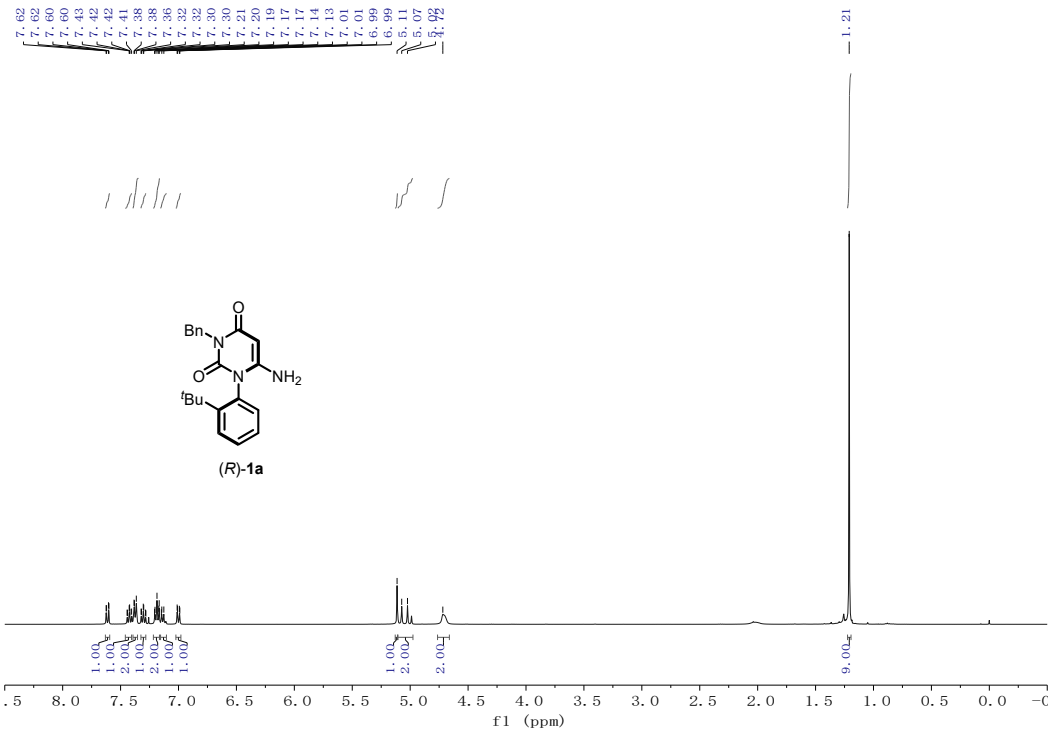
12. NMR spectra



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7.30
7.21
7.20
7.19
7.17
7.17
7.14
7.13
7.01
7.01
6.99
5.11
5.07
5.02
1.21
Bn
N
O
O
N
NH2
tBu
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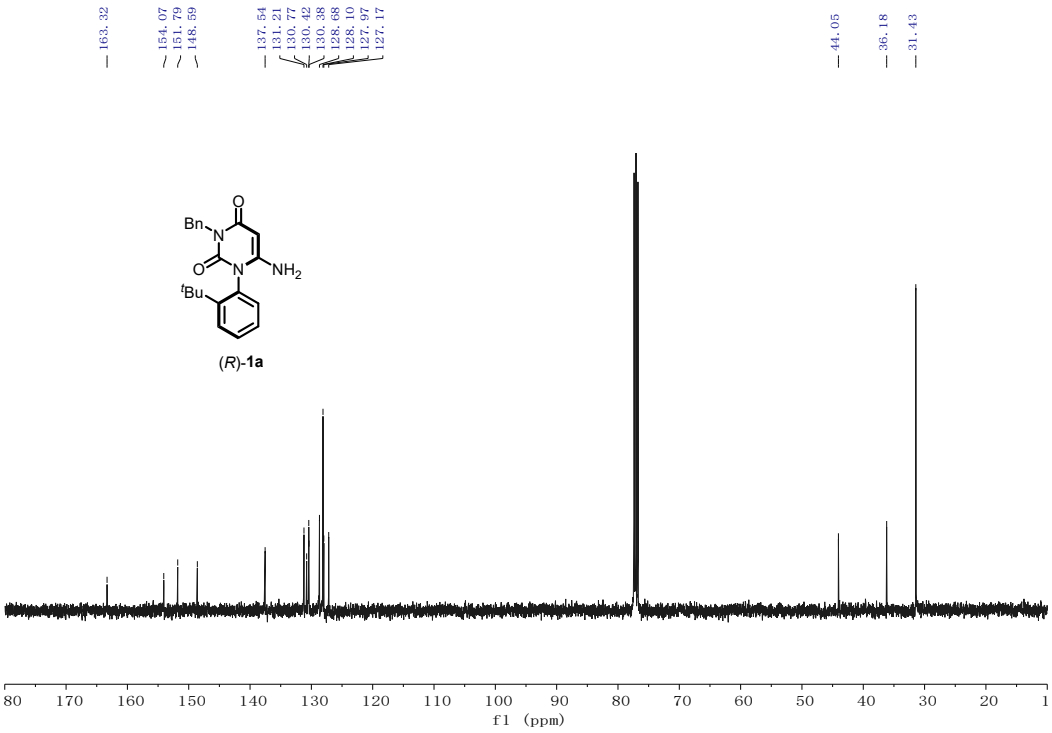
f1 (ppm)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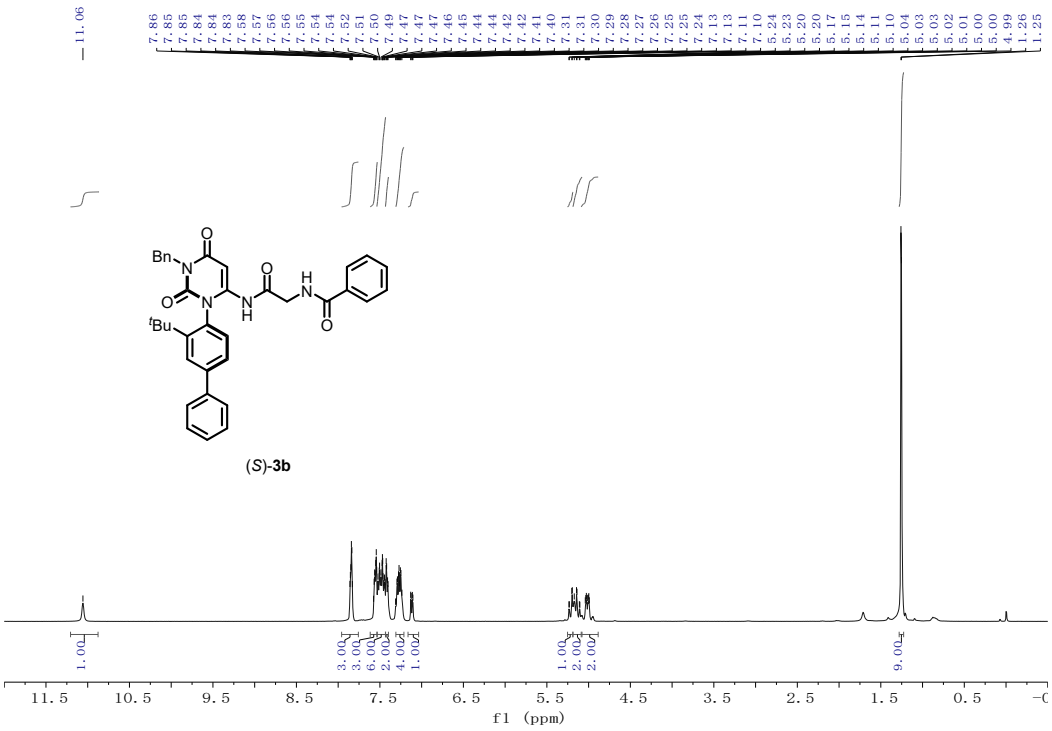
NH2
tBu
(R)-1a
f1 (ppm)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Bn
tBu
(S)-3b
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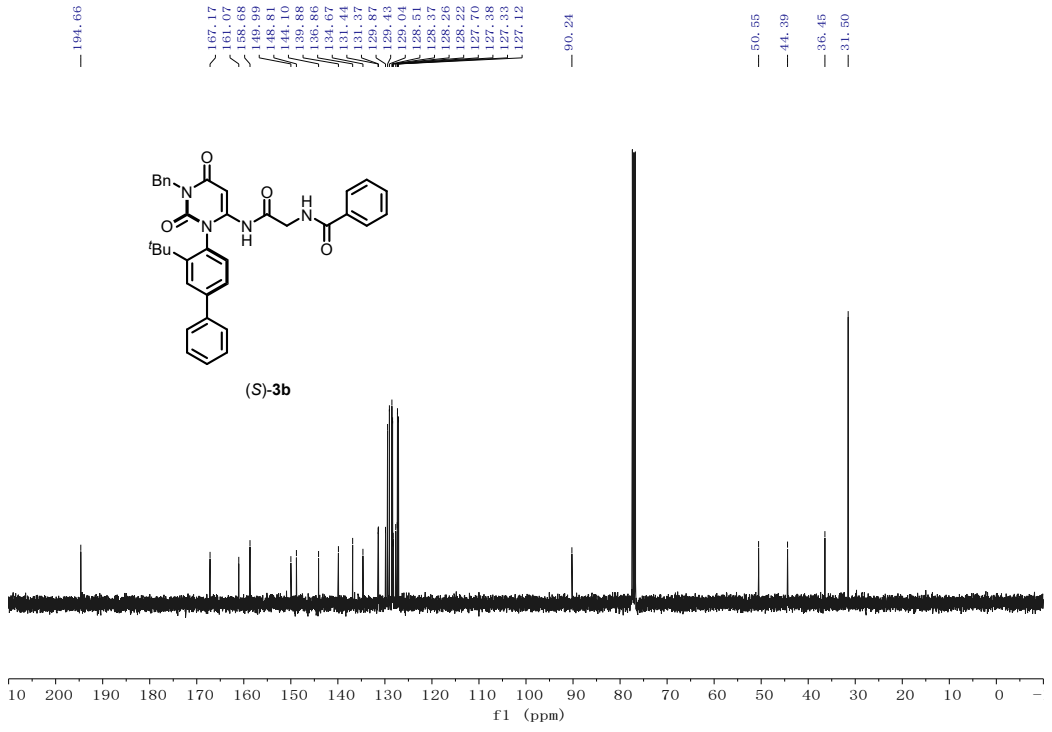
f1 (ppm)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90.24
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tBu
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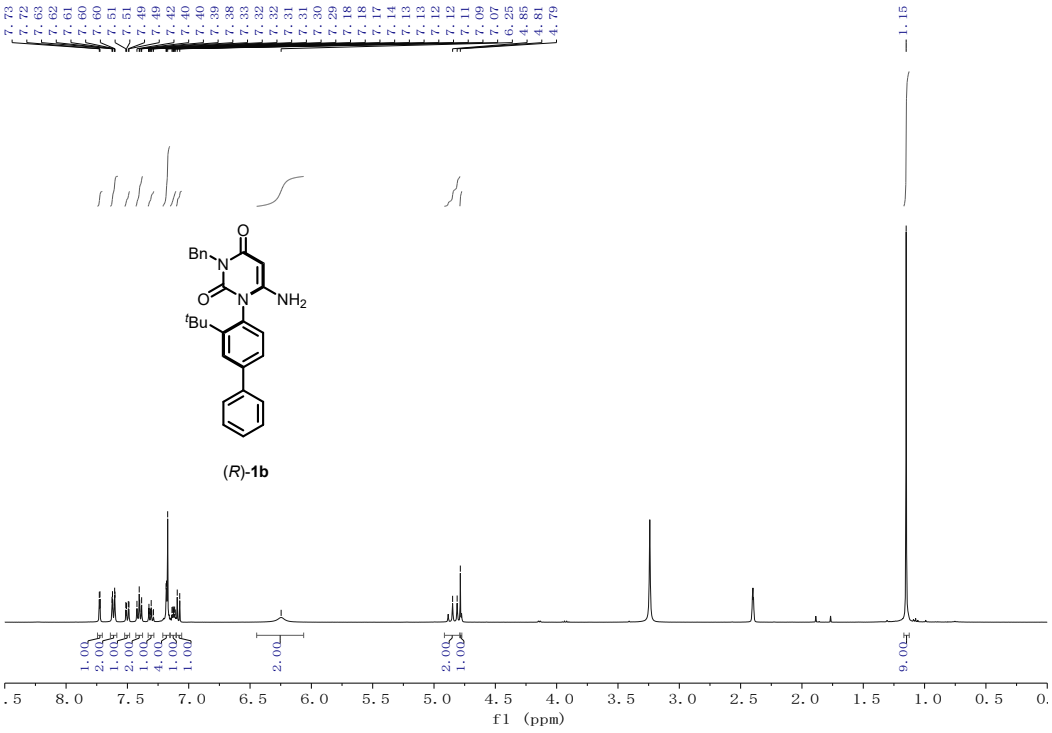
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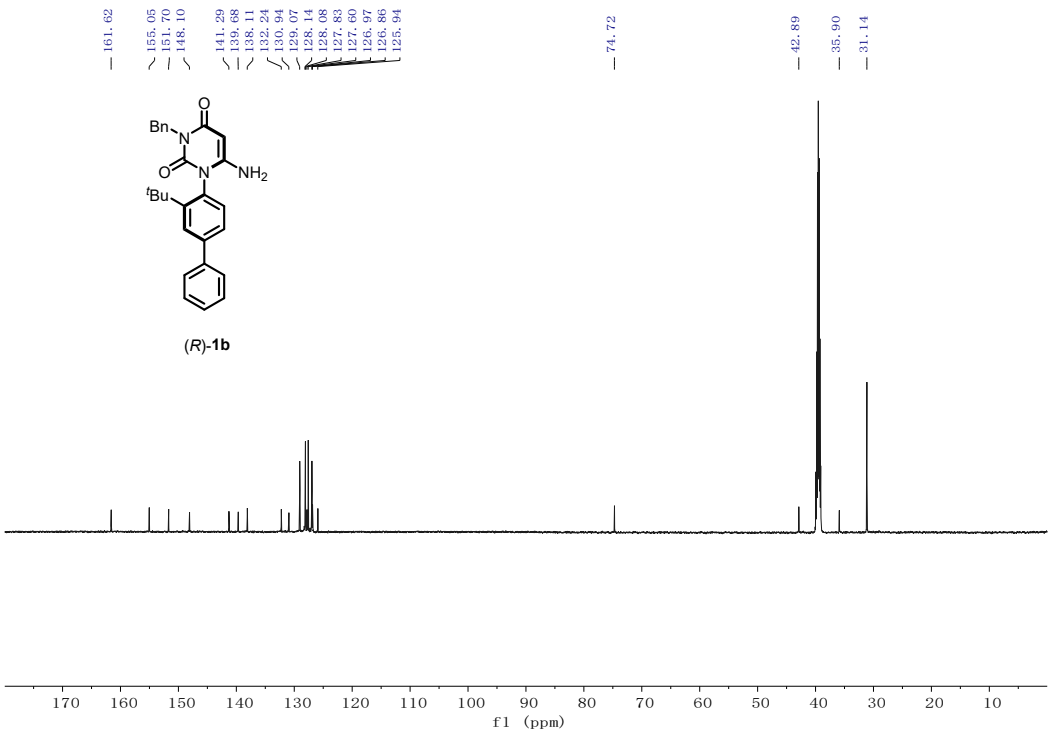
f1 (ppm)

(*R*)-**1b**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N
NH2
tBu
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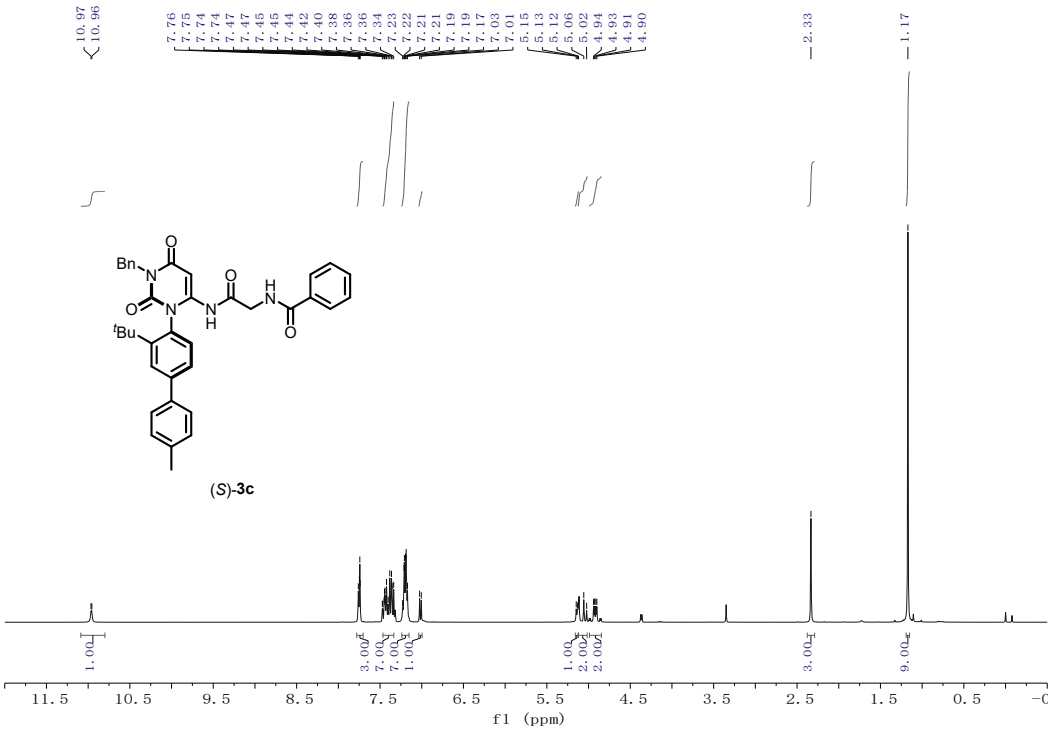
f1 (ppm)

(*R*)-**1b**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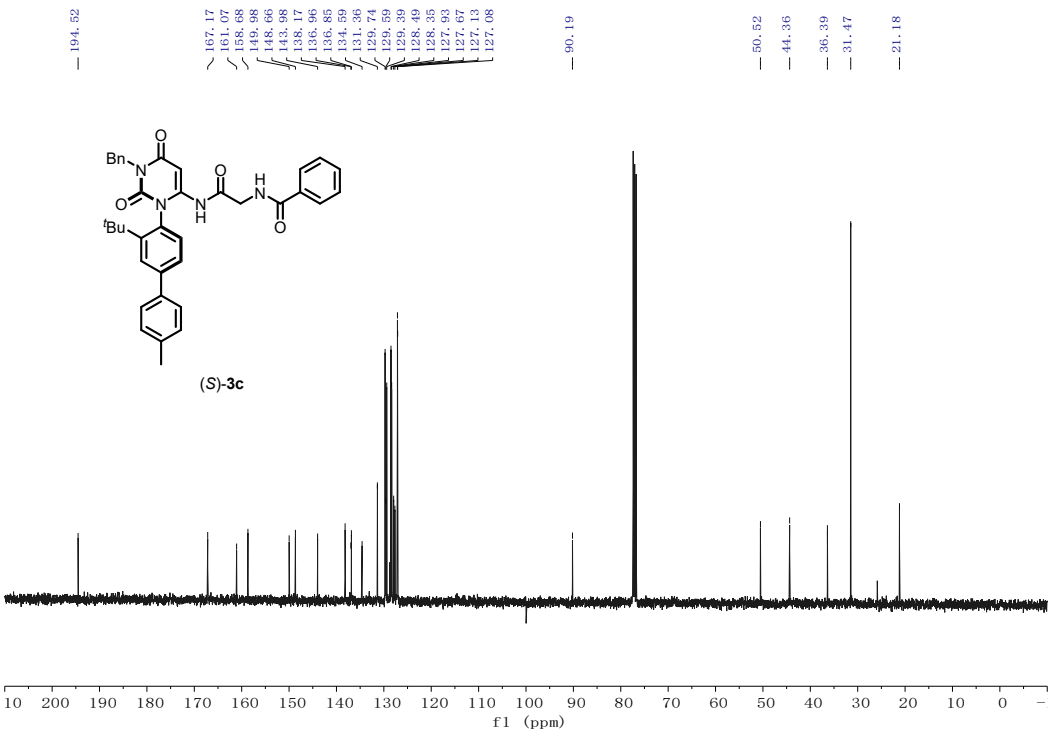
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tBu
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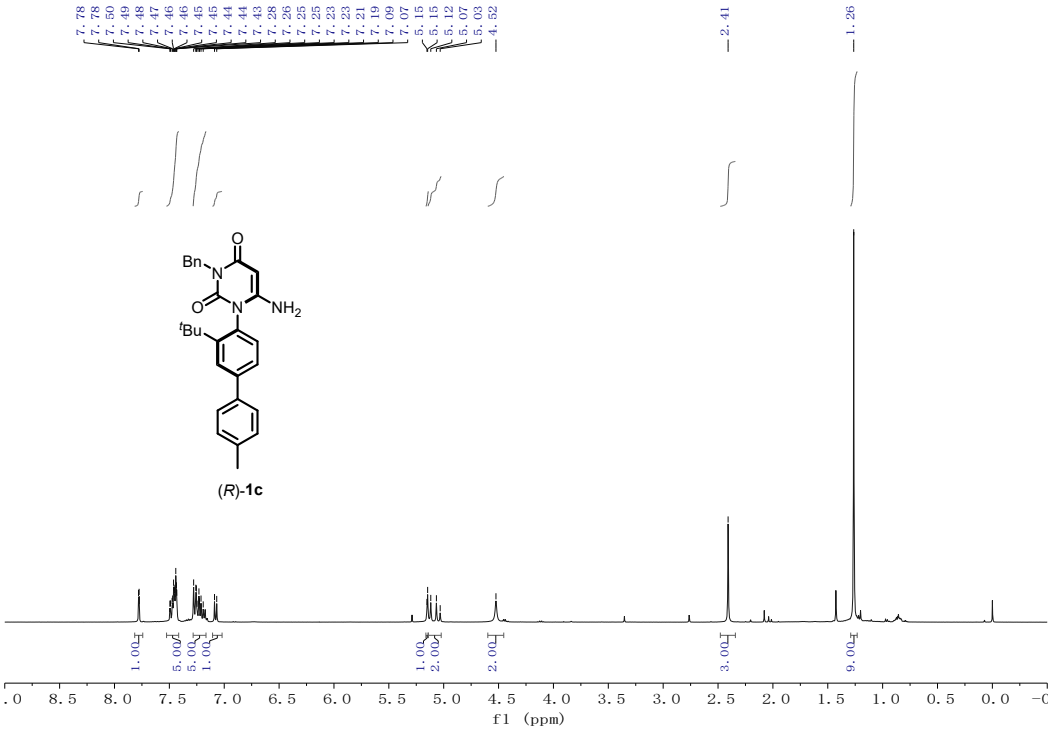
f1 (ppm)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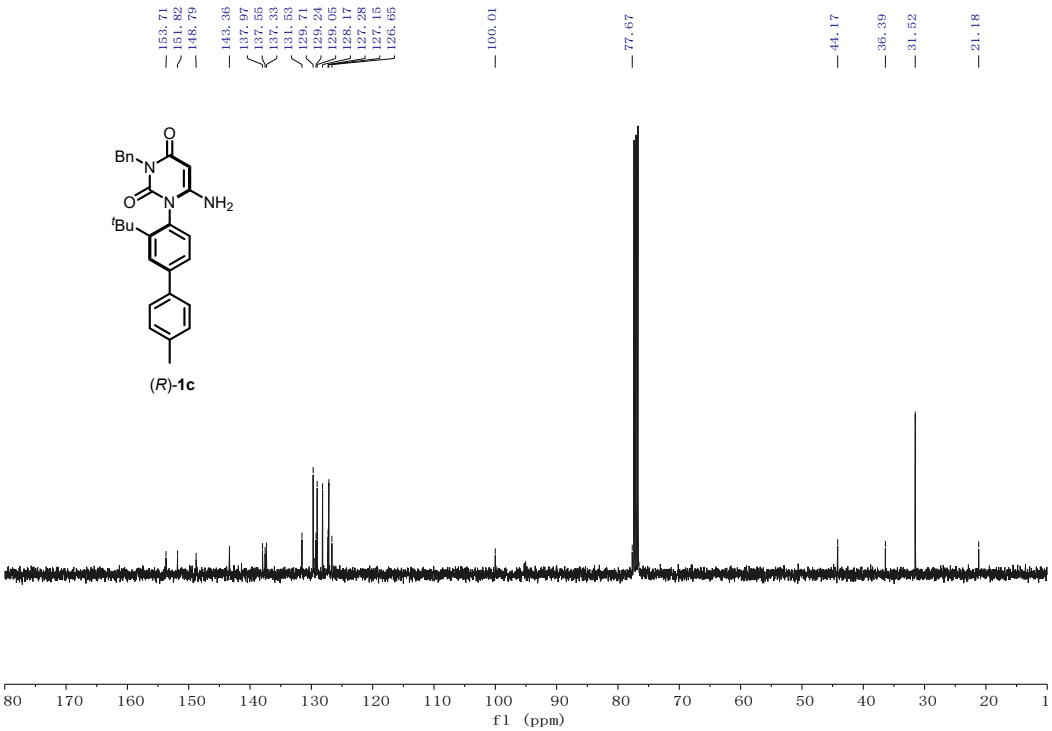
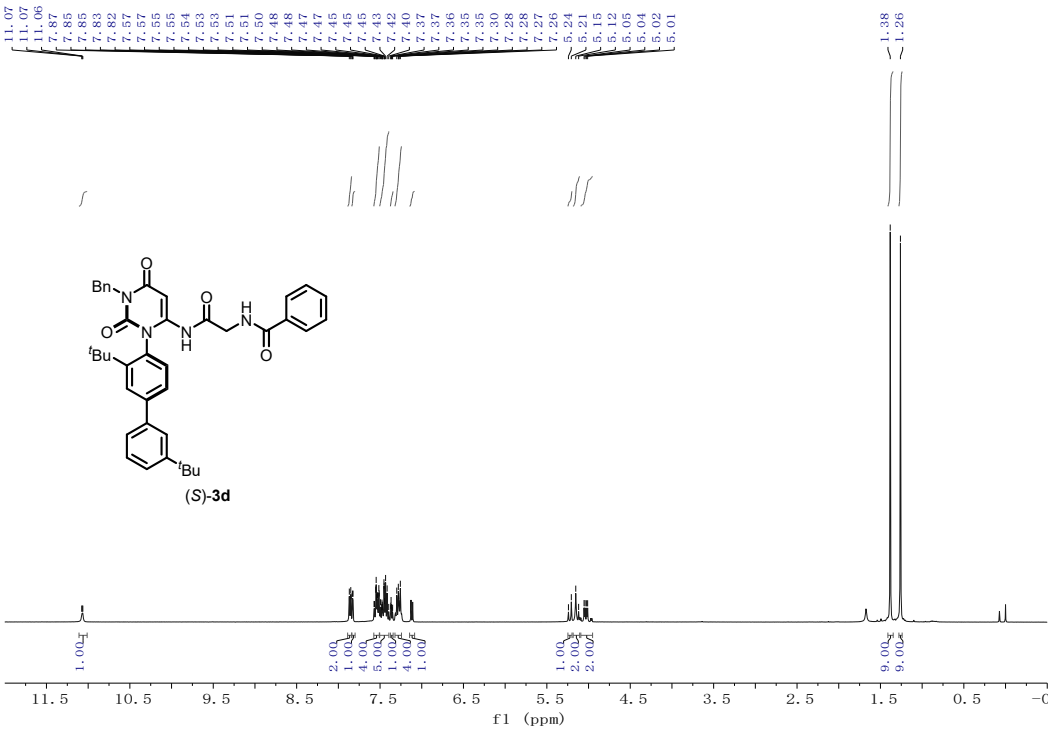
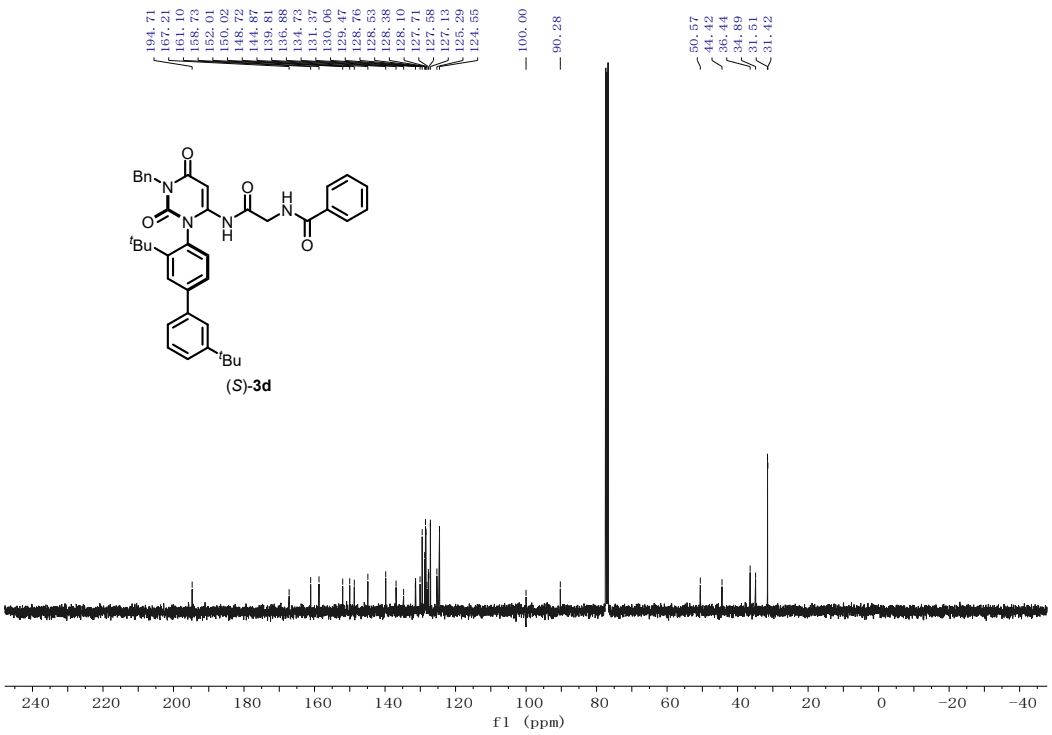
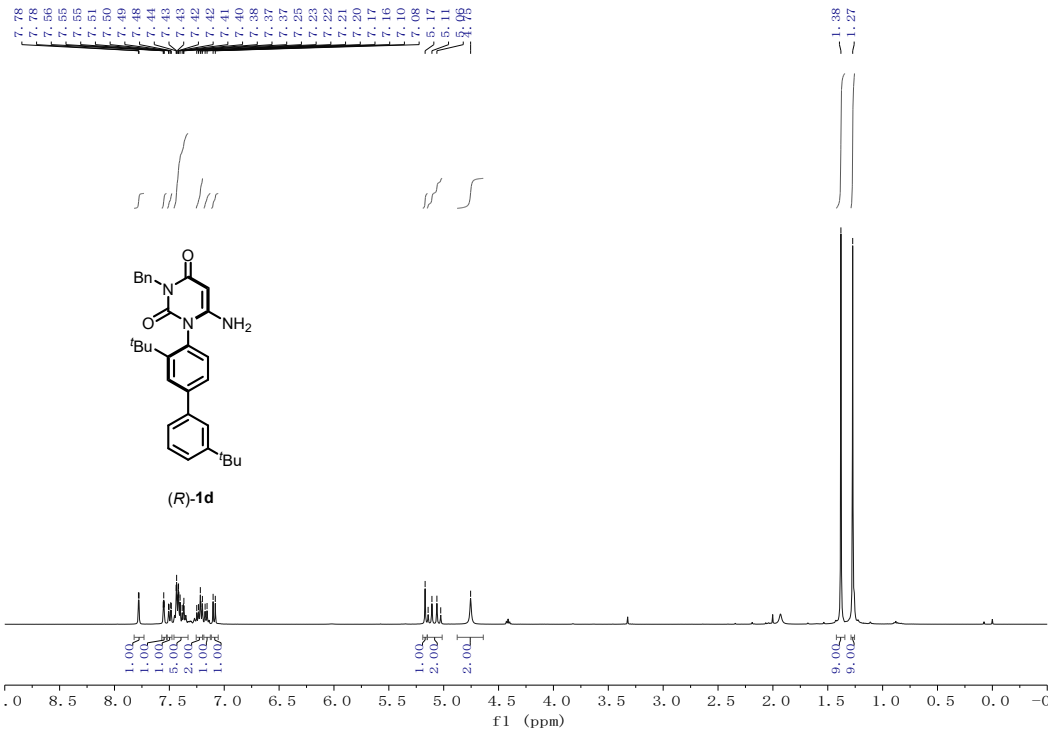
9.00
f1 (ppm)

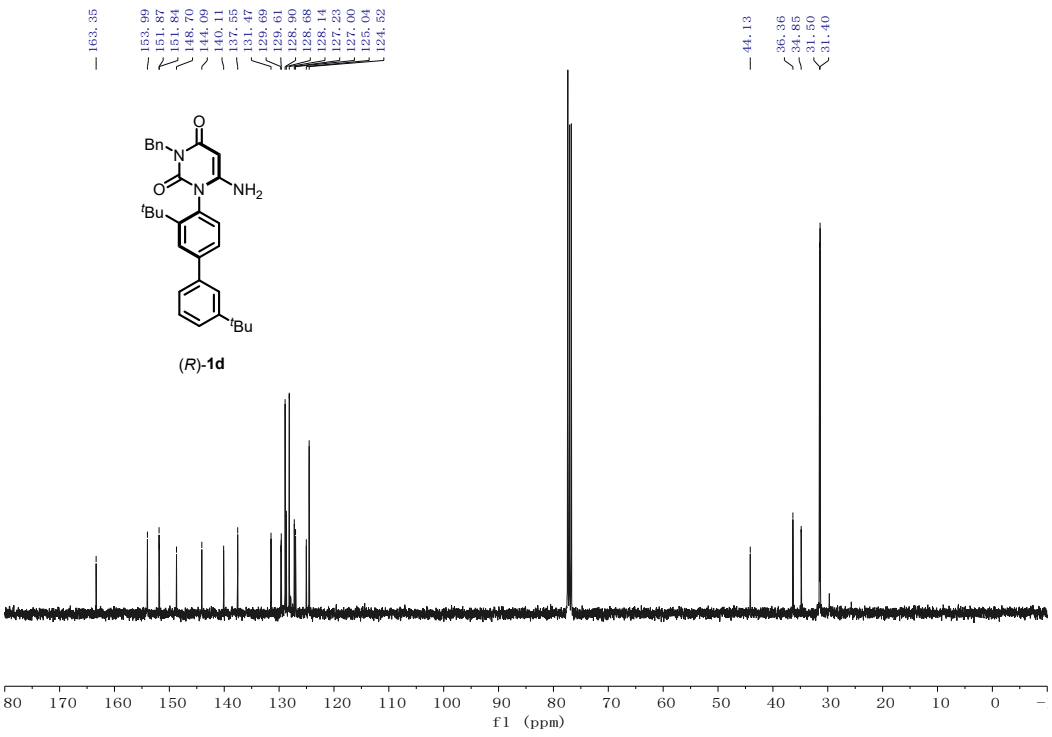

153.71
151.82
148.79
143.36
137.97
137.55
137.33
131.53
129.71
129.24
129.05
128.17
127.28
127.15
126.65
100.01
77.67
44.17
36.39
31.52
21.18
Bn
N
O
O
N
NH2
tBu
(R)-1c
f1 (ppm)


11.07
11.07
11.06
7.87
7.85
7.85
7.83
7.82
7.57
7.57
7.55
7.55
7.54
7.53
7.53
7.51
7.51
7.50
7.48
7.48
7.47
7.47
7.45
7.45
7.43
7.42
7.40
7.37
7.37
7.36
7.35
7.35
7.30
7.28
7.28
7.27
7.26
5.24
5.21
5.15
5.12
5.05
5.04
5.02
5.01
1.38
1.26
Bn
tBu
tBu
(S)-3d
1.00
2.00
1.00
4.00
5.00
1.00
4.00
1.00
1.00
2.00
2.00
9.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

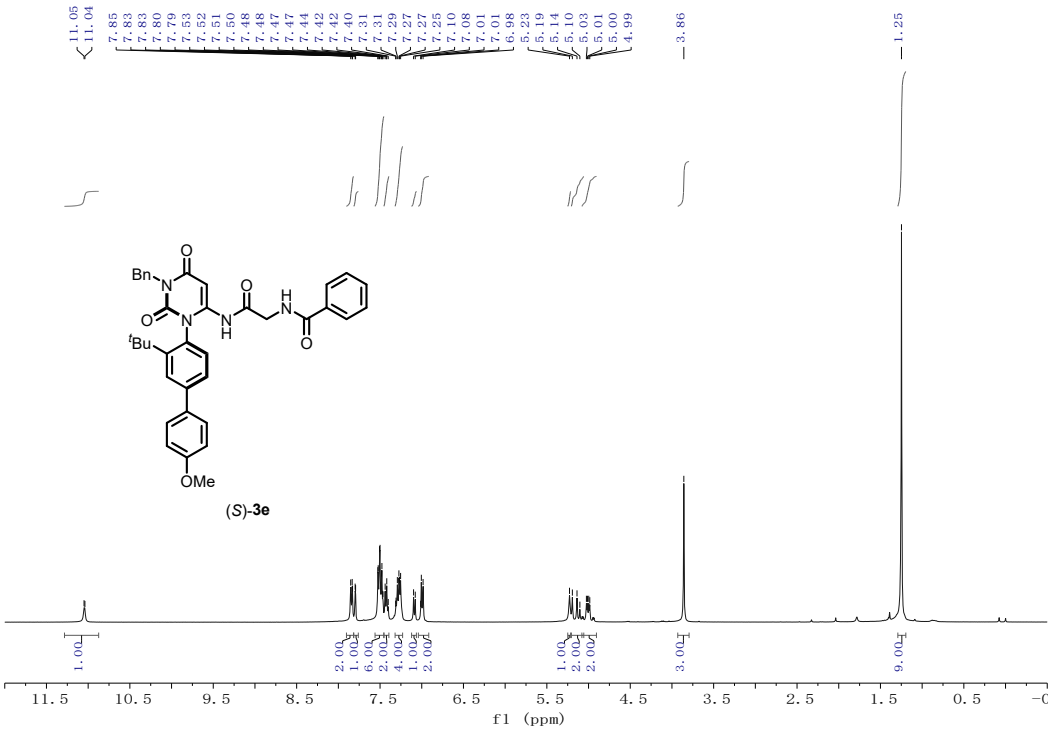

194.71
167.21
161.10
158.73
152.01
150.02
148.72
144.87
139.81
136.88
134.73
131.37
130.06
129.47
128.76
128.53
128.38
128.10
127.71
127.58
127.13
125.29
124.55
100.00
90.28
50.57
44.42
36.44
34.89
31.51
31.42
Bn
tBu
tBu
(S)-3d
240
220
200
180
160
140
120
100
80
60
40
20
0
−20
−40
f1 (ppm)

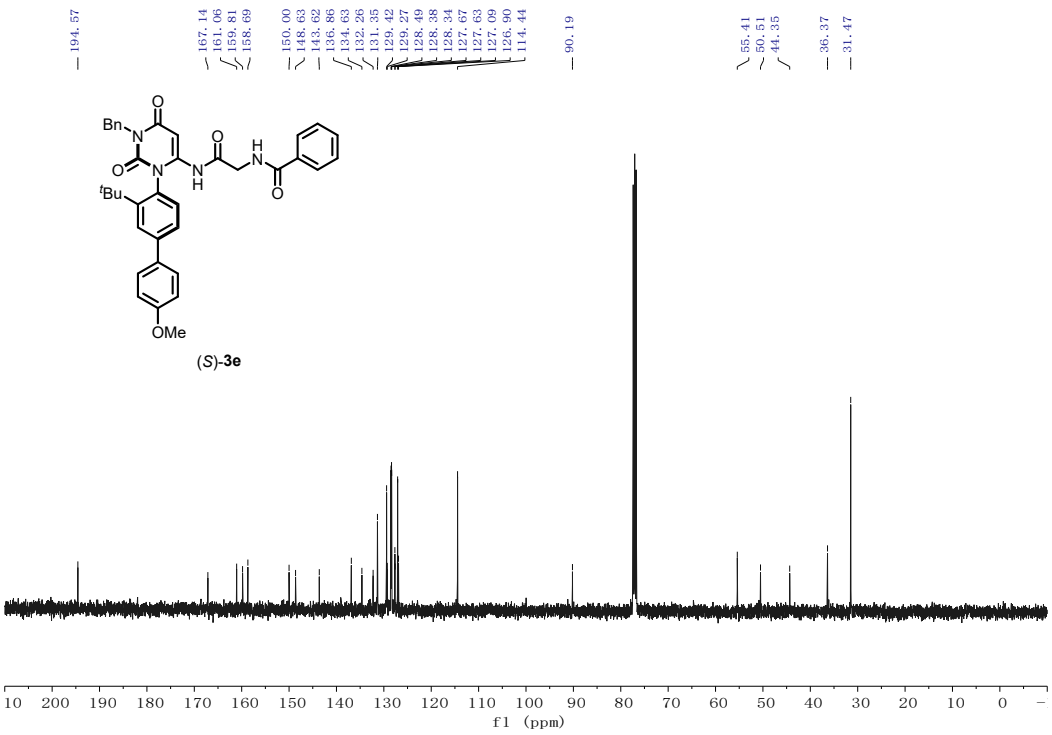

7.78
7.78
7.56
7.55
7.55
7.51
7.50
7.49
7.48
7.44
7.43
7.43
7.42
7.42
7.41
7.40
7.38
7.37
7.37
7.25
7.23
7.22
7.21
7.20
7.17
7.16
7.10
7.08
5.17
5.11
5.06
5.05
1.38
1.27
Bn
N
O
O
N
NH2
tBu
tBu
1.00
1.00
1.00
5.00
2.00
1.00
1.00
1.00
2.00
2.00
9.00
9.00
f1 (ppm)

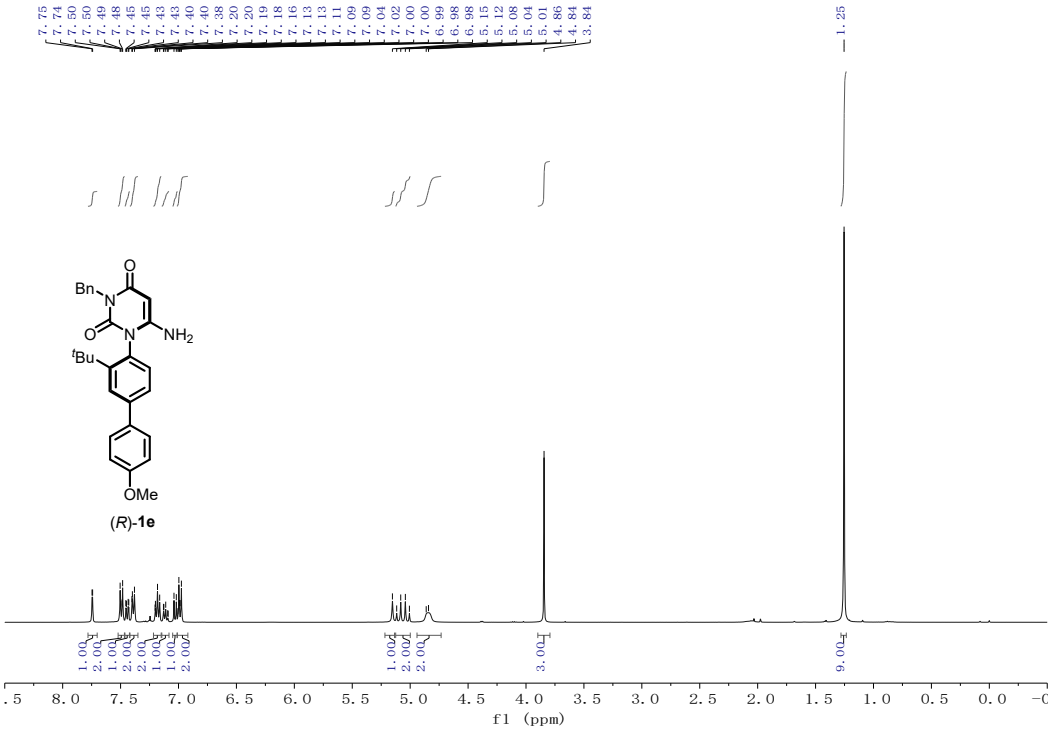
(*R*)-**1d**

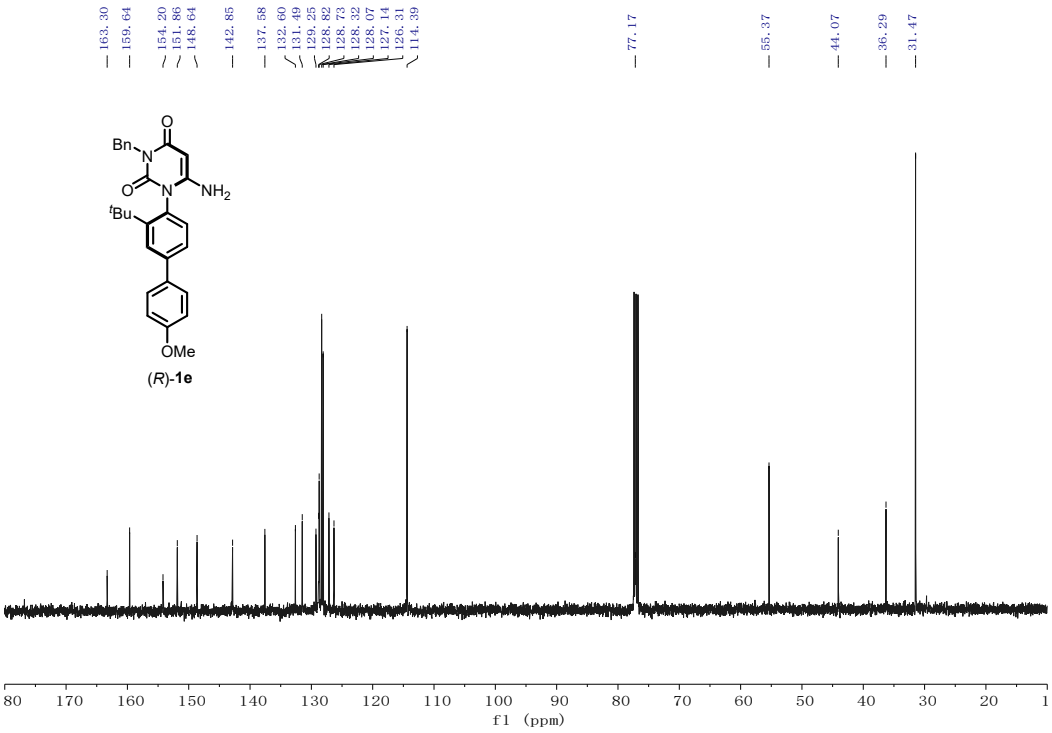

163.35
153.99
151.87
151.84
148.70
144.09
140.11
137.55
131.47
129.69
129.61
128.90
128.68
128.14
127.23
127.00
125.04
124.52
44.13
36.36
34.85
31.50
31.40
Bn
N
O
O
N
NH2
tBu
tBu
f1 (ppm)

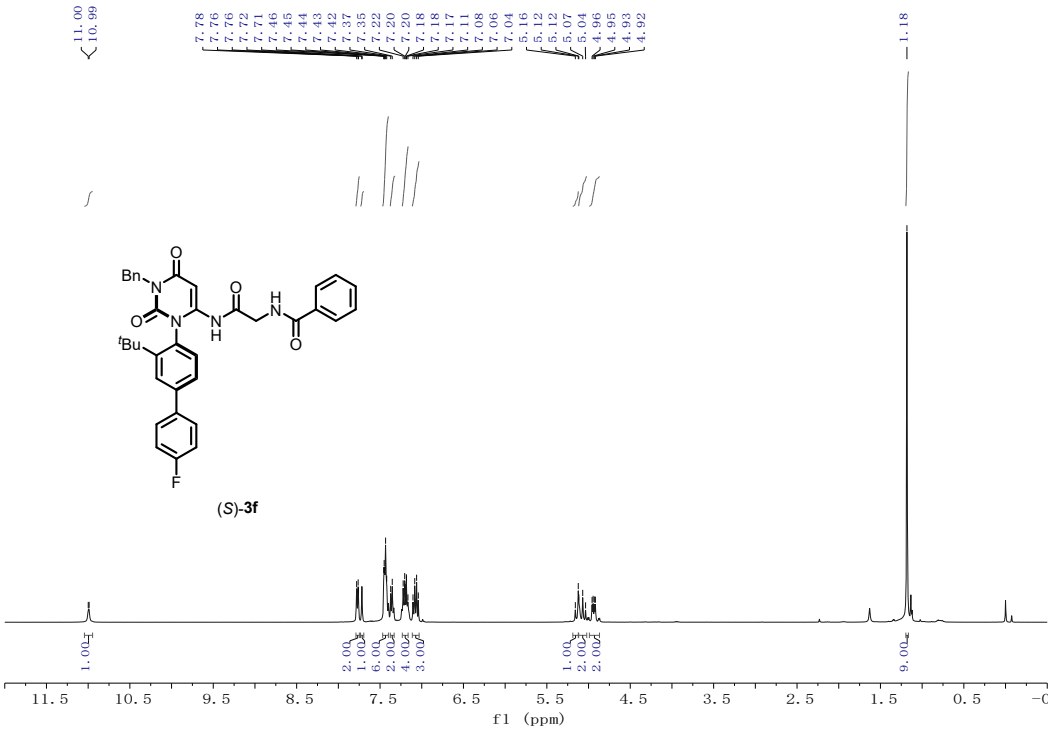
(*R*)-**1d**

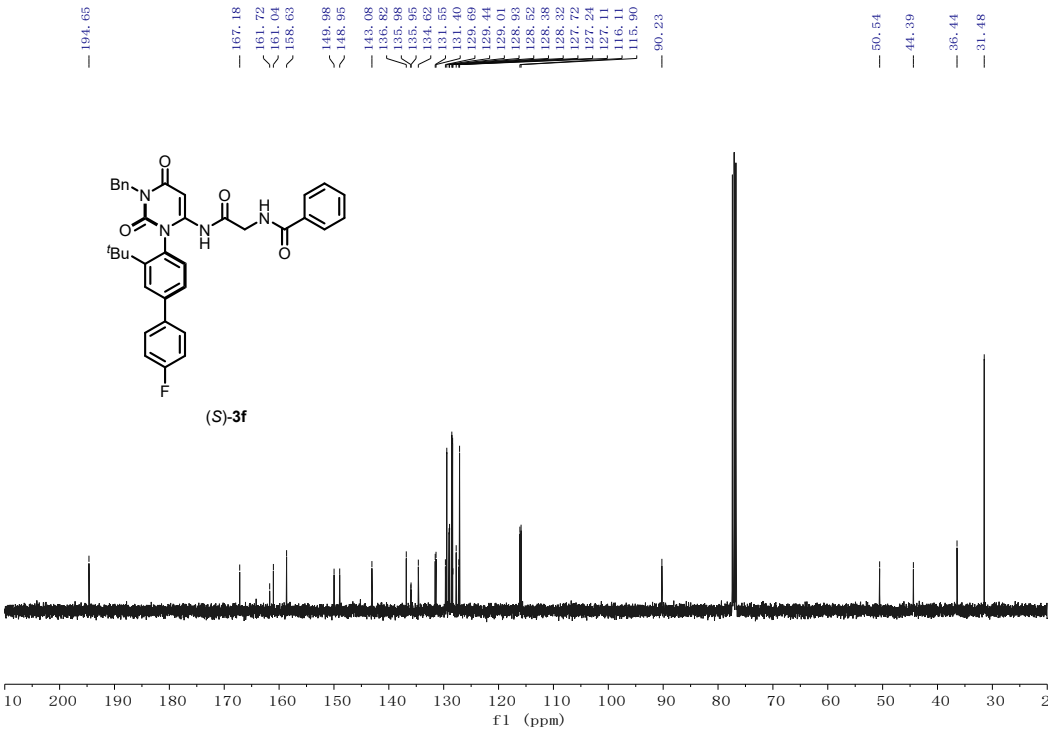

11.05
11.04
7.85
7.83
7.83
7.80
7.79
7.53
7.52
7.51
7.50
7.48
7.48
7.47
7.47
7.44
7.42
7.42
7.40
7.31
7.31
7.29
7.27
7.27
7.25
7.10
7.08
7.01
7.01
6.98
5.23
5.19
5.14
5.10
5.03
5.01
5.00
4.99
3.86
1.25
Bn
tBu
OMe
(S)-3e
1.00
2.00
1.00
6.00
2.00
4.00
1.00
2.00
1.00
2.00
3.00
9.00
f1 (ppm)

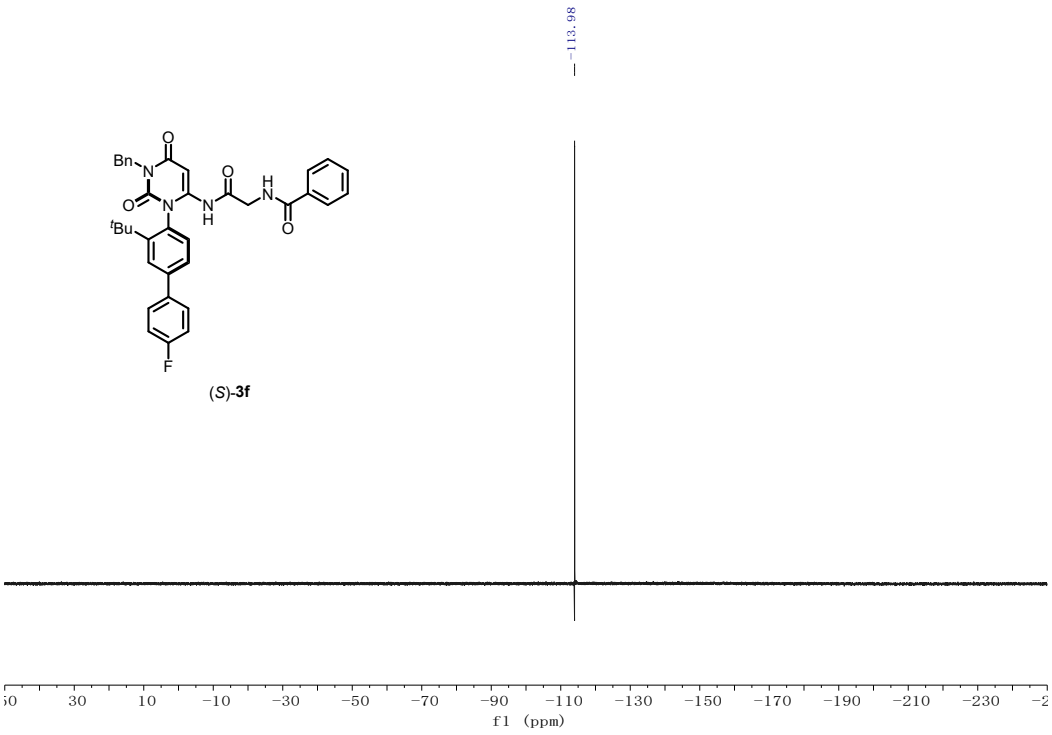

194.57
167.14
161.06
159.81
158.69
150.00
148.63
143.62
136.86
134.63
132.26
131.35
129.42
129.27
128.49
128.38
128.34
127.67
127.63
127.09
126.90
114.44
90.19
55.41
50.51
44.35
36.37
31.47
Bn
tBu
OMe
(S)-3e
f1 (ppm)


7.75 7.74 7.50 7.50 7.49 7.48 7.45 7.45 7.43 7.43 7.40 7.40 7.38 7.20 7.19 7.18 7.16 7.13 7.11 7.09 7.09 7.04 7.02 7.00 7.00 6.99 6.98 5.15 5.12 5.08 5.04 5.01 4.86 4.84 3.84
1.25
Bn
NH2
tBu
OMe
(R)-1e
1.00 2.04 1.04 2.00 2.00 1.00 2.00 1.00 2.00 2.00 3.00 9.00
f1 (ppm)

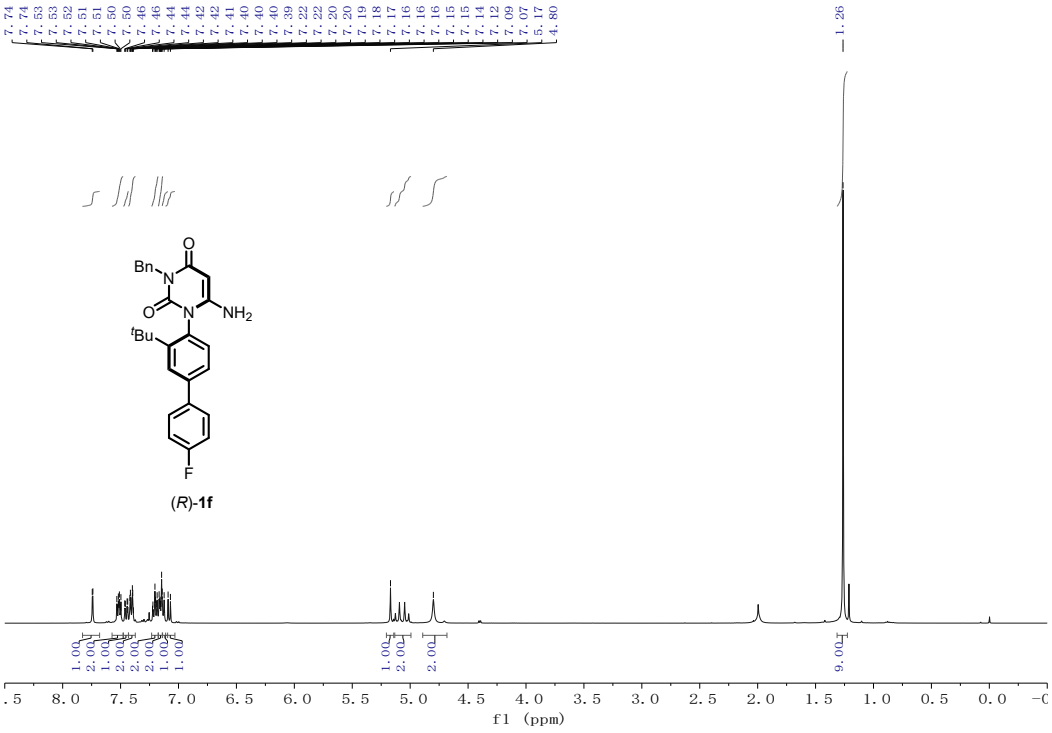

163.30 159.64 154.20 151.86 148.64 142.85 137.58 132.60 131.49 129.25 128.82 128.73 128.32 128.07 127.14 126.31 114.39
77.17
55.37
44.07
36.29
31.47
Bn
NH2
tBu
OMe
(R)-1e
f1 (ppm)


11.00
10.99
7.78
7.76
7.76
7.72
7.71
7.46
7.45
7.44
7.43
7.42
7.37
7.35
7.22
7.20
7.20
7.18
7.18
7.17
7.11
7.08
7.06
7.04
5.16
5.12
5.12
5.07
5.04
4.96
4.95
4.93
4.92
1.18
Bn
tBu
F
(S)-3f
1.00
2.00
1.00
6.00
2.00
4.00
3.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

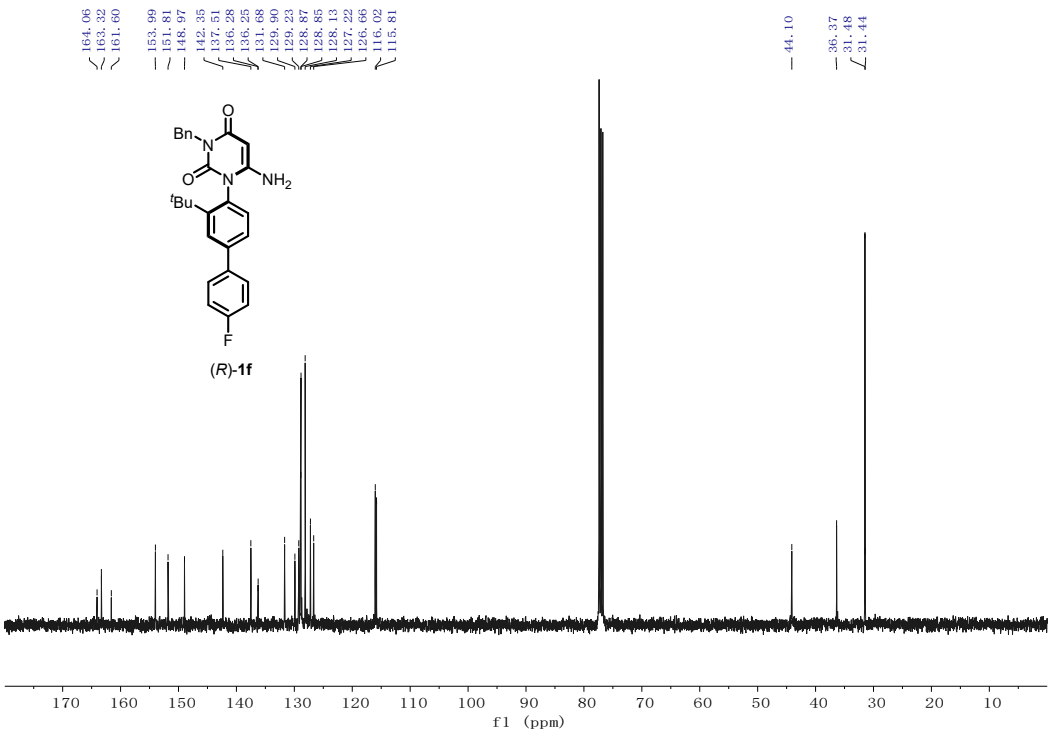

194.65
167.18
161.72
161.04
158.63
149.98
148.95
143.08
136.82
135.98
135.95
134.62
131.55
131.40
129.69
129.44
129.01
128.93
128.52
128.38
128.32
127.72
127.24
127.11
116.11
115.90
90.23
50.54
44.39
36.44
31.48
Bn
tBu
F
(S)-3f
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)


−113.98
Bn
N
O
O
N
tBu
F
O
N
H
O
H
N
O
50
30
10
−10
−30
−50
−70
−90
−110
−130
−150
−170
−190
−210
−230
f1 (ppm)

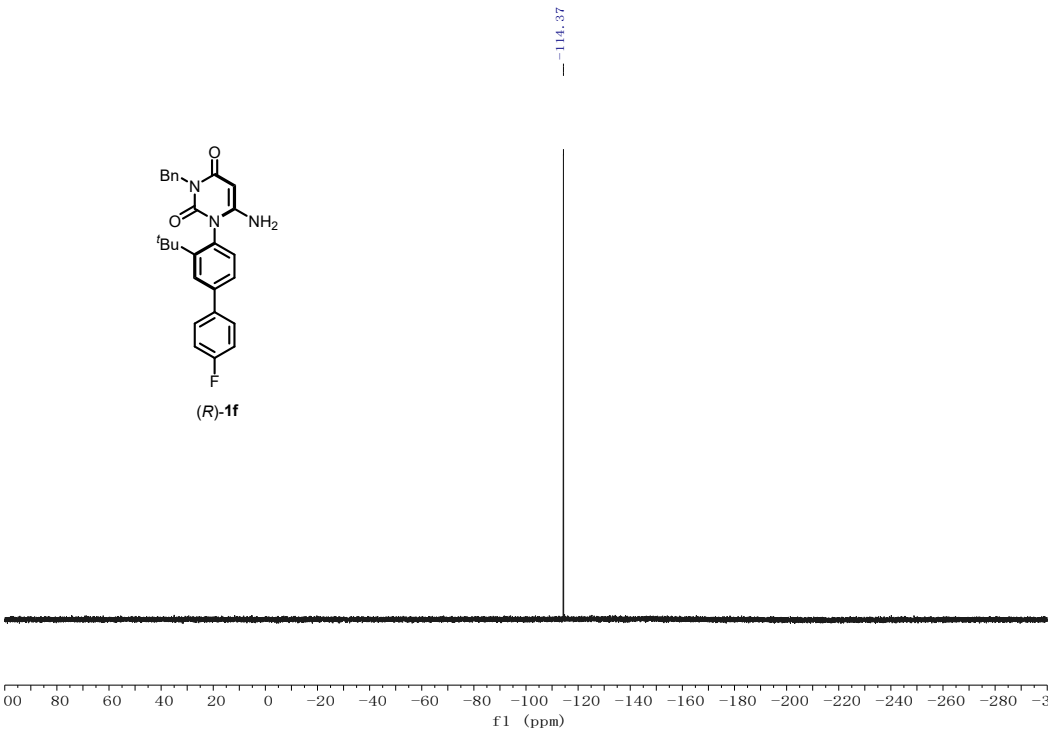
(*S*)-**3f**


7.74
7.74
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.46
7.46
7.44
7.44
7.42
7.42
7.41
7.40
7.40
7.40
7.39
7.22
7.22
7.20
7.20
7.19
7.18
7.17
7.16
7.16
7.16
7.15
7.15
7.14
7.12
7.09
7.07
5.17
4.80
1.26
Bn
N
O
O
N
NH2
tBu
F
1.00
2.00
1.00
2.00
2.00
2.00
1.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

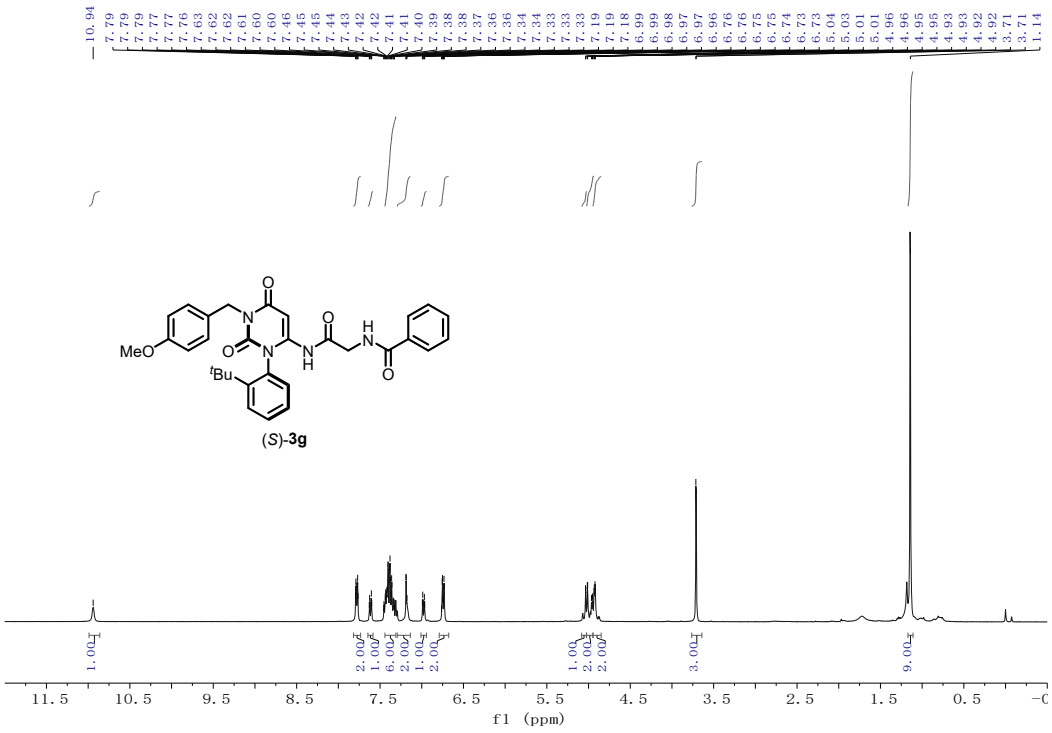
(*R*)-**1f**

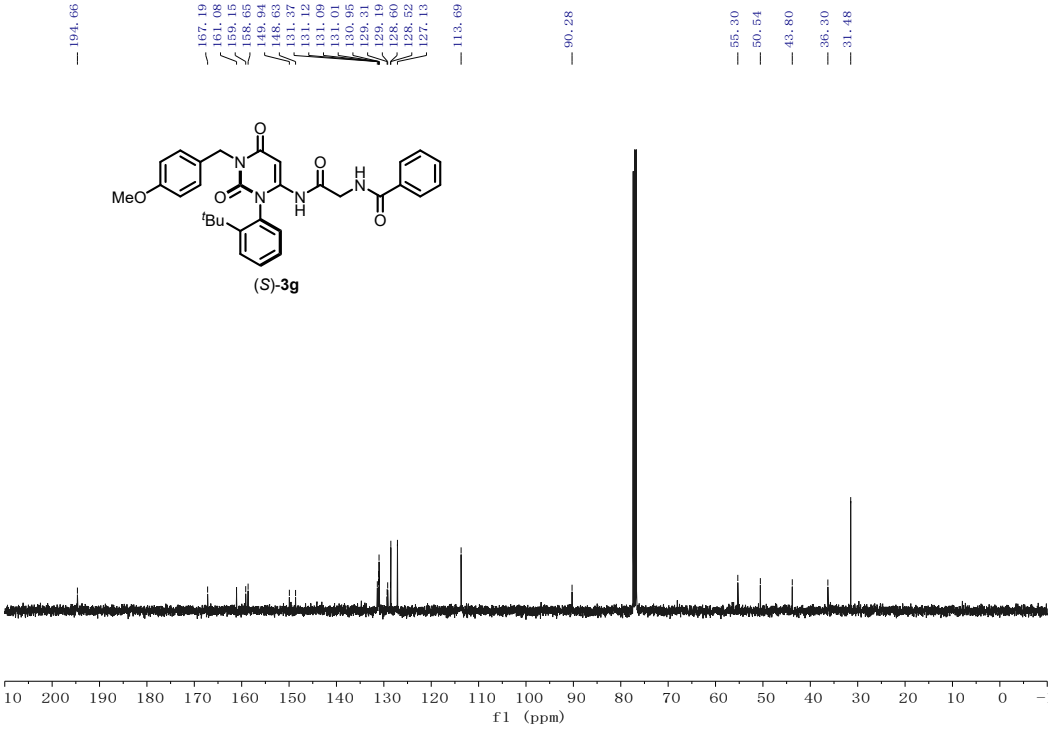

164.06
163.32
161.60
153.99
151.81
148.97
142.35
137.51
136.28
136.25
131.68
129.90
129.23
128.87
128.85
128.13
127.22
126.66
116.02
115.81
44.10
36.37
31.48
31.44
Bn
N
O
O
N
NH2
tBu
F
f1 (ppm)

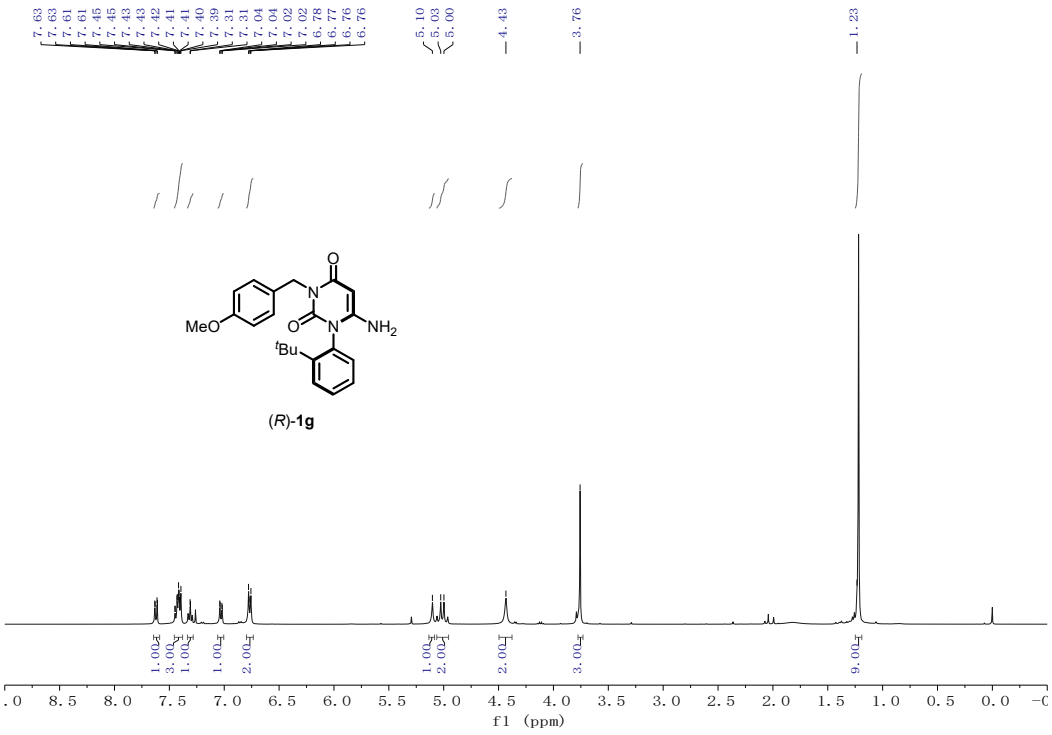
(*R*)-**1f**

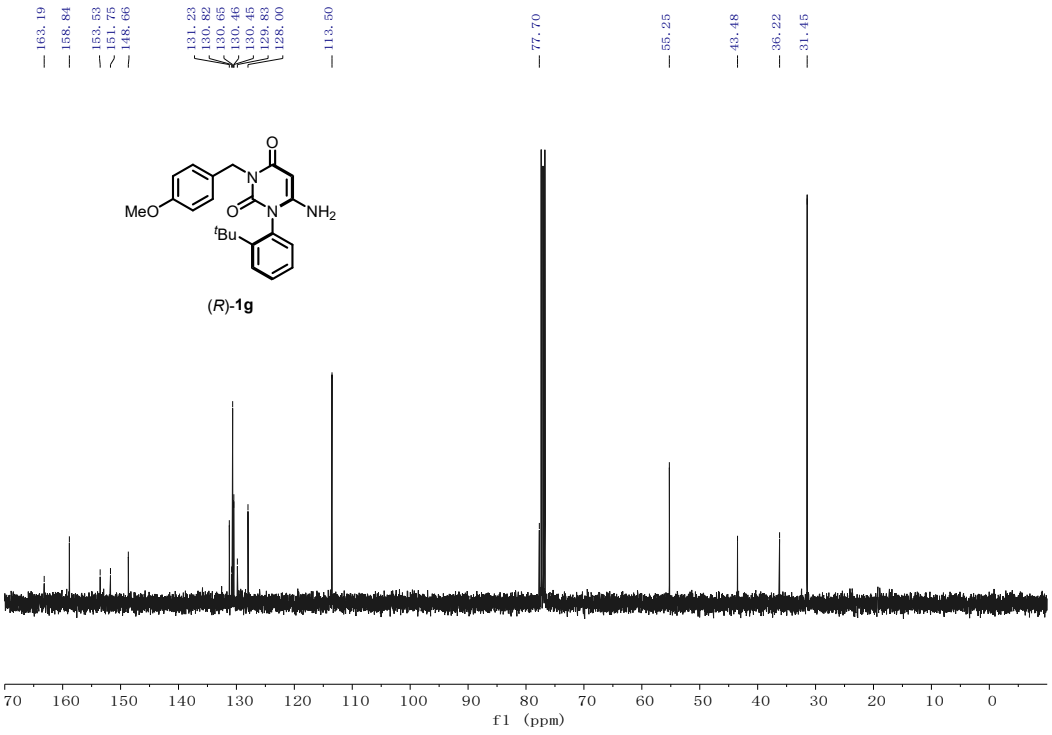

−114.37
Bn
O
N
O
N
NH2
tBu
F
00 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 −220 −240 −260 −280 −3
f1 (ppm)

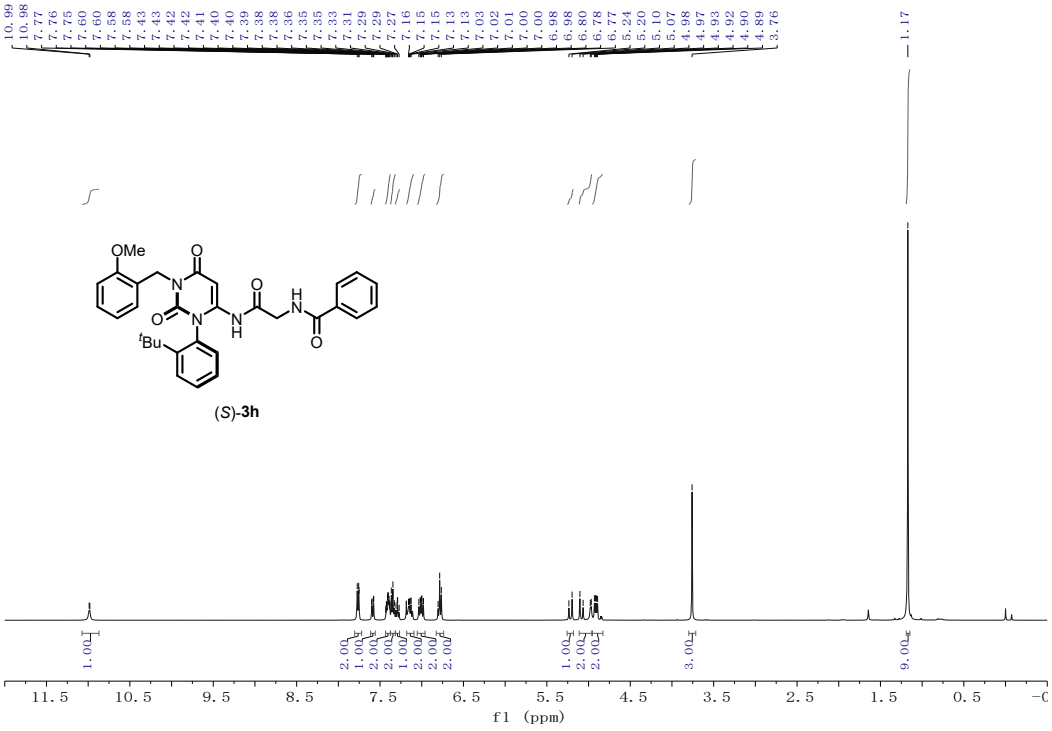
(*R*)-**1f**


10.94
7.79
7.79
7.79
7.77
7.77
7.76
7.63
7.62
7.62
7.61
7.60
7.60
7.46
7.45
7.45
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.34
7.34
7.33
7.33
7.19
7.19
7.18
6.99
6.99
6.98
6.97
6.97
6.96
6.76
6.76
6.75
6.75
6.74
6.73
6.73
5.04
5.03
5.01
5.01
4.96
4.96
4.95
4.95
4.93
4.92
4.92
3.71
3.71
1.14
MeO
tBu
(S)-3g
1.00
2.00
1.00
6.00
2.00
1.00
2.00
1.00
2.00
2.00
3.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

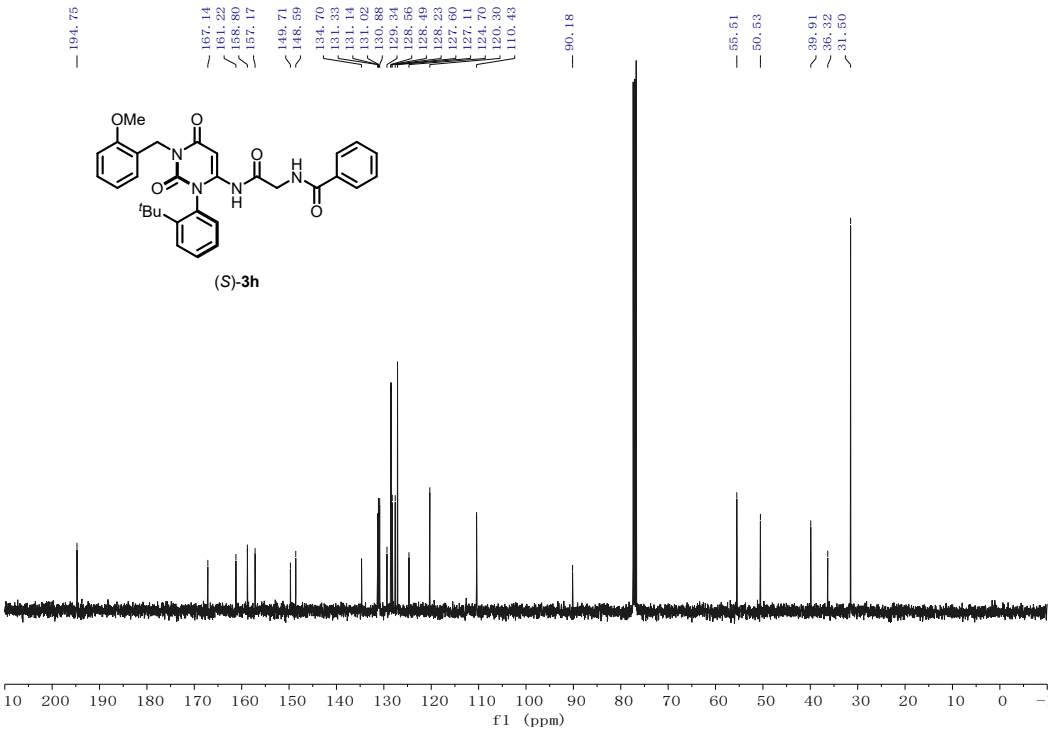

194.66
167.19
161.08
159.15
158.65
149.94
148.63
131.37
131.12
131.09
131.01
130.95
129.31
129.19
128.60
128.52
127.13
113.69
90.28
55.30
50.54
43.80
36.30
31.48
MeO
tBu
(S)-3g
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.63
7.63
7.61
7.61
7.45
7.45
7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.31
7.04
7.04
7.02
6.78
6.77
6.76
6.76
5.10
5.03
5.00
4.43
3.76
1.23
MeO
NH2
tBu
(R)-1g
1.00
3.01
1.00
1.00
2.00
1.00
2.00
2.00
3.00
9.00
f1 (ppm)

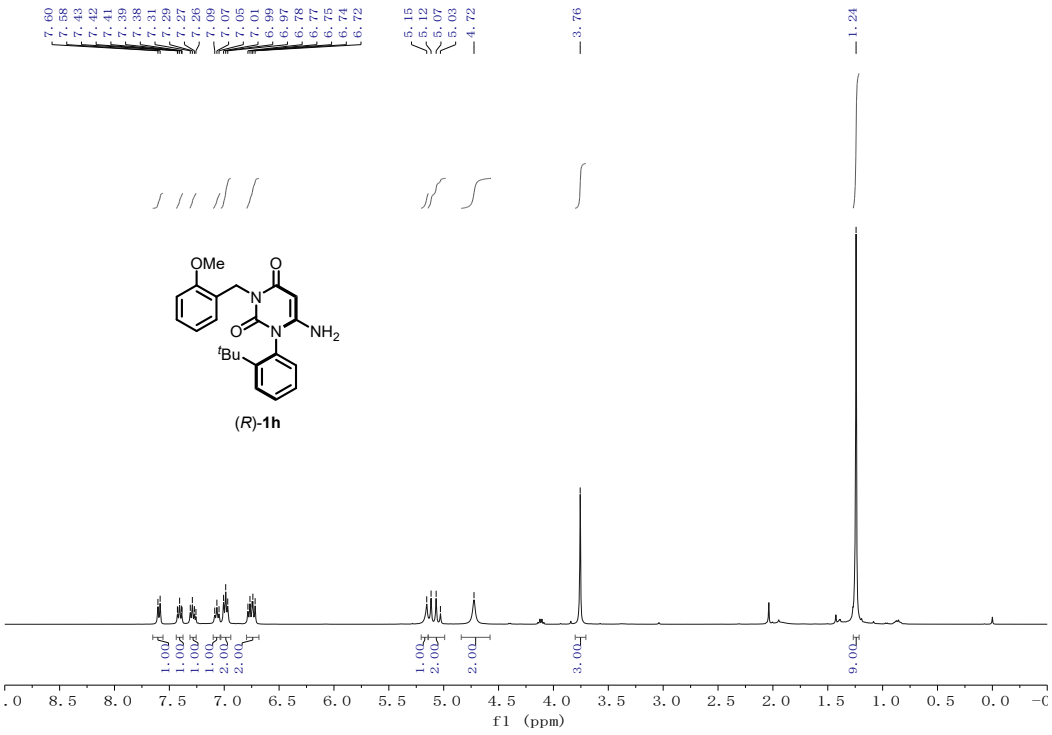

163.19
158.84
153.53
151.75
148.66
131.23
130.82
130.65
130.46
130.45
129.83
128.00
113.50
77.70
55.25
43.48
36.22
31.45
MeO
NH2
tBu
(R)-1g
f1 (ppm)


10.99
10.98
7.77
7.76
7.75
7.60
7.60
7.58
7.58
7.43
7.43
7.42
7.42
7.41
7.40
7.40
7.39
7.38
7.38
7.36
7.35
7.35
7.33
7.31
7.29
7.29
7.27
7.16
7.15
7.15
7.13
7.13
7.03
7.02
7.01
7.00
7.00
6.98
6.98
6.80
6.78
6.77
5.24
5.20
5.10
5.07
4.98
4.97
4.93
4.92
4.90
4.89
3.76
1.17
OMe
tBu
1.00
2.00
1.00
2.00
2.00
1.00
2.00
2.00
1.00
2.00
2.00
3.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

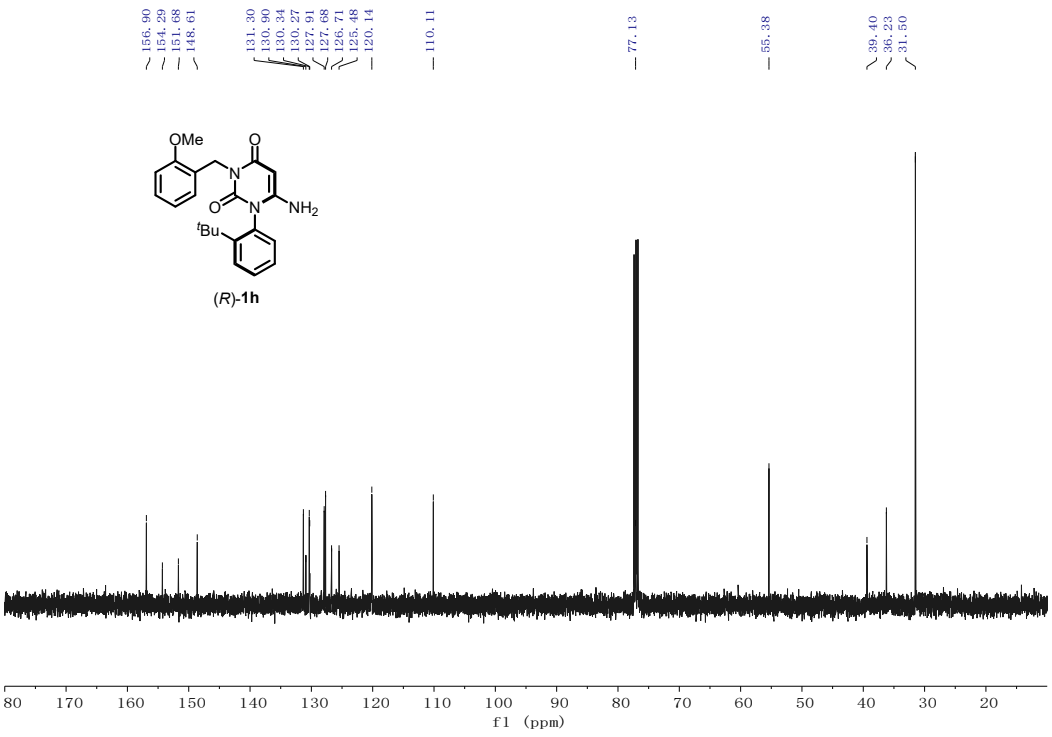
(*S*)-**3h**


194.75
167.14
161.22
158.80
157.17
149.71
148.59
134.70
131.33
131.14
131.02
130.88
129.34
128.56
128.49
128.23
127.60
127.11
124.70
120.30
110.43
90.18
55.51
50.53
39.91
36.32
31.50
OMe
tBu
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

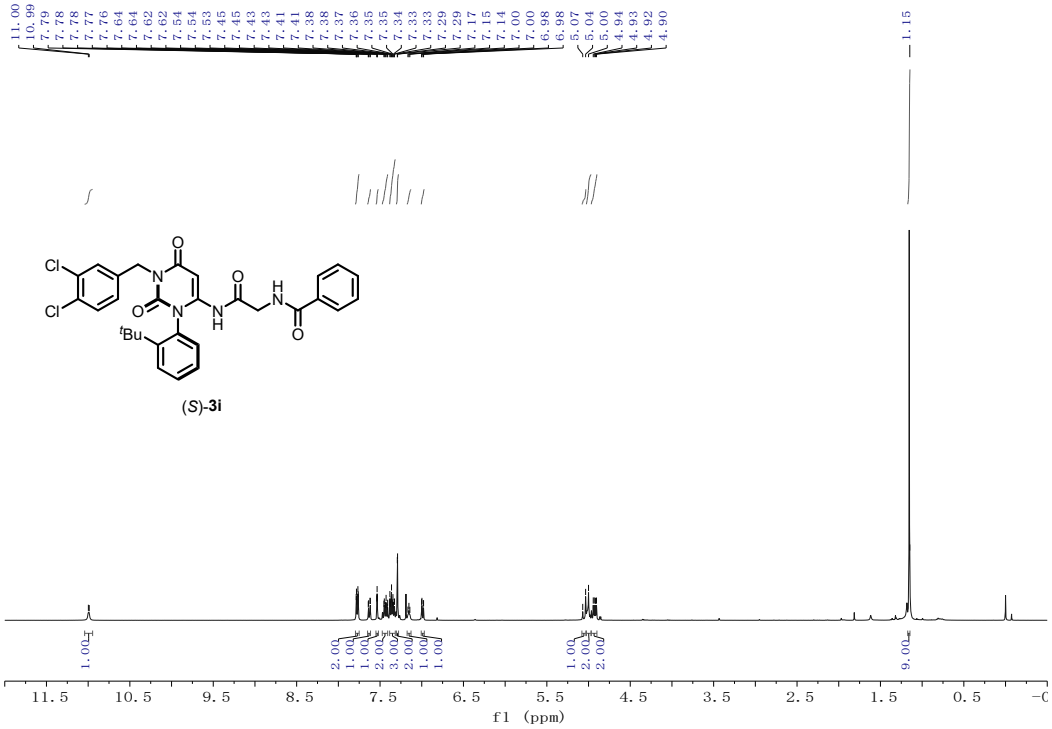
(*S*)-**3h**


7.60
7.58
7.43
7.42
7.41
7.39
7.38
7.31
7.29
7.27
7.26
7.09
7.07
7.05
7.01
6.99
6.97
6.78
6.77
6.75
6.74
6.72
5.15
5.12
5.07
5.03
4.72
3.76
1.24
OMe
O
N
O
N
NH2
tBu
1.00
1.00
1.00
1.00
2.00
2.00
1.00
2.00
2.00
3.00
9.00
f1 (ppm)

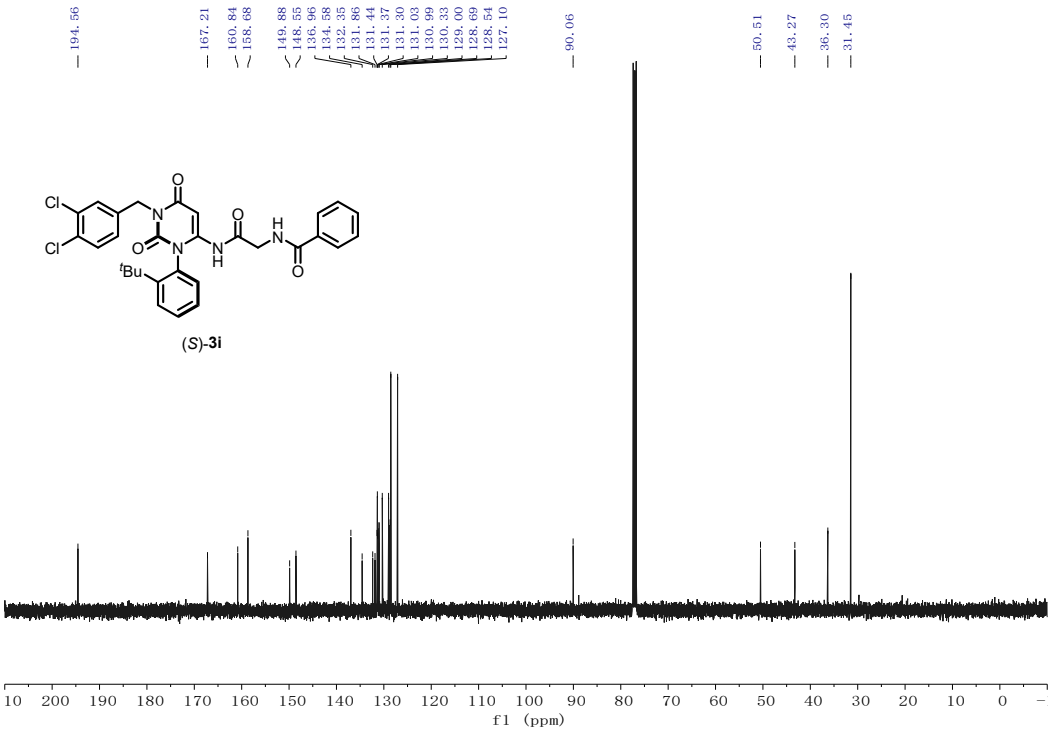
(*R*)-**1h**


156.90
154.29
151.68
148.61
131.30
130.90
130.34
130.27
127.91
127.68
126.71
125.48
120.14
110.11
77.13
55.38
39.40
36.23
31.50
OMe
O
N
O
N
NH2
tBu
f1 (ppm)

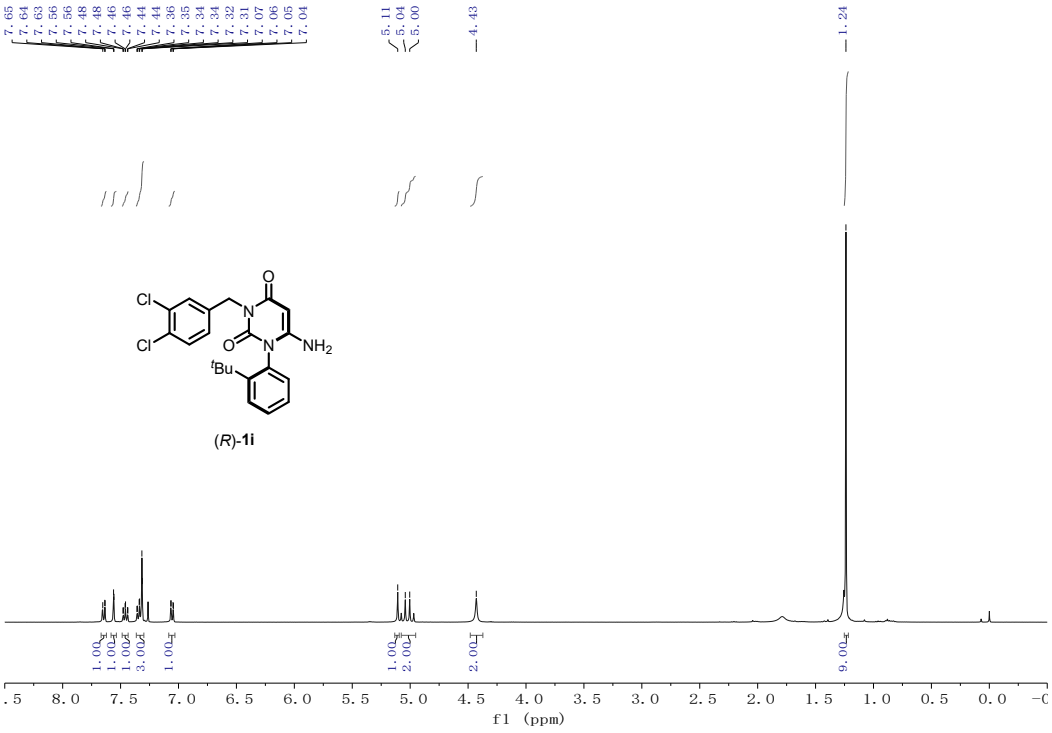
(*R*)-**1h**

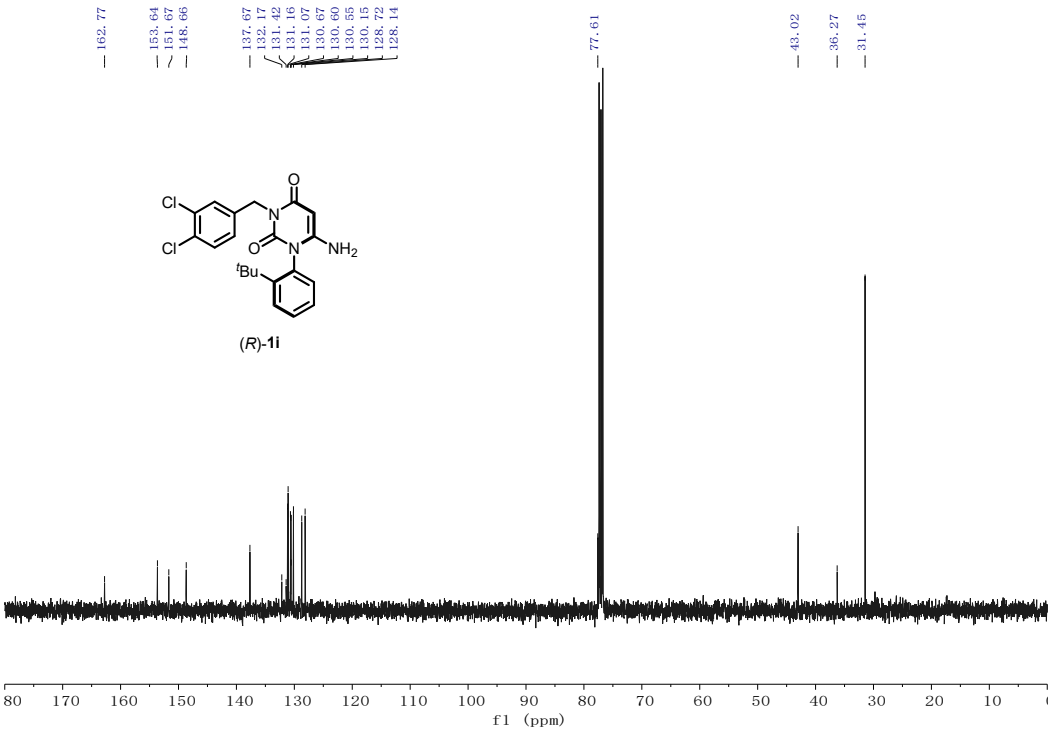

11.00
10.99
7.79
7.78
7.78
7.77
7.76
7.64
7.62
7.54
7.53
7.45
7.43
7.41
7.38
7.37
7.36
7.35
7.34
7.33
7.29
7.29
7.17
7.15
7.14
7.00
7.00
6.98
6.98
5.07
5.04
5.00
4.94
4.93
4.92
4.90
1.15
Cl
Cl
O
N
O
N
O
N
H
H
N
O
tBu
1.00
2.00
1.00
1.00
2.00
3.00
2.00
1.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

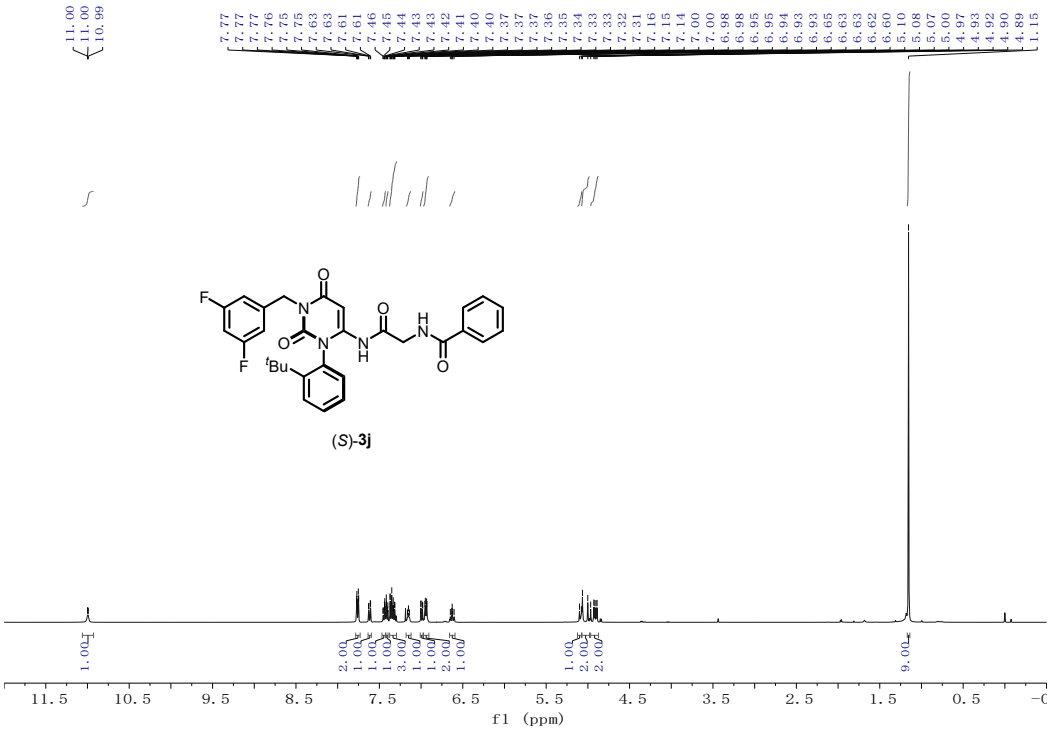
(*S*)-**3i**


194.56
167.21
160.84
158.68
149.88
148.55
136.96
134.58
132.35
131.86
131.44
131.37
131.30
131.03
130.99
130.33
129.00
128.69
128.54
127.10
90.06
50.51
43.27
36.30
31.45
Cl
Cl
O
N
O
N
O
N
H
H
N
O
tBu
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

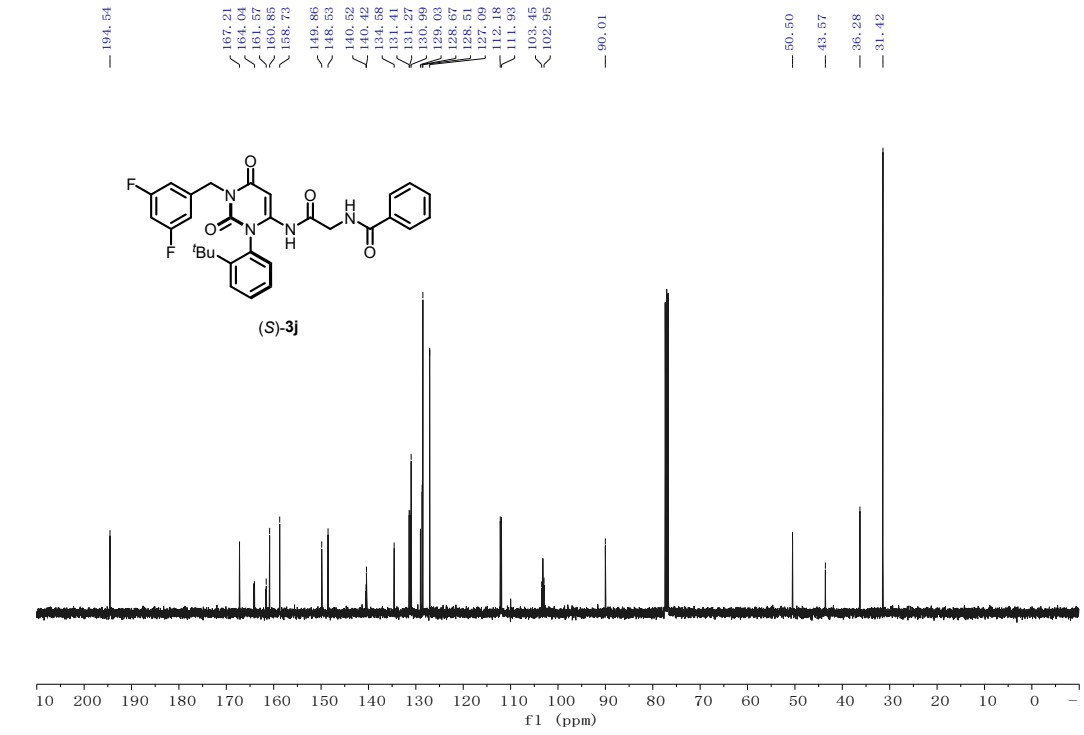
(*S*)-**3i**


7.65
7.64
7.63
7.56
7.56
7.48
7.48
7.46
7.46
7.44
7.44
7.36
7.35
7.34
7.34
7.32
7.31
7.07
7.06
7.05
7.04
5.11
5.04
5.00
4.43
1.24
Cl
Cl
O
N
O
N
NH2
tBu
(R)-1i
1.00
1.00
1.00
3.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

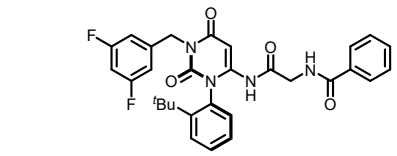

162.77
153.64
151.67
148.66
137.67
132.17
131.42
131.16
131.07
130.67
130.60
130.55
130.15
128.72
128.14
77.61
43.02
36.27
31.45
Cl
Cl
O
N
O
N
NH2
tBu
(R)-1i
f1 (ppm)


11.00
11.00
10.99
7.77
7.77
7.77
7.76
7.75
7.75
7.63
7.63
7.61
7.61
7.46
7.45
7.44
7.43
7.43
7.42
7.41
7.40
7.40
7.37
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.16
7.15
7.14
7.00
7.00
6.98
6.98
6.95
6.95
6.94
6.93
6.93
6.65
6.63
6.63
6.62
6.60
5.10
5.08
5.07
5.00
4.97
4.93
4.92
4.90
4.89
1.15
1.00
2.00
1.00
1.00
1.00
3.00
1.00
1.00
2.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

(*S*)-**3j**

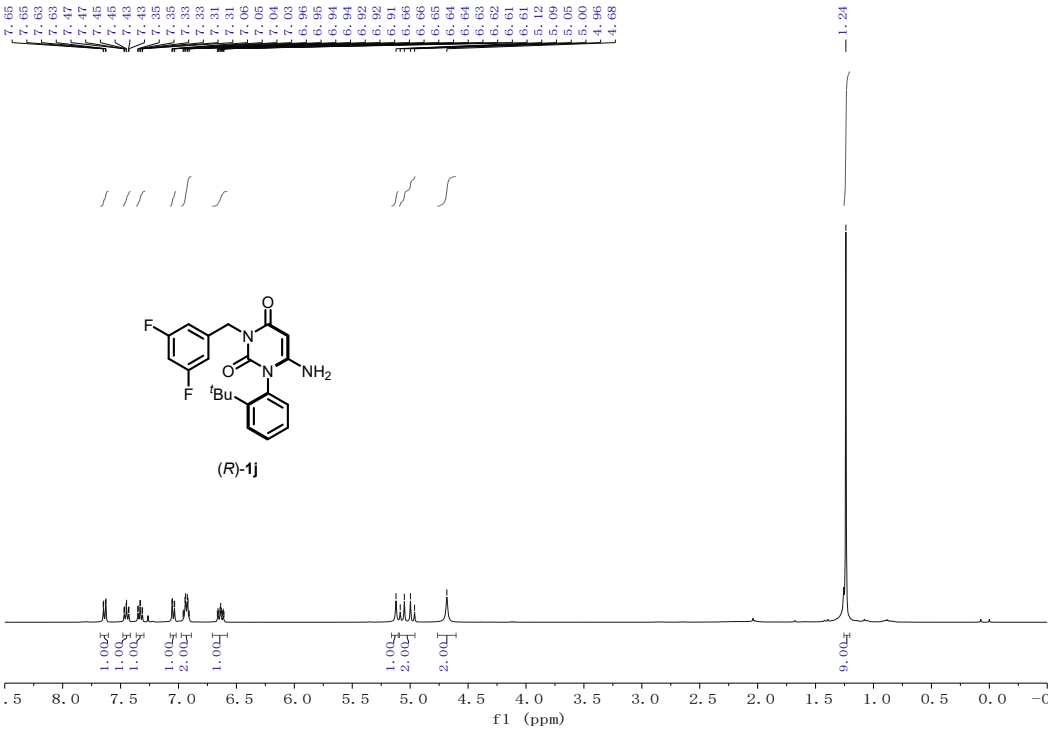

194.54
167.21
164.04
161.57
160.85
158.73
149.86
148.53
140.52
140.42
134.58
131.41
131.27
130.99
129.03
128.67
128.51
127.09
112.18
111.93
103.45
102.95
90.01
50.50
43.57
36.28
31.42
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

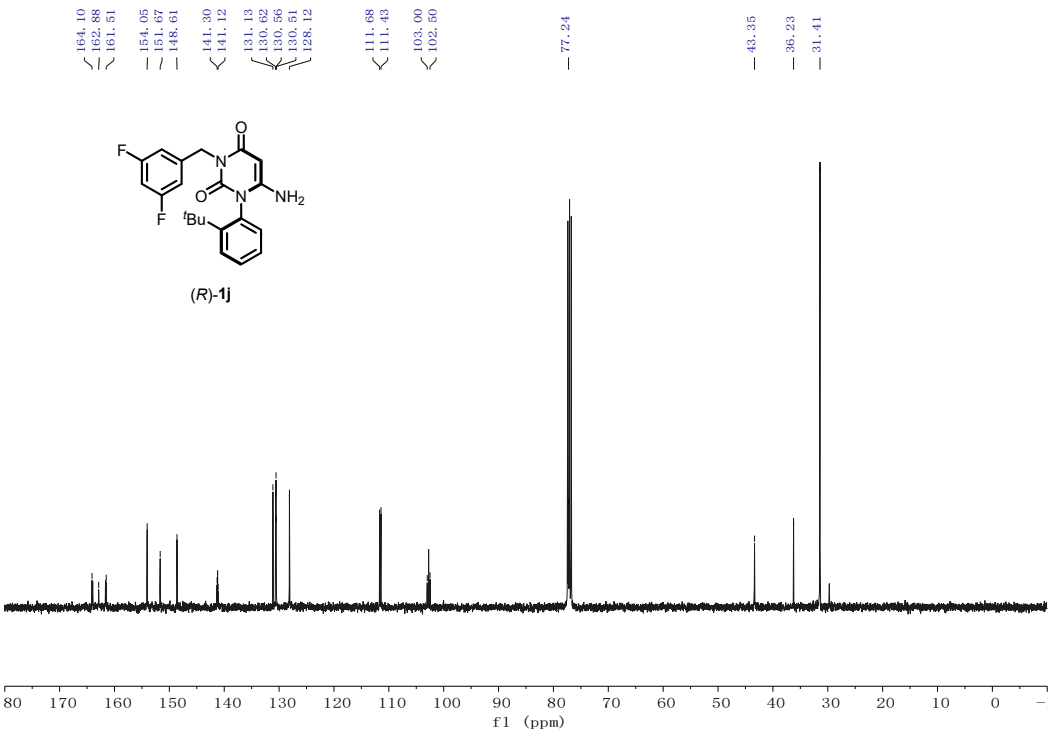
(*S*)-**3j**

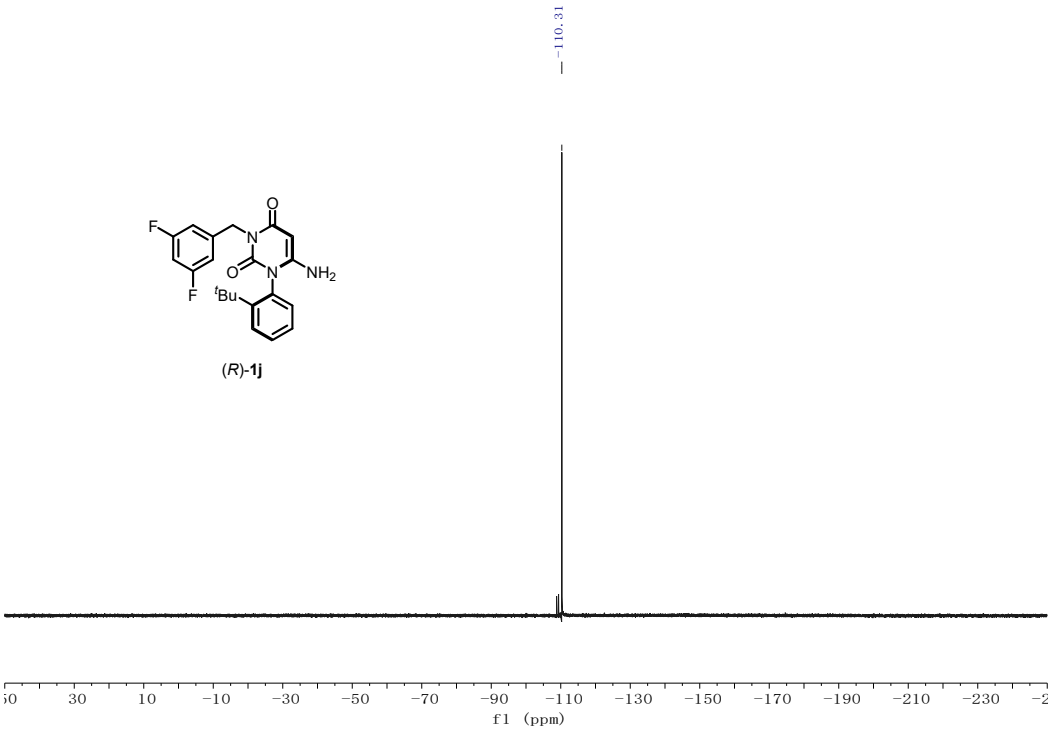

F
O
N
O
N
F
tBu
O
H
N
N
H
O

(*S*)-**3j**

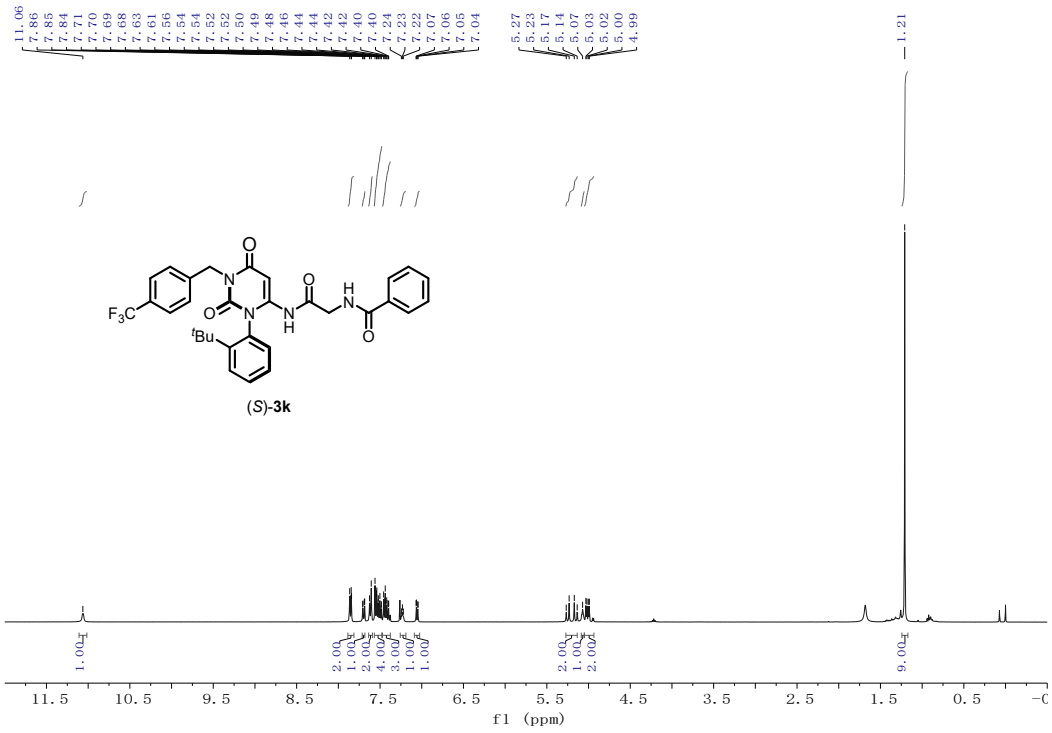
-109.79
90
70
50
30
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


7.65
7.63
7.47
7.45
7.43
7.35
7.33
7.31
7.06
7.05
7.04
7.03
6.96
6.95
6.94
6.92
6.91
6.66
6.65
6.64
6.63
6.62
6.61
5.12
5.09
5.05
5.00
4.96
4.68
1.24
F
O
N
O
N
NH2
F
tBu
(R)-1j
1.00
1.00
1.00
1.00
2.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

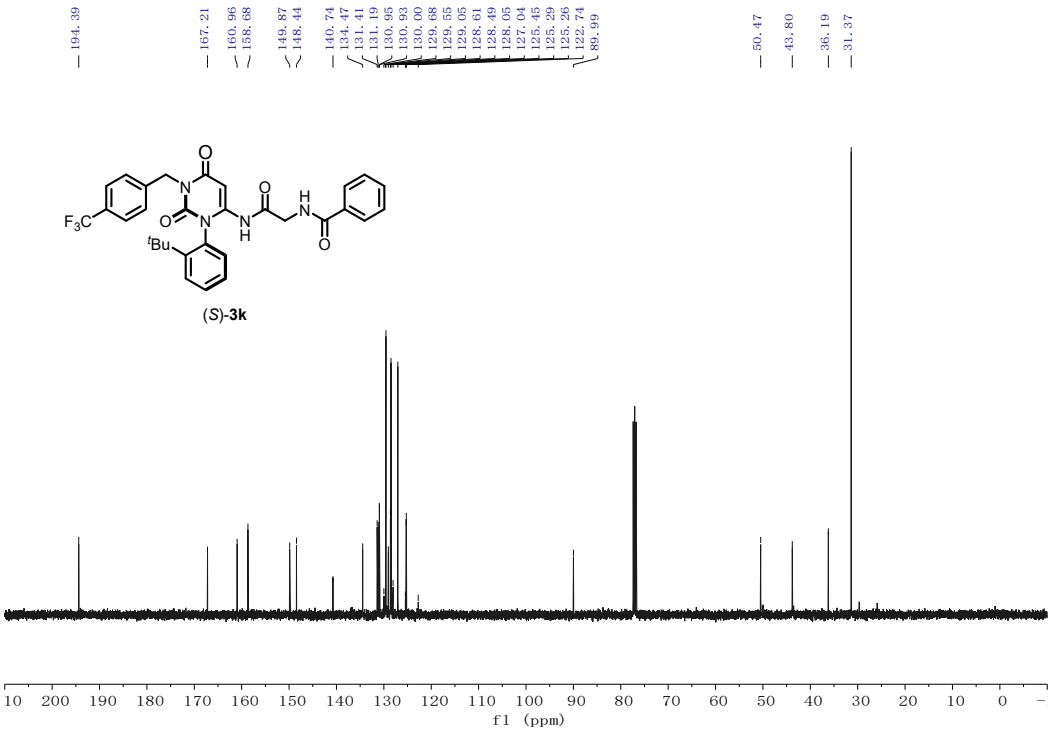

164.10
162.88
161.51
154.05
151.67
148.61
141.30
141.12
131.13
130.62
130.56
130.51
128.12
111.68
111.43
103.00
102.50
77.24
43.35
36.23
31.41
F
O
N
O
N
NH2
F
tBu
(R)-1j
f1 (ppm)


−110.31
F
O
N
O
N
NH2
F
tBu
50
30
10
−10
−30
−50
−70
−90
−110
−130
−150
−170
−190
−210
−230
f1 (ppm)

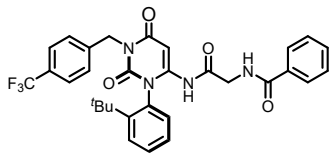
(*R*)-**1j**


11.06
7.86
7.85
7.84
7.71
7.70
7.69
7.68
7.63
7.61
7.56
7.54
7.54
7.52
7.52
7.50
7.49
7.48
7.46
7.44
7.44
7.42
7.42
7.40
7.40
7.24
7.23
7.22
7.07
7.06
7.05
7.04
5.27
5.23
5.17
5.14
5.07
5.03
5.02
5.00
4.99
1.21
1.00
2.00
1.00
2.00
4.00
3.00
1.00
1.00
2.00
1.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

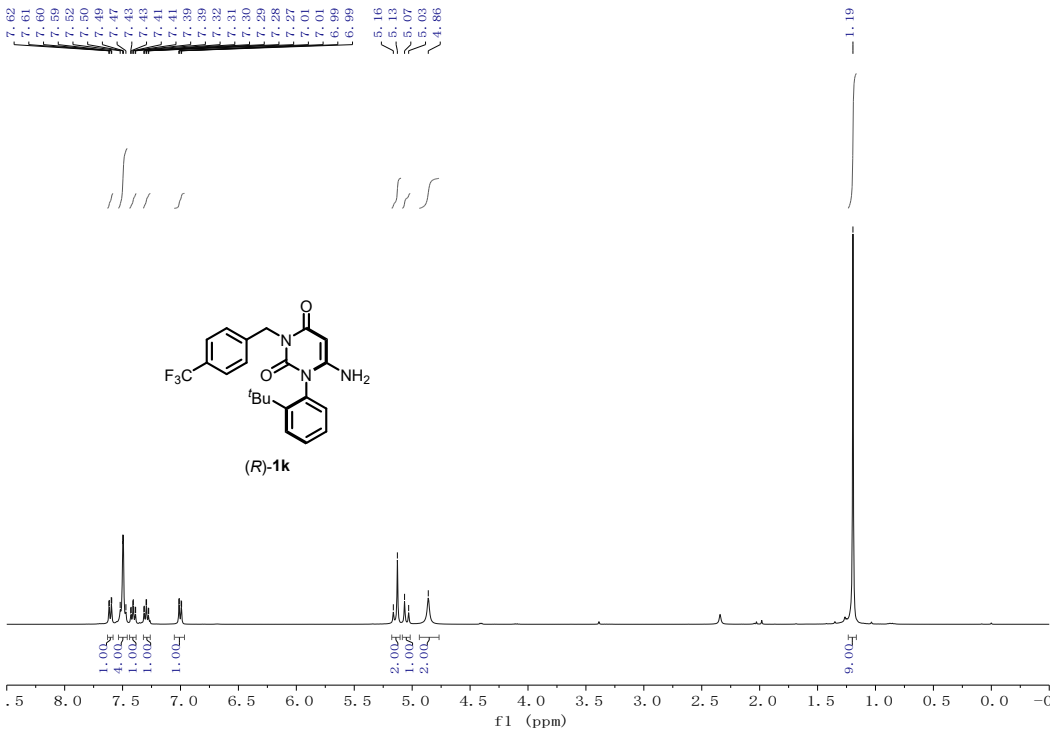
(*S*)-**3k**

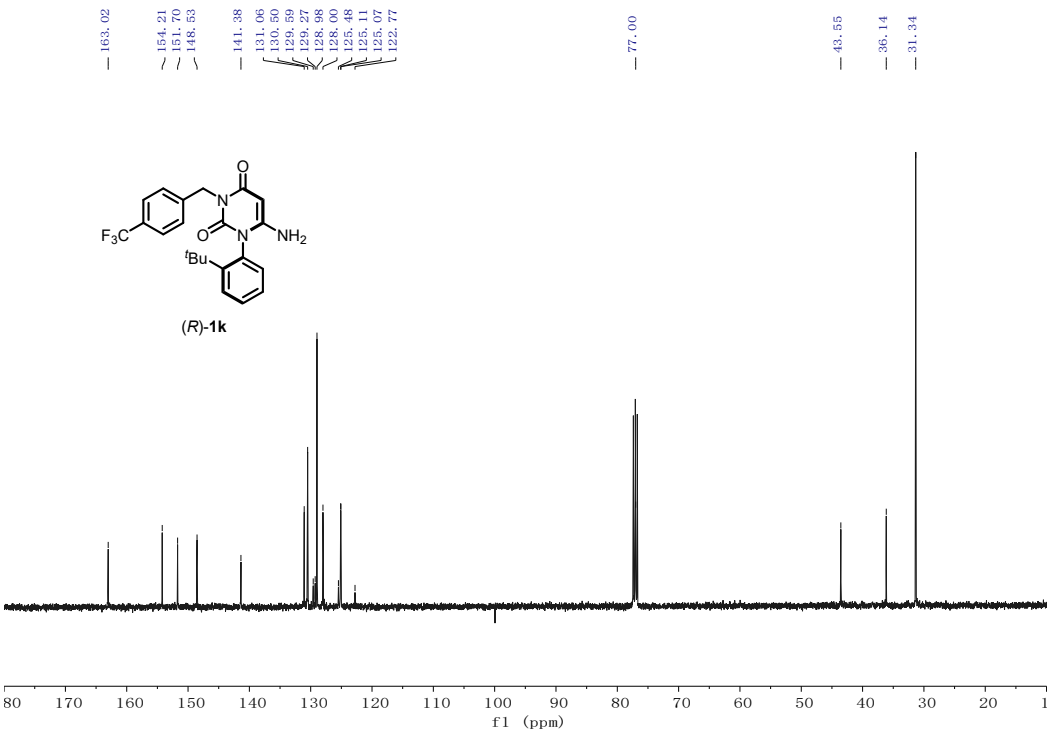

194.39
167.21
160.96
158.68
149.87
148.44
140.74
134.47
131.41
131.19
130.95
130.93
130.00
129.68
129.55
129.05
128.61
128.49
128.05
127.04
125.45
125.29
125.26
122.74
89.99
50.47
43.80
36.19
31.37
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

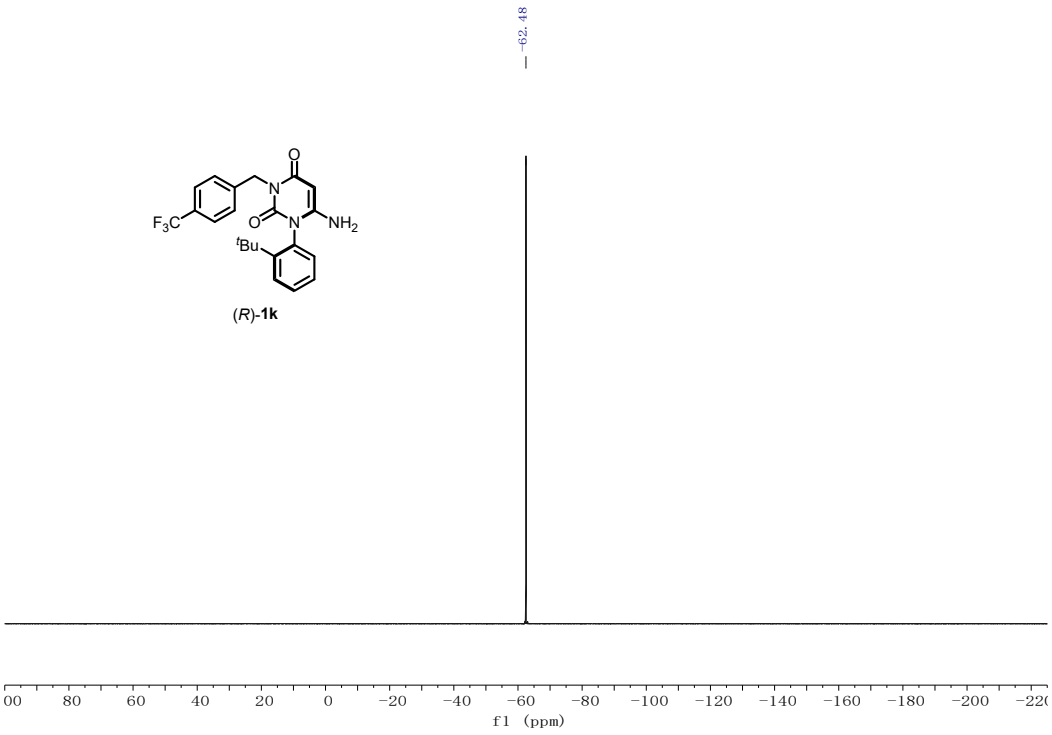
(*S*)-**3k**



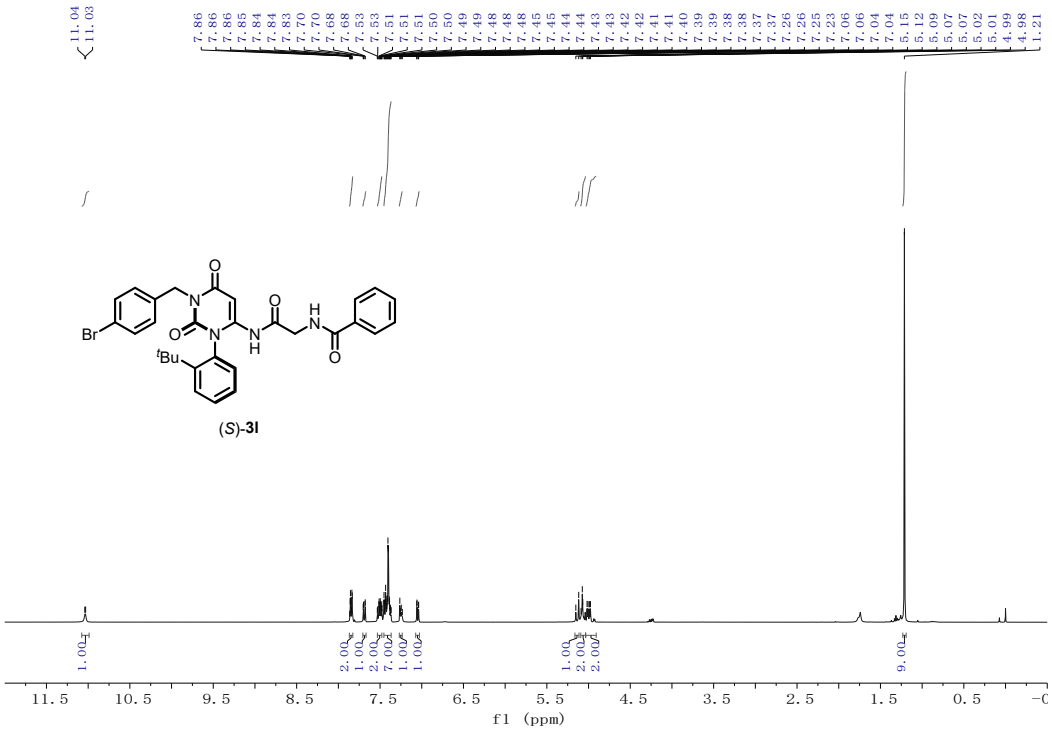
(*S*)-**3k**

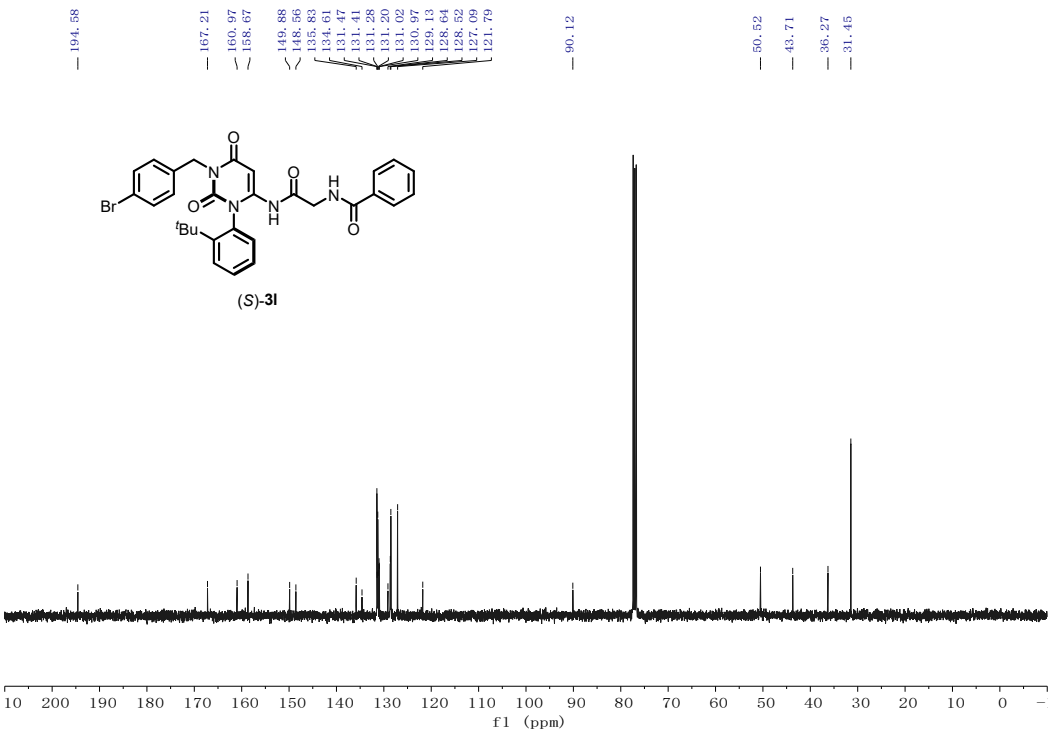

7.62
7.61
7.60
7.59
7.52
7.50
7.49
7.47
7.43
7.43
7.41
7.41
7.39
7.39
7.32
7.31
7.30
7.29
7.28
7.27
7.01
7.01
6.99
6.99
5.16
5.13
5.07
5.03
4.86
1.19
F3C
O
N
O
N
NH2
tBu
(R)-1k
1.00
4.00
1.00
1.00
1.00
2.00
1.00
2.00
9.00
f1 (ppm)

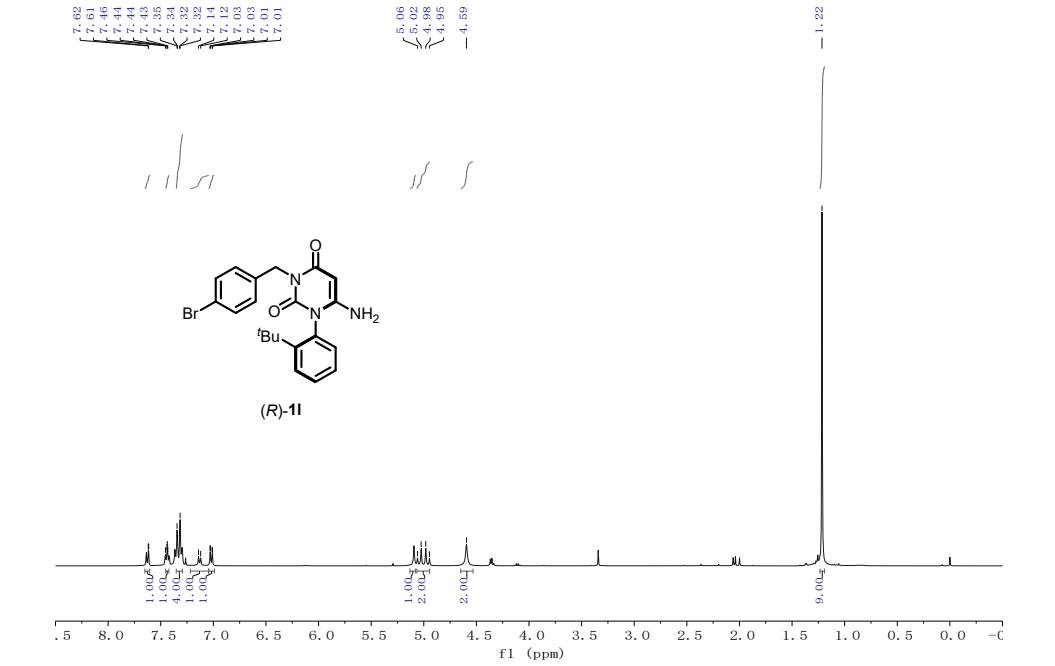

163.02
154.21
151.70
148.53
141.38
131.06
130.50
129.59
129.27
128.98
128.00
125.48
125.11
125.07
122.77
77.00
43.55
36.14
31.34
F3C
O
N
O
N
NH2
tBu
(R)-1k
f1 (ppm)


−62.48
O
N
O
N
NH2
F3C
tBu
00
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−22(
f1 (ppm)

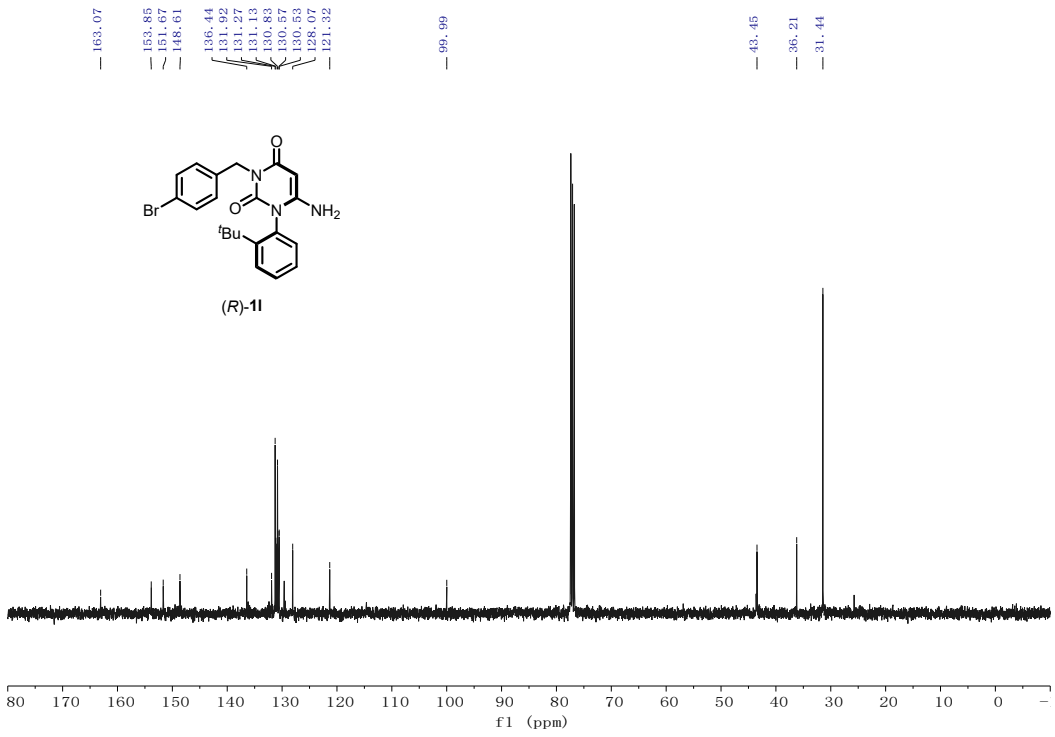
(*R*)-**1k**


11.04
11.03
7.86
7.86
7.86
7.85
7.84
7.84
7.83
7.70
7.70
7.68
7.68
7.53
7.51
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.45
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.26
7.26
7.25
7.23
7.06
7.06
7.04
7.04
5.15
5.12
5.09
5.07
5.07
5.02
5.01
4.99
4.98
1.21
Br
tBu
(S)-3l
1.00
2.00
1.00
2.00
7.00
1.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

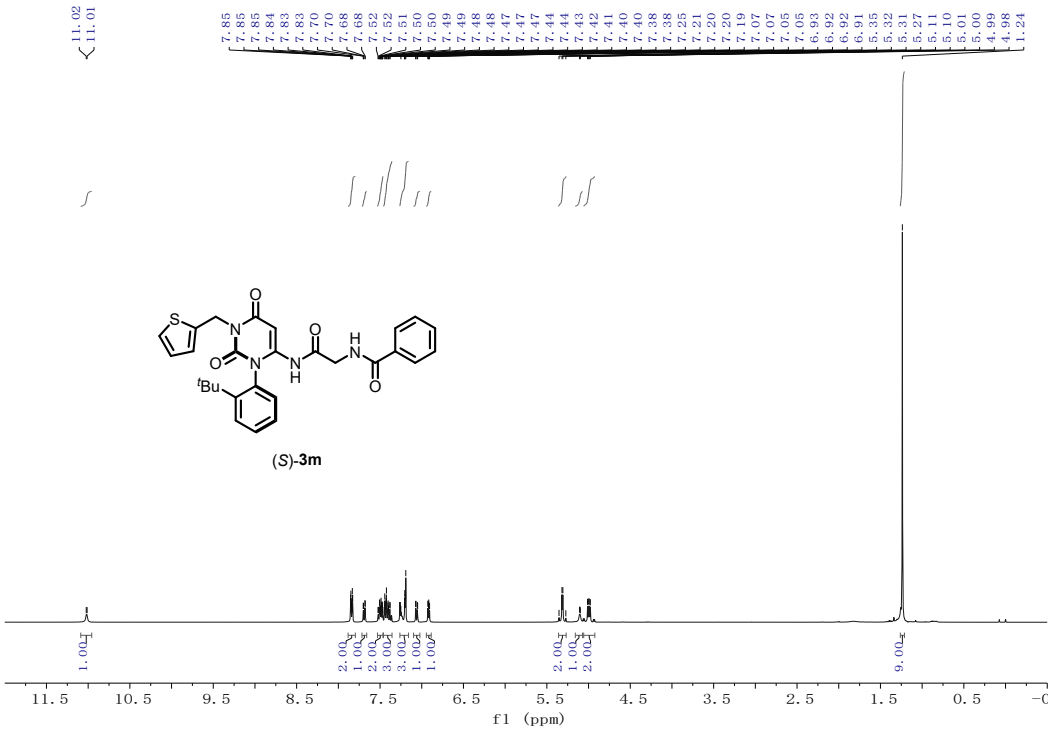

194.58
167.21
160.97
158.67
149.88
148.56
135.83
134.61
131.47
131.41
131.28
131.20
131.02
130.97
129.13
128.64
128.52
127.09
121.79
90.12
50.52
43.71
36.27
31.45
Br
tBu
(S)-3l
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.62
7.61
7.46
7.44
7.44
7.43
7.35
7.34
7.32
7.32
7.14
7.12
7.03
7.01
7.01
5.06
5.02
4.98
4.95
4.59
1.22
Br
NH2
tBu
1.00
1.00
4.00
1.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

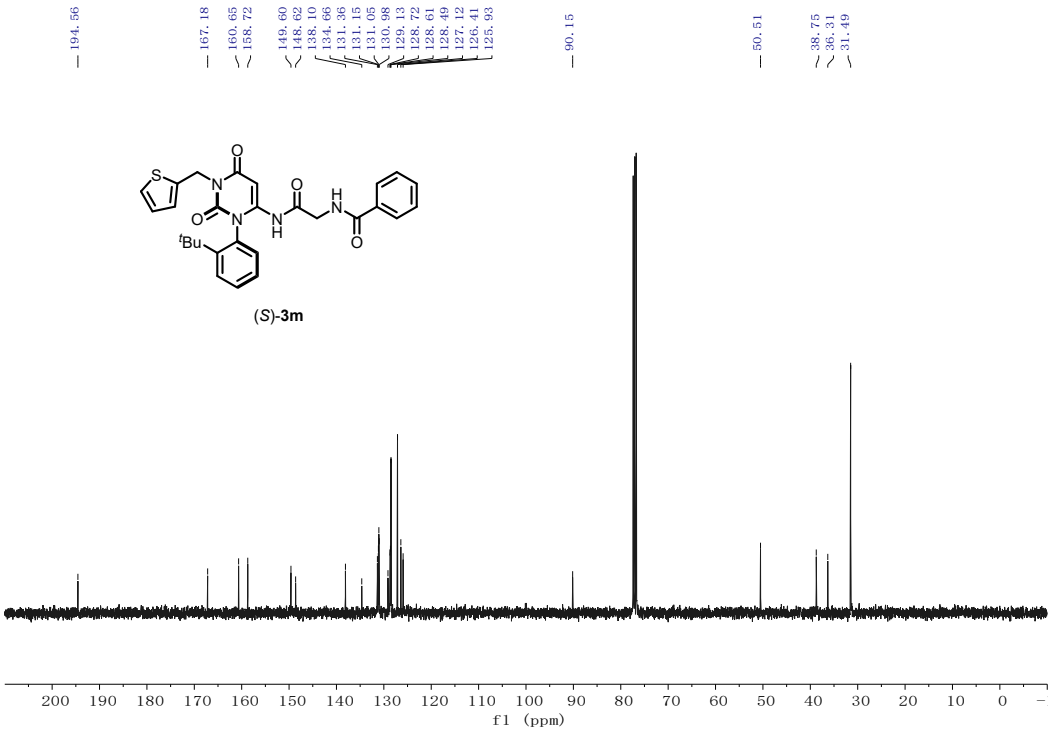
(*R*)-**1l**


163.07
153.85
151.67
148.61
136.44
131.92
131.27
131.13
130.83
130.57
130.53
128.07
121.32
99.99
43.45
36.21
31.44
Br
NH2
tBu
f1 (ppm)

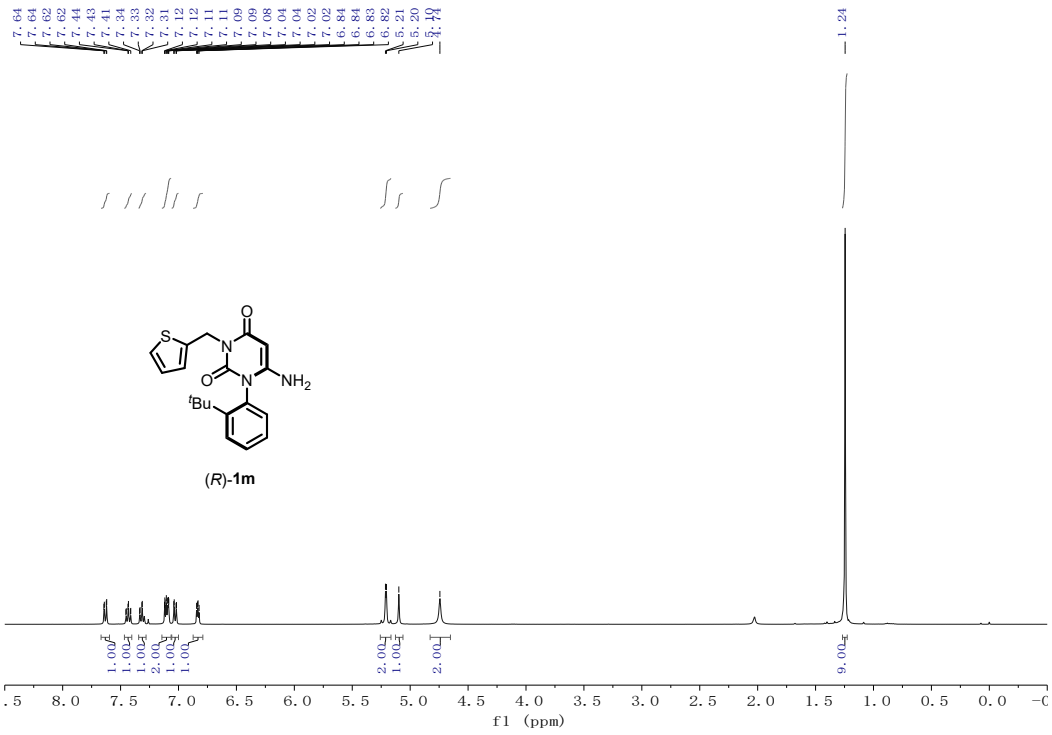
(*R*)-**1l**


11.02
11.01
7.85
7.85
7.85
7.84
7.83
7.83
7.70
7.70
7.68
7.68
7.52
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.47
7.44
7.44
7.43
7.42
7.41
7.40
7.40
7.38
7.38
7.25
7.21
7.20
7.20
7.19
7.07
7.07
7.05
7.05
6.93
6.92
6.92
6.91
5.35
5.32
5.31
5.27
5.11
5.10
5.01
5.00
4.99
4.98
1.24
1.00
2.00
1.00
2.00
3.00
3.00
1.00
1.00
2.00
1.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

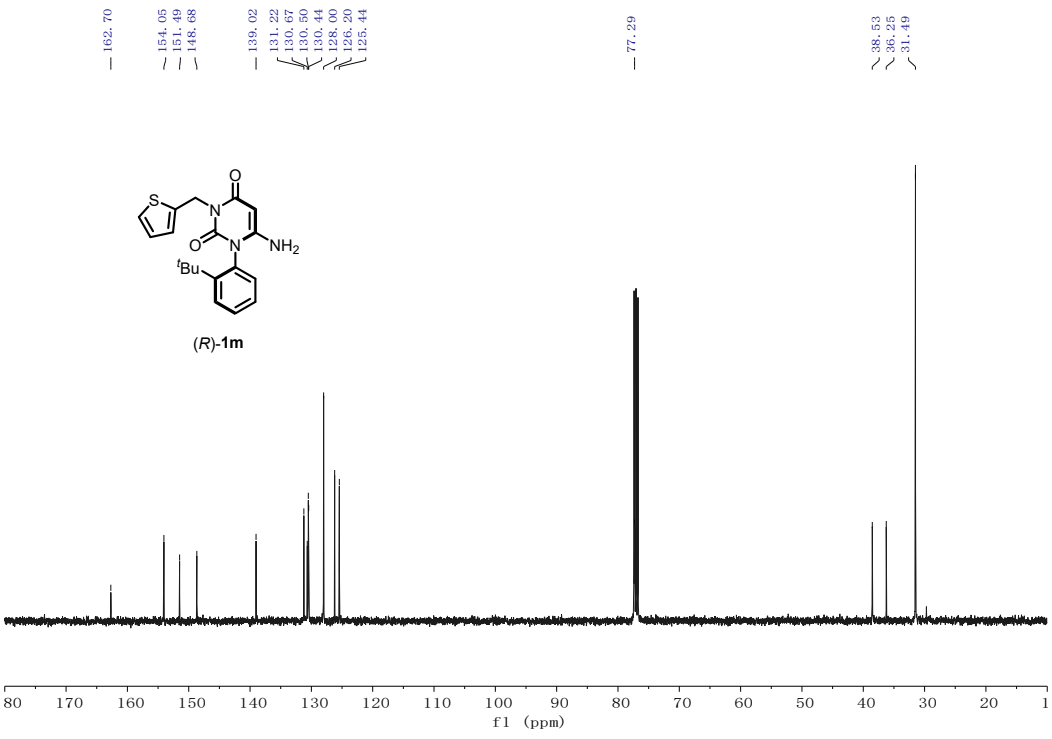
(*S*)-**3m**


194.56
167.18
160.65
158.72
149.60
148.62
138.10
134.66
131.36
131.15
131.05
130.98
129.13
128.72
128.61
128.49
127.12
126.41
125.93
90.15
50.51
38.75
36.31
31.49
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

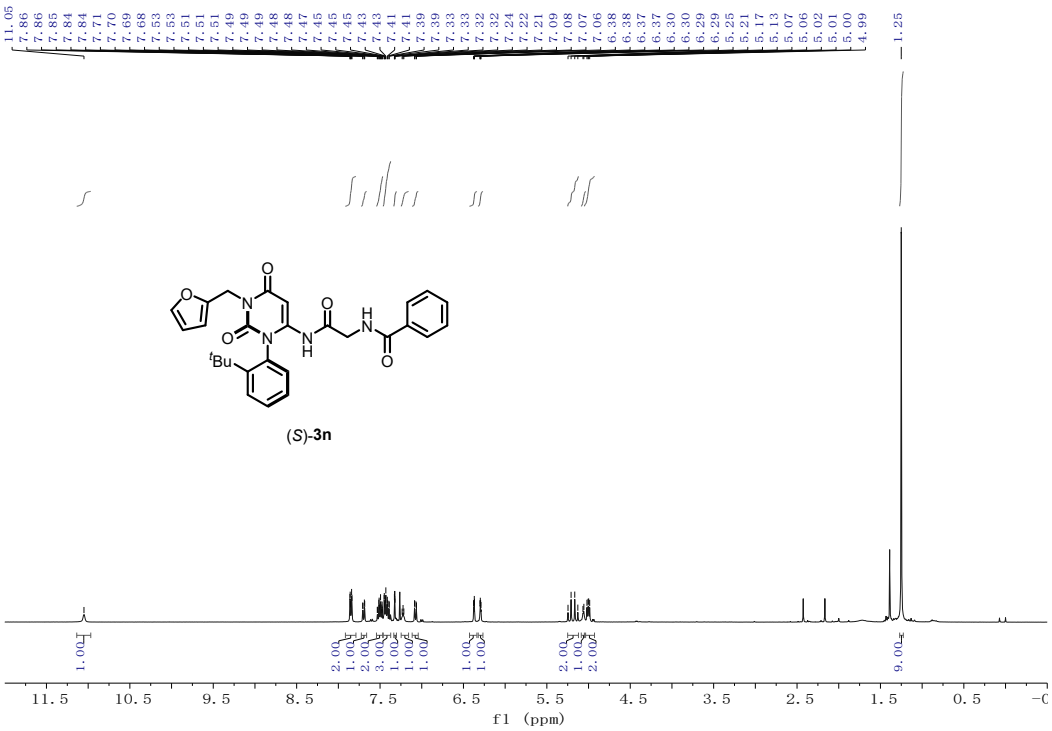
(*S*)-**3m**


7.64
7.64
7.62
7.62
7.44
7.43
7.41
7.34
7.33
7.32
7.31
7.12
7.12
7.11
7.11
7.09
7.09
7.08
7.04
7.04
7.02
7.02
6.84
6.84
6.83
6.82
5.21
5.20
1.24
1.00
1.00
1.00
2.00
1.00
1.00
2.00
1.00
2.00
9.00
f1 (ppm)

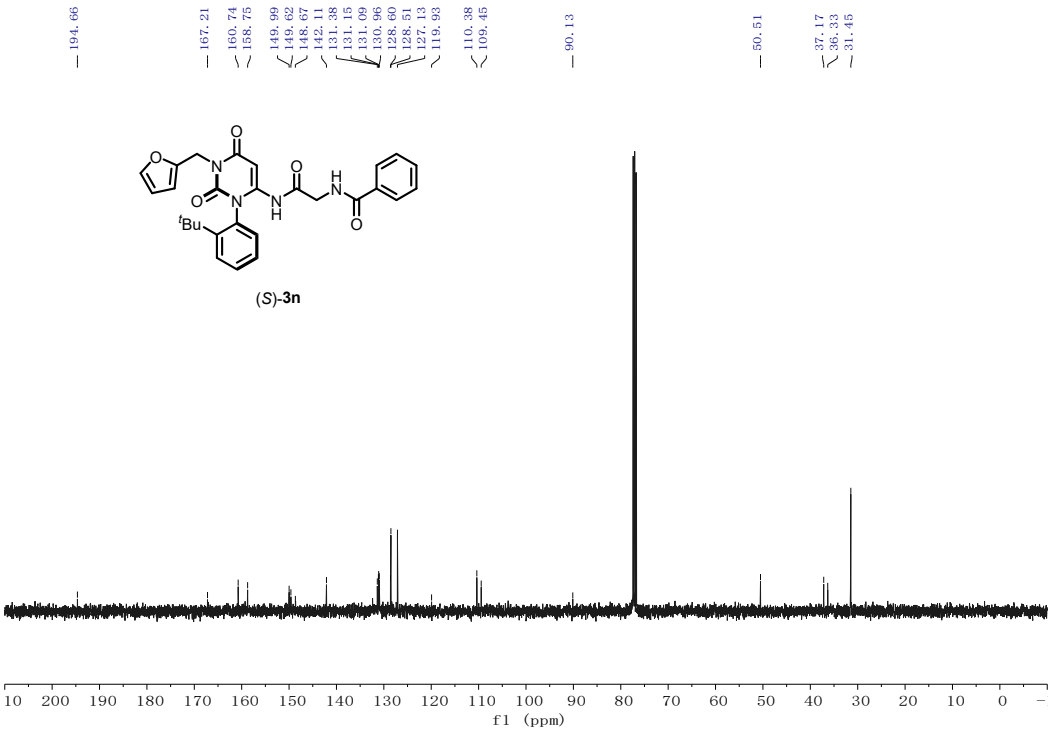
(*R*)-**1m**


162.70
154.05
151.49
148.68
139.02
131.22
130.67
130.50
130.44
128.00
126.20
125.44
77.29
38.53
36.25
31.49
f1 (ppm)

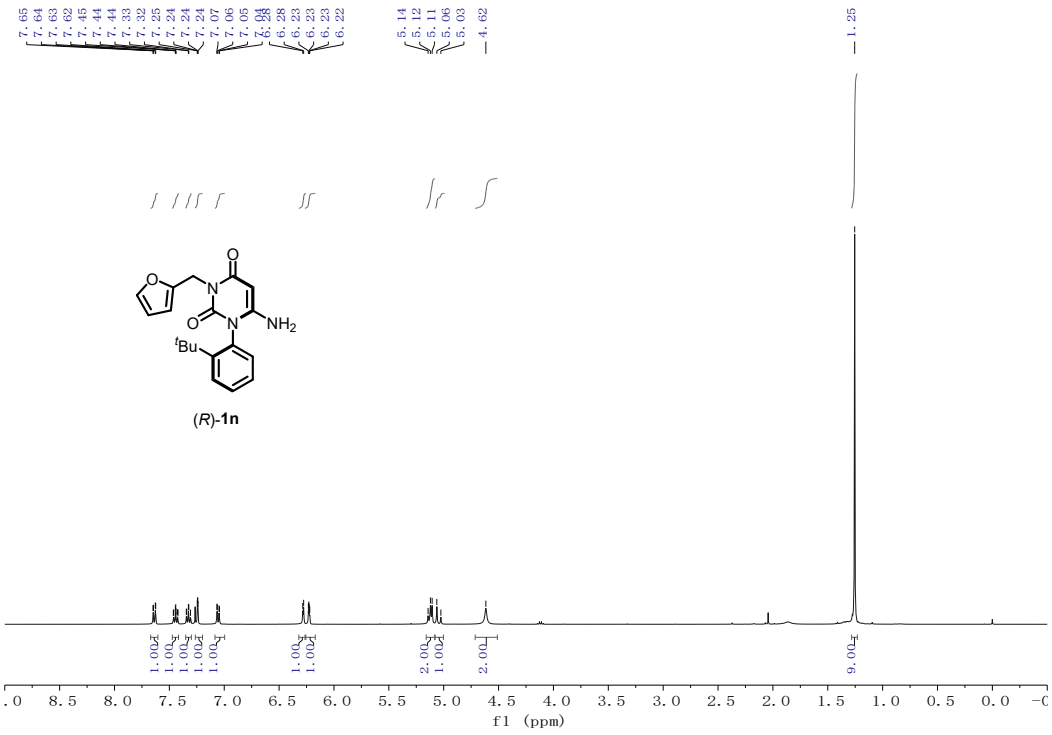
(*R*)-**1m**


11.05
7.86
7.86
7.85
7.84
7.84
7.71
7.70
7.69
7.68
7.53
7.53
7.51
7.51
7.51
7.49
7.49
7.49
7.48
7.48
7.47
7.45
7.45
7.45
7.43
7.43
7.41
7.41
7.39
7.39
7.33
7.33
7.32
7.32
7.24
7.22
7.21
7.09
7.08
7.07
7.06
6.38
6.38
6.37
6.37
6.30
6.30
6.29
6.29
5.25
5.21
5.17
5.13
5.07
5.06
5.02
5.01
5.00
4.99
1.25
1.00
2.00
1.00
2.00
3.00
1.00
1.00
1.00
1.00
2.00
1.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

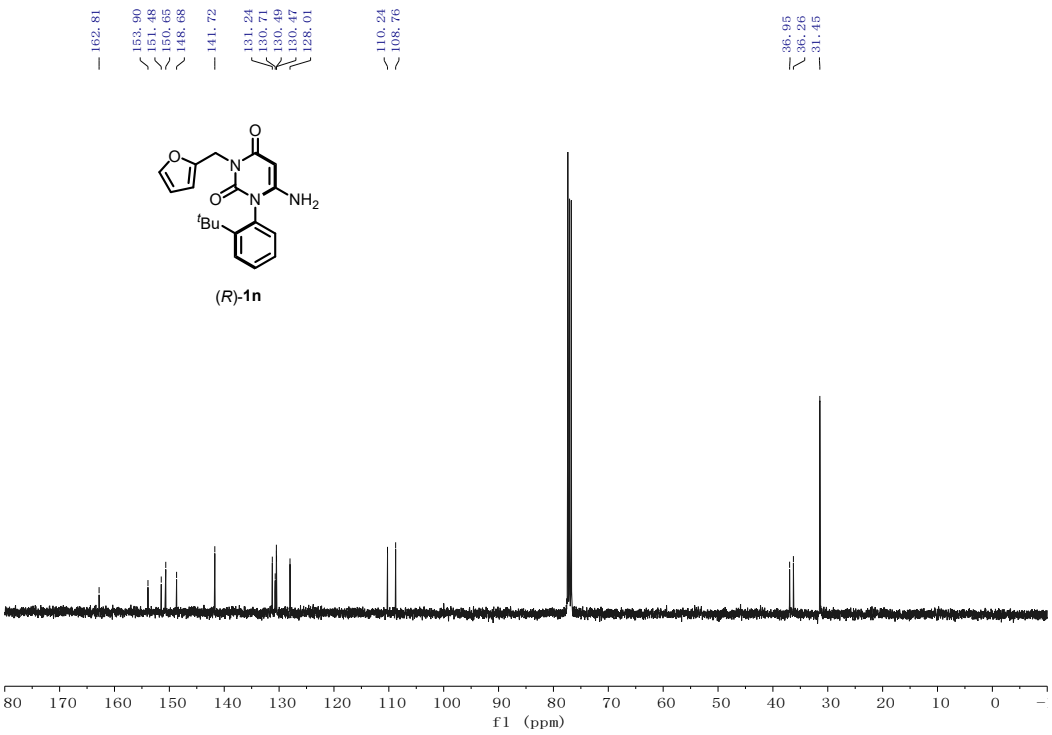
(*S*)-**3n**


194.66
167.21
160.74
158.75
149.99
149.62
148.67
142.11
131.38
131.15
131.09
130.96
128.60
128.51
127.13
119.93
110.38
109.45
90.13
50.51
37.17
36.33
31.45
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

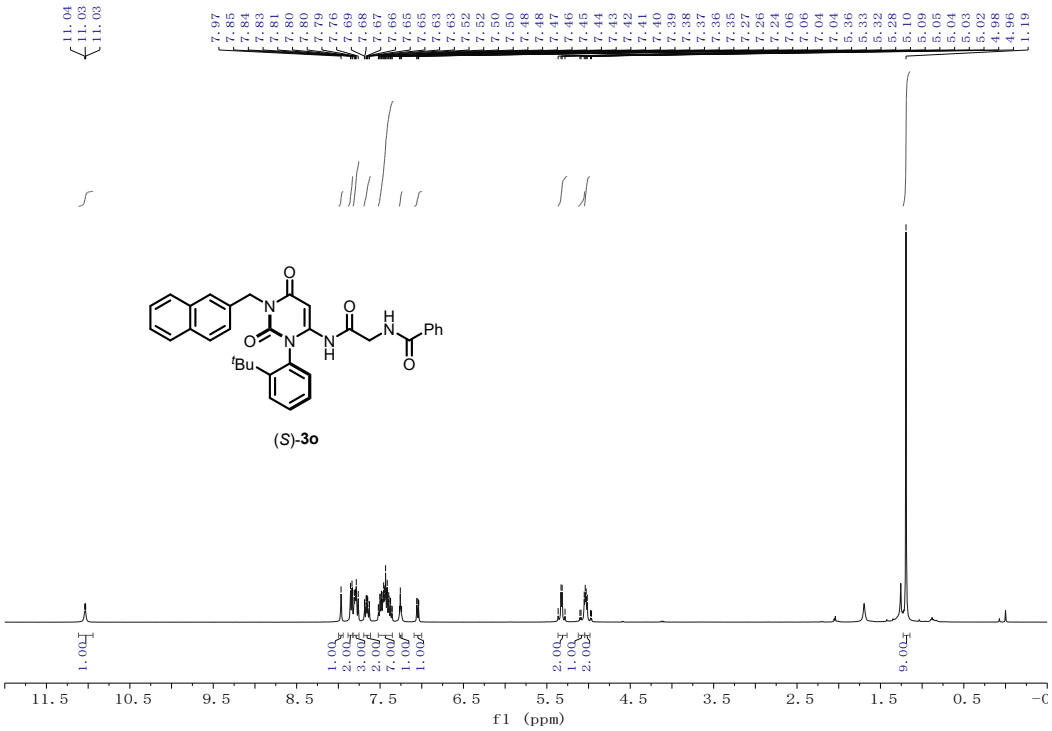
(*S*)-**3n**


7.65
7.64
7.63
7.62
7.45
7.44
7.44
7.33
7.25
7.24
7.24
7.24
7.07
7.06
7.05
6.28
6.28
6.23
6.23
6.23
6.22
5.14
5.12
5.11
5.06
5.03
4.62
1.25
1.00
1.00
1.00
1.00
1.00
1.00
1.00
2.00
1.00
2.00
9.00
f1 (ppm)

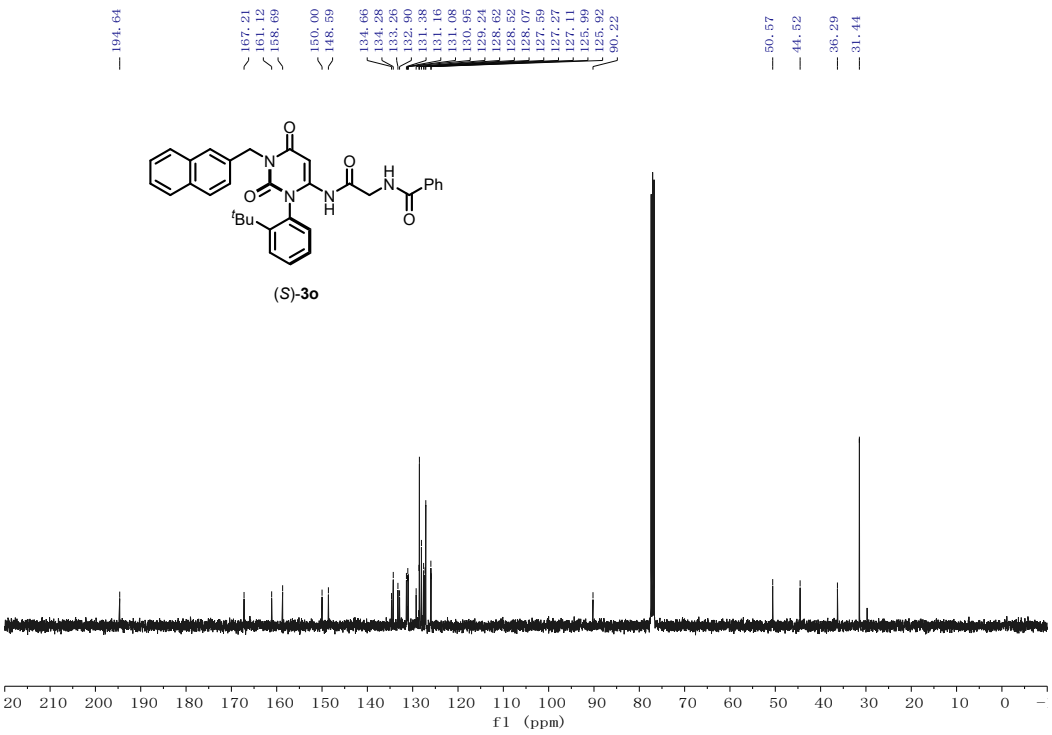
(*R*)-**1n**


162.81
153.90
151.48
150.65
148.68
141.72
131.24
130.71
130.49
130.47
128.01
110.24
108.76
36.95
36.26
31.45
f1 (ppm)

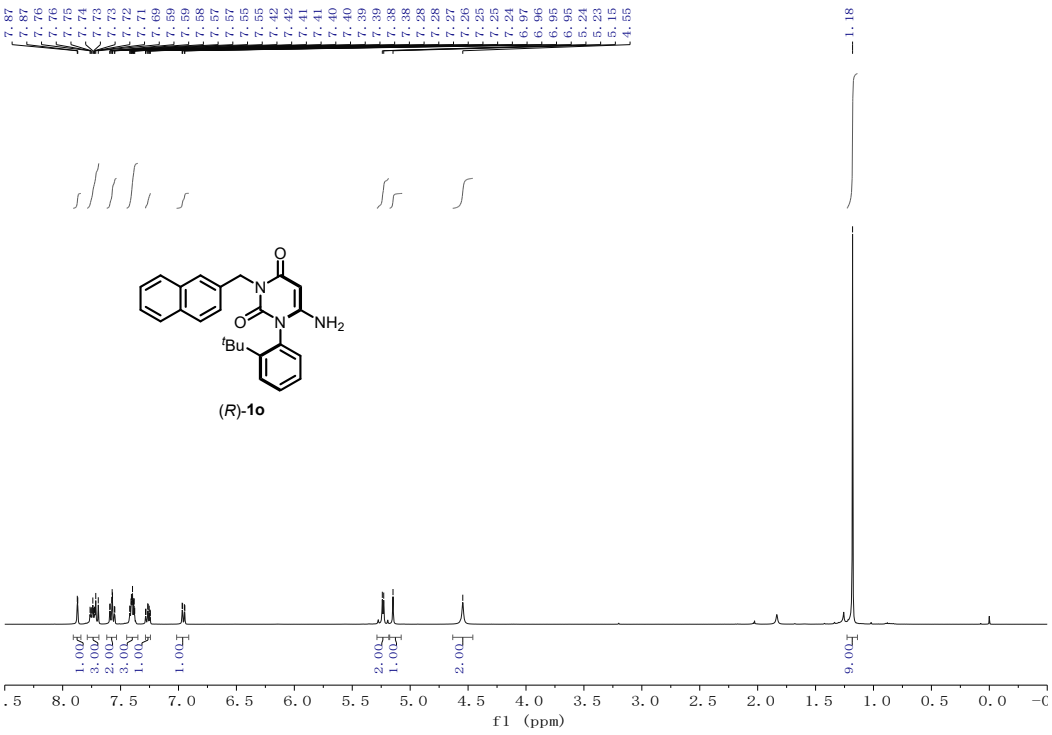
(*R*)-**1n**

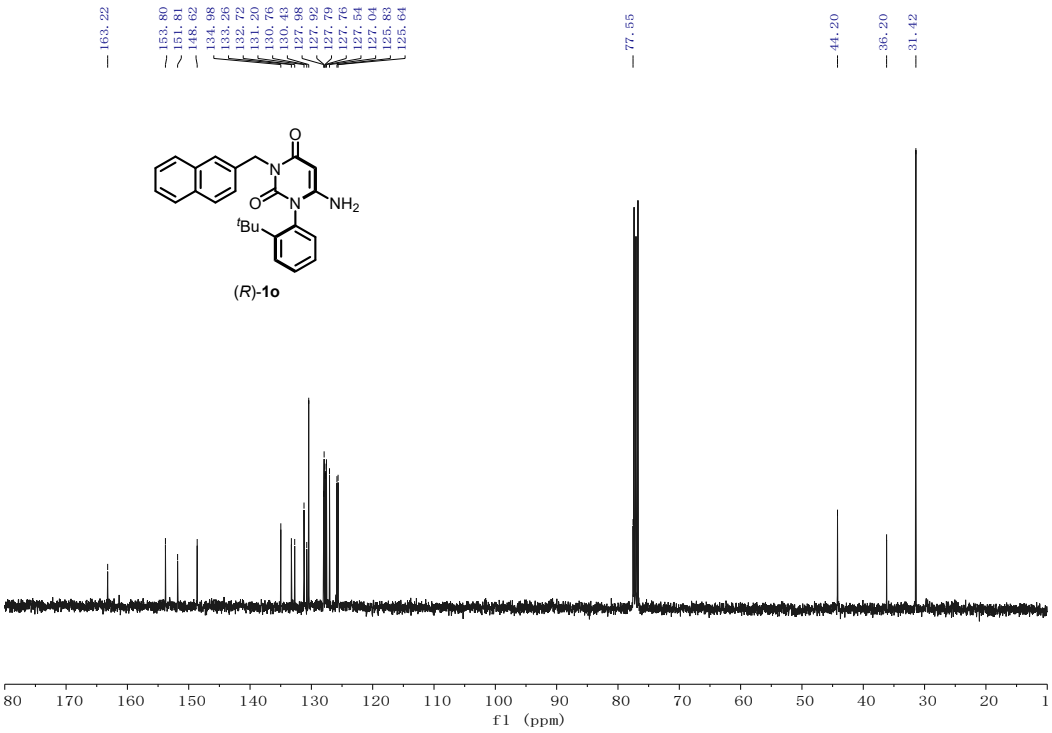

11.04
11.03
11.03
7.97
7.85
7.84
7.83
7.81
7.80
7.80
7.79
7.76
7.69
7.68
7.67
7.66
7.65
7.65
7.63
7.63
7.52
7.52
7.50
7.50
7.48
7.48
7.47
7.46
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.27
7.26
7.24
7.06
7.06
7.04
7.04
5.36
5.33
5.32
5.28
5.10
5.09
5.05
5.04
5.03
5.02
4.98
4.96
1.19
O
N
O
N
H
O
N
H
Ph
O
tBu
1.00
1.00
2.00
3.00
2.00
7.00
1.00
1.00
2.00
1.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

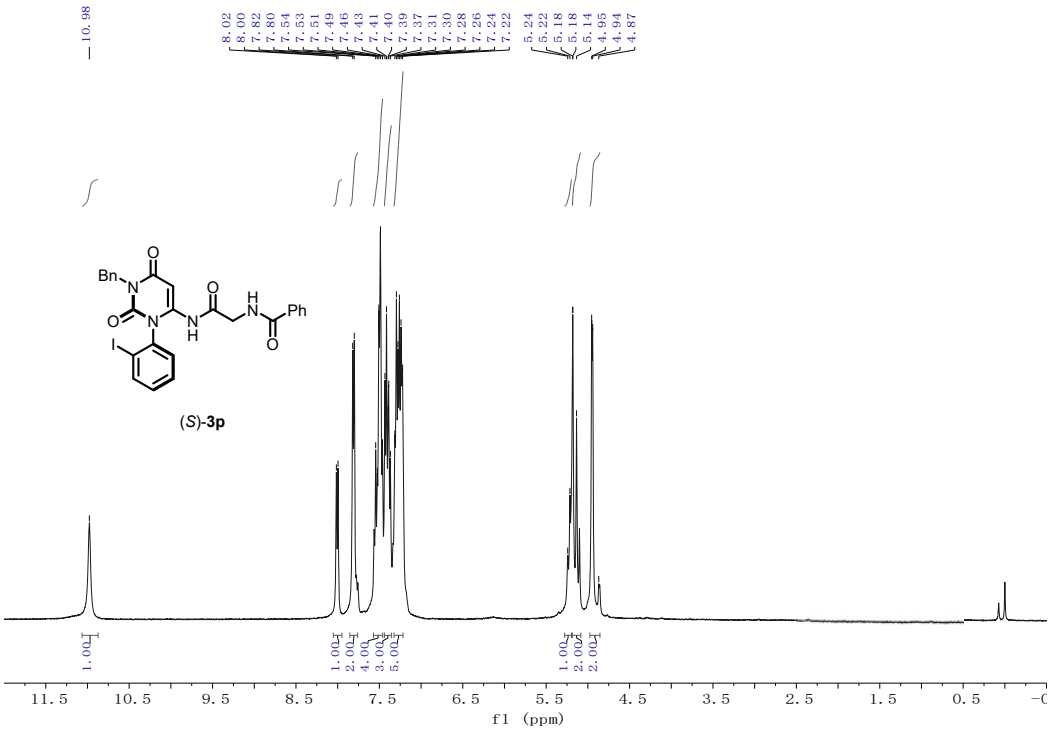
(*S*)-**3o**


194.64
167.21
161.12
158.69
150.00
148.59
134.66
134.28
133.26
132.90
131.38
131.16
131.08
130.95
129.24
128.62
128.52
128.07
127.59
127.27
127.11
125.99
125.92
90.22
50.57
44.52
36.29
31.44
O
N
O
N
H
O
N
H
Ph
O
tBu
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

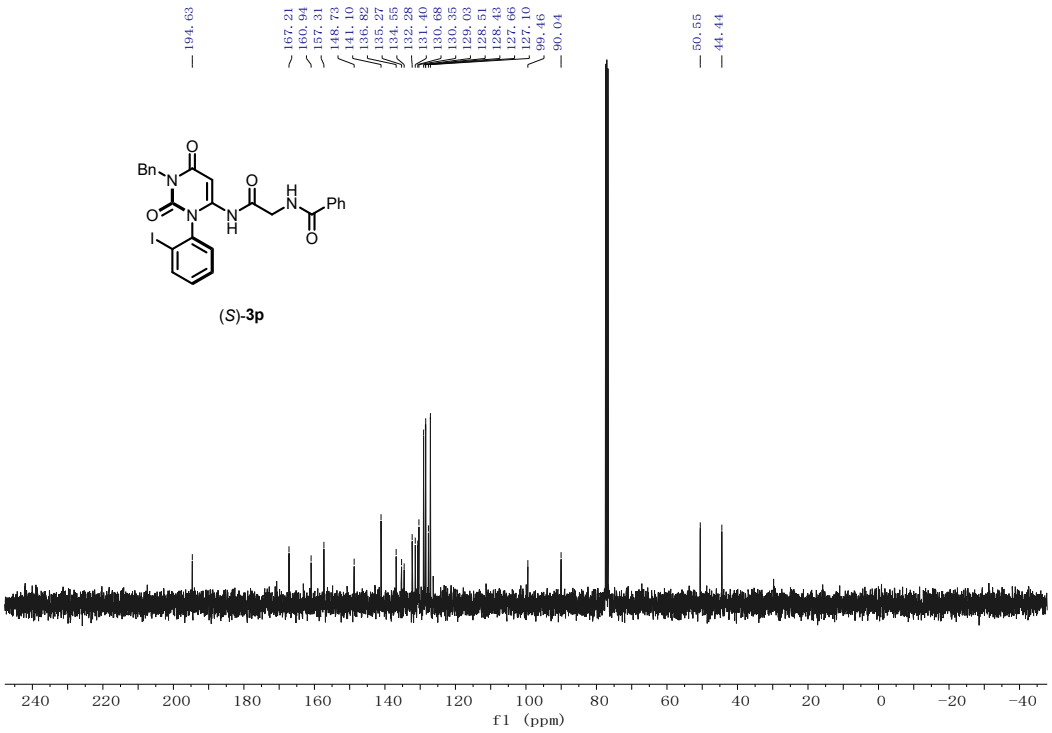
(*S*)-**3o**


7.87
7.87
7.76
7.76
7.75
7.74
7.73
7.73
7.72
7.71
7.69
7.59
7.59
7.58
7.57
7.57
7.55
7.55
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.28
7.28
7.27
7.26
7.25
7.25
7.24
6.97
6.96
6.95
6.95
5.24
5.23
5.15
4.55
1.18
O
N
O
N
NH2
tBu
(R)-1o
1.00
3.00
2.00
3.00
1.00
1.00
2.00
1.00
2.00
9.00
f1 (ppm)

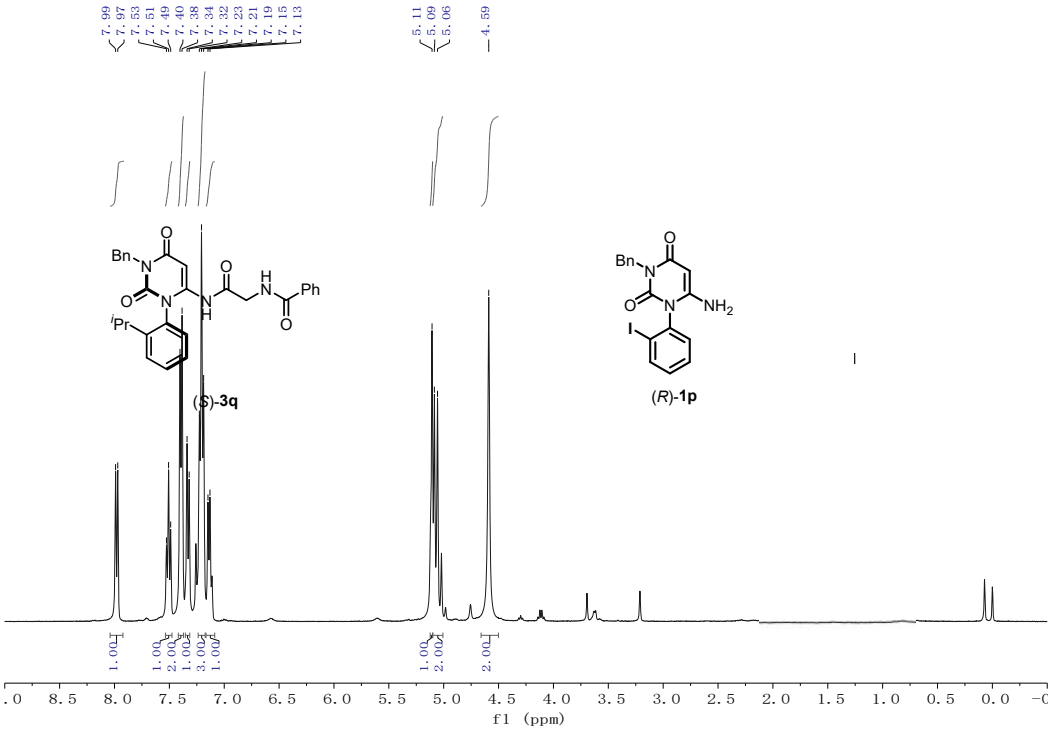

163.22
153.80
151.81
148.62
134.98
133.26
132.72
131.20
130.76
130.43
127.98
127.92
127.79
127.76
127.54
127.04
125.83
125.64
77.55
44.20
36.20
31.42
O
N
O
N
NH2
tBu
(R)-1o
f1 (ppm)

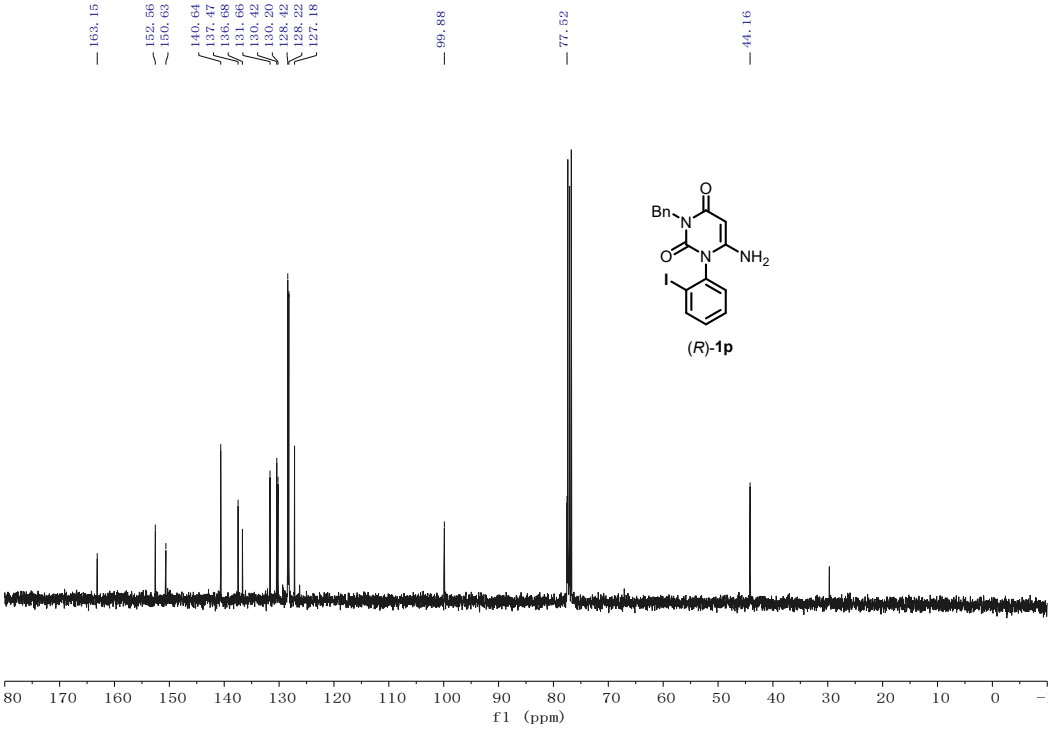

10.98
8.02
8.00
7.82
7.80
7.54
7.53
7.51
7.49
7.46
7.43
7.41
7.40
7.39
7.37
7.31
7.30
7.28
7.26
7.24
7.22
5.24
5.22
5.18
5.18
5.14
4.95
4.94
4.87
Bn
O
N
O
N
H
N
O
H
N
Ph
O
I
1.00
1.00
2.00
4.00
3.00
5.00
1.00
2.00
2.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

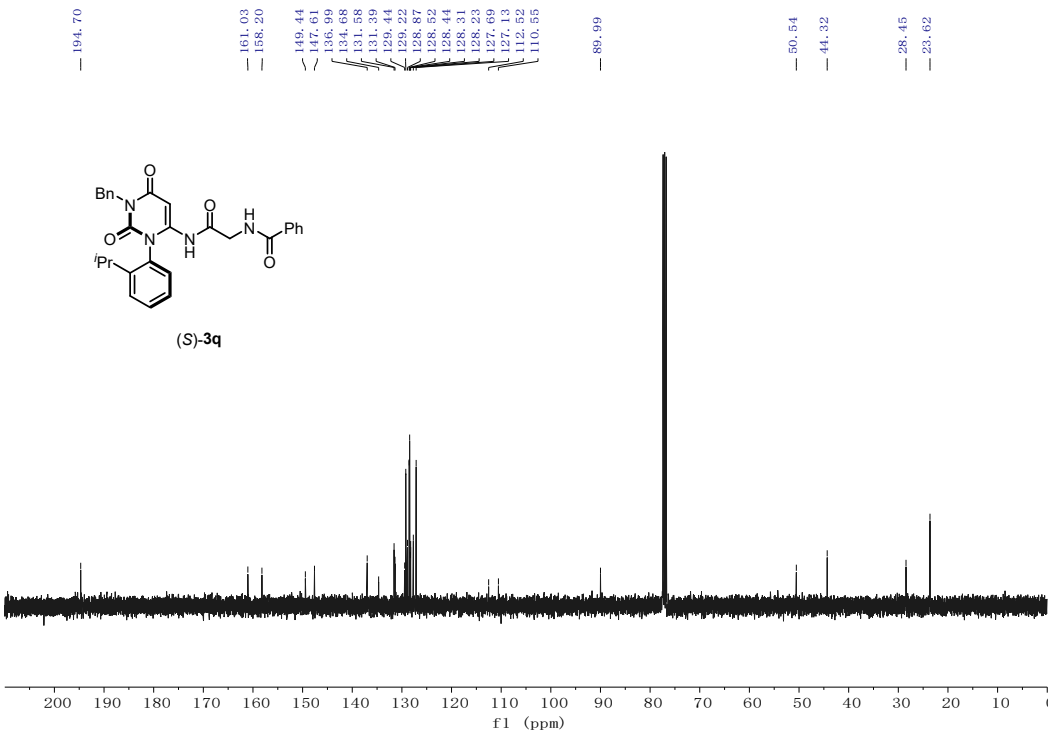
(*S*)-**3p**

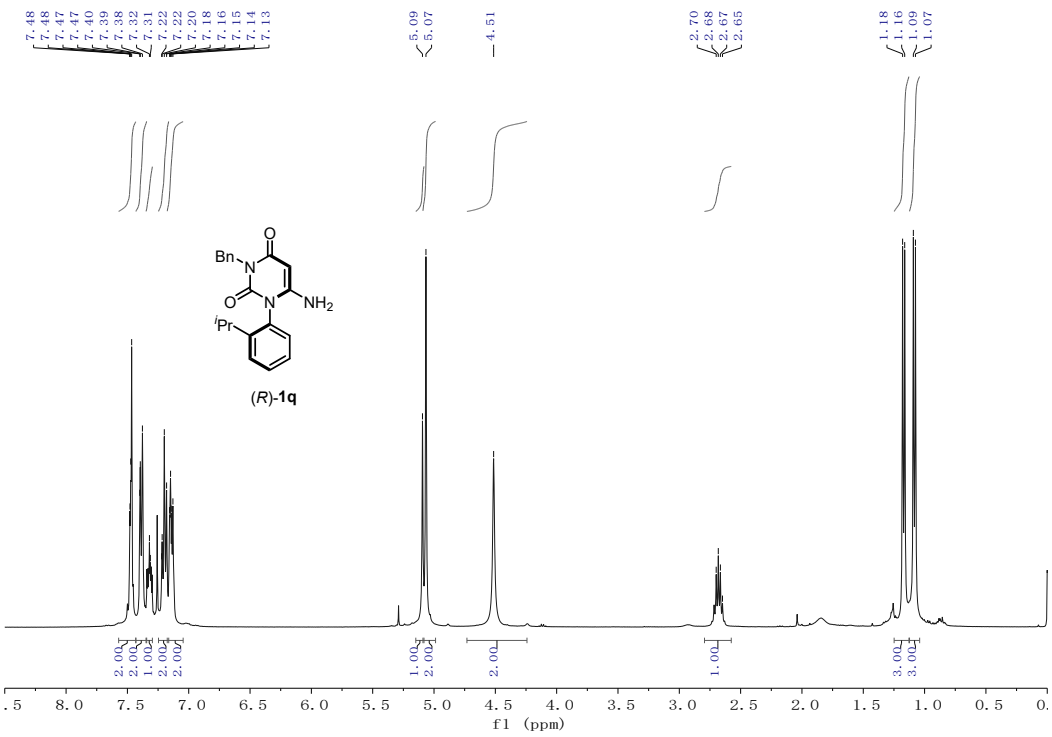

194.63
167.21
160.94
157.31
148.73
141.10
136.82
135.27
134.55
132.28
131.40
130.68
130.35
129.03
128.51
128.43
127.66
127.10
99.46
90.04
50.55
44.44
Bn
O
N
O
N
H
N
O
H
N
Ph
O
I
240
220
200
180
160
140
120
100
80
60
40
20
0
−20
−40
f1 (ppm)

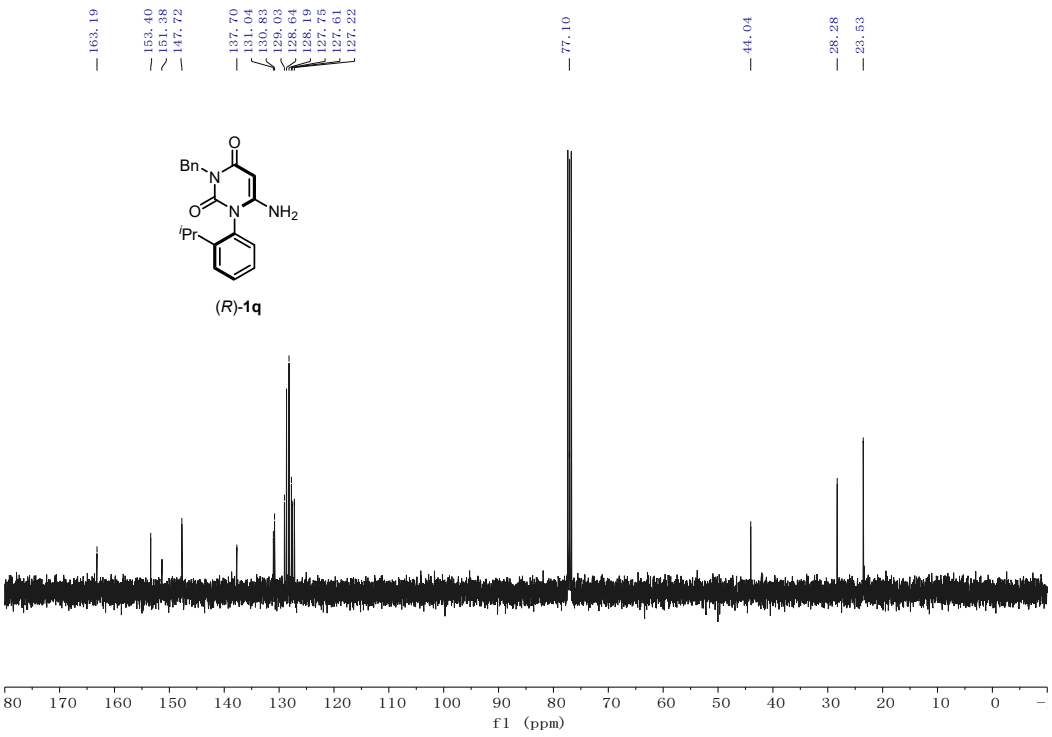
(*S*)-**3p**

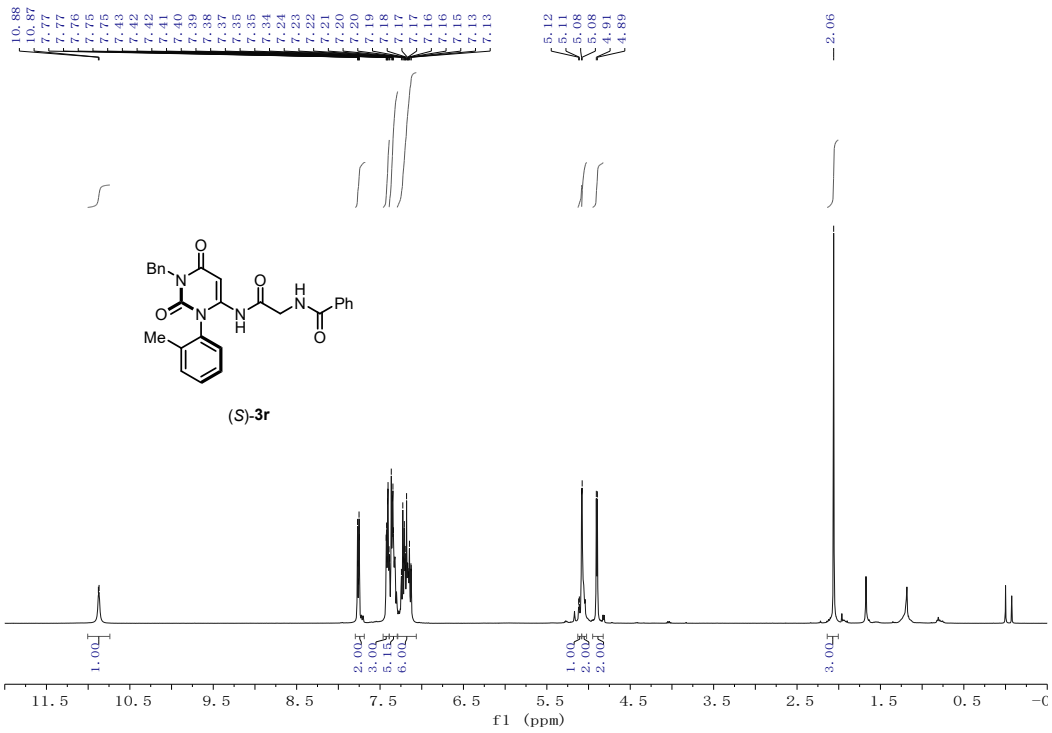

7.99
7.97
7.53
7.51
7.49
7.40
7.38
7.34
7.32
7.23
7.21
7.19
7.15
7.13
5.11
5.09
5.06
4.59
Bn
N
O
O
N
H
O
N
H
Ph
O
iPr
(S)-3q
Bn
N
O
O
N
NH2
I
(R)-1p
1.00
1.00
2.00
1.00
3.00
1.00
1.00
2.00
2.00
f1 (ppm)

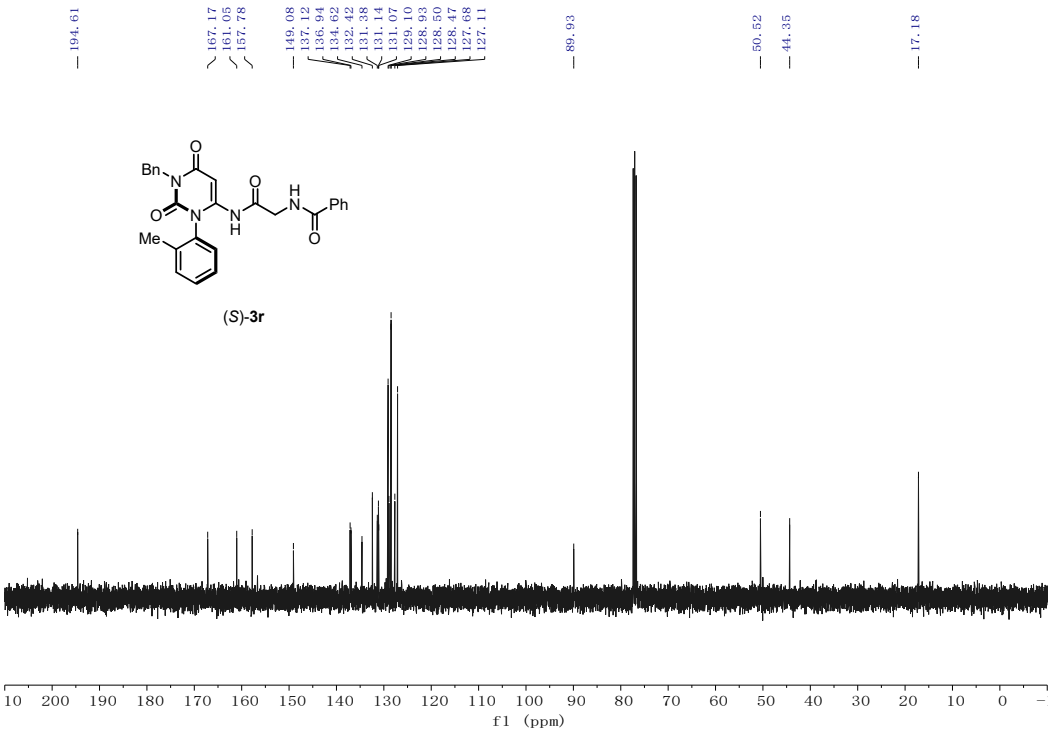

163.15
152.56
150.63
140.64
137.47
136.68
131.66
130.42
130.20
128.42
128.22
127.18
99.88
77.52
44.16
Bn
N
O
O
N
NH2
I
(R)-1p
f1 (ppm)

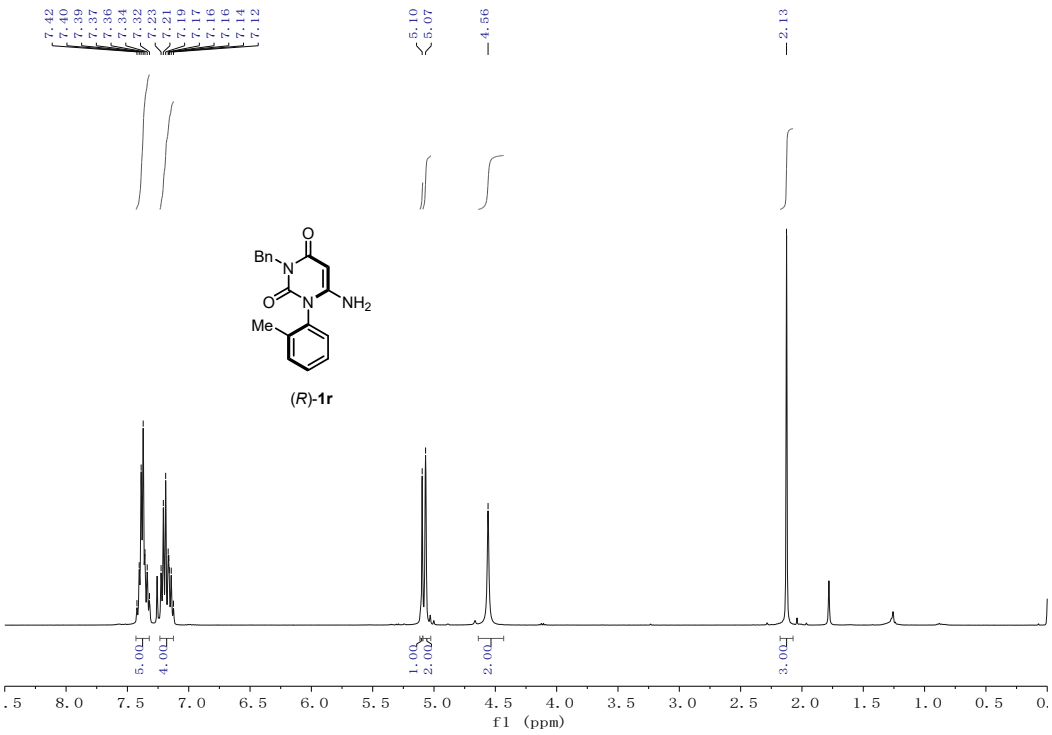

194.70
161.03
158.20
149.44
147.61
136.99
134.68
131.58
131.39
129.44
129.22
128.87
128.52
128.44
128.31
128.23
127.69
127.13
112.52
110.55
89.99
50.54
44.32
28.45
23.62
Bn
O
N
O
N
H
N
H
O
N
H
Ph
O
iPr
(S)-3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

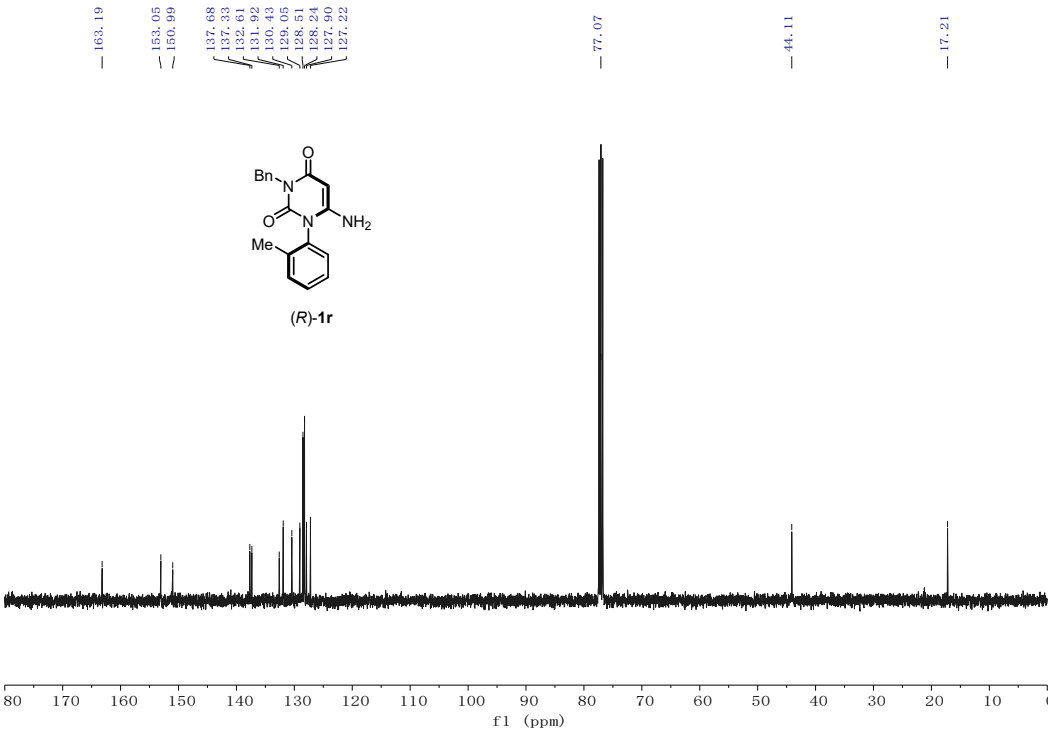

7.48
7.48
7.47
7.47
7.40
7.39
7.38
7.32
7.31
7.22
7.22
7.20
7.18
7.16
7.15
7.14
7.13
5.09
5.07
4.51
2.70
2.68
2.67
2.65
1.18
1.16
1.09
1.07
Bn
O
N
O
N
NH2
iPr
(R)-1q
2.00
2.00
1.03
2.00
2.00
1.00
2.00
2.00
1.00
3.00
3.00
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

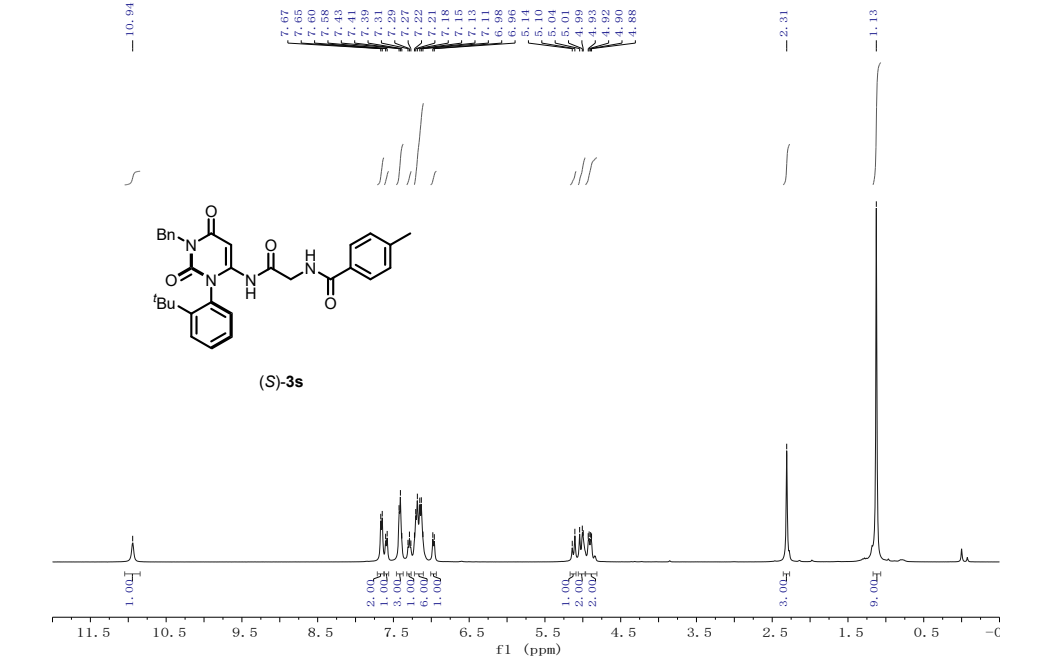

163.19
153.40
151.38
147.72
137.70
131.04
130.83
129.03
128.64
128.19
127.75
127.61
127.22
77.10
44.04
28.28
23.53
Bn
N
O
O
N
NH2
iPr
(R)-1q
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

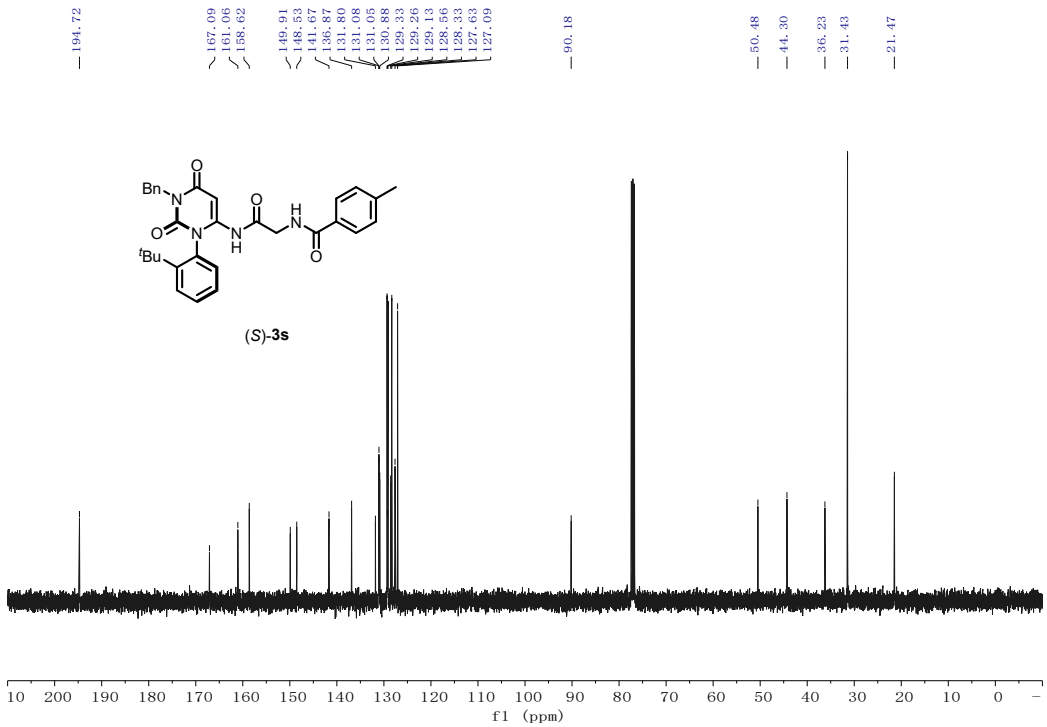

10.88
10.87
7.77
7.77
7.76
7.75
7.75
7.43
7.42
7.42
7.41
7.40
7.39
7.38
7.37
7.35
7.35
7.34
7.24
7.23
7.22
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.16
7.16
7.15
7.13
5.12
5.11
5.08
5.08
4.91
4.89
2.06
Bn
N
O
O
N
H
N
O
H
N
Ph
O
Me
(S)-3r
1.00
2.01
3.00
5.15
6.04
1.00
2.00
2.02
3.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

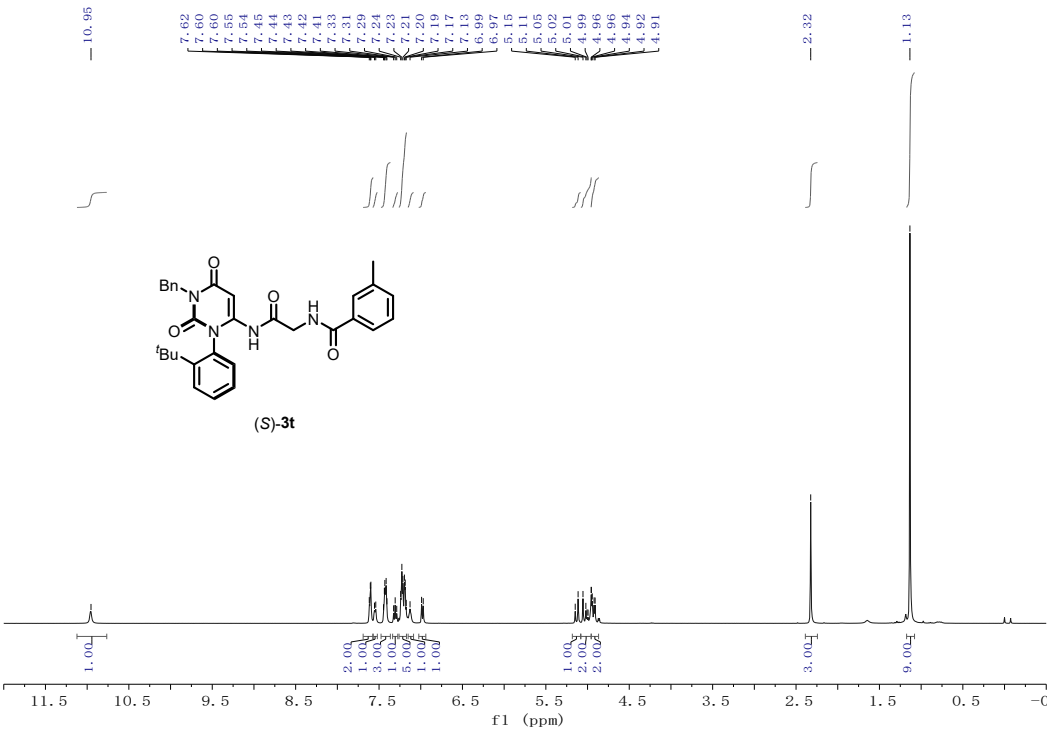

194.61
167.17
161.05
157.78
149.08
137.12
136.94
134.62
132.42
131.38
131.14
131.07
129.10
128.93
128.50
128.47
127.68
127.11
89.93
50.52
44.35
17.18
Bn
O
N
O
N
H
N
O
Me
O
H
N
Ph
O
(S)-3r
f1 (ppm)

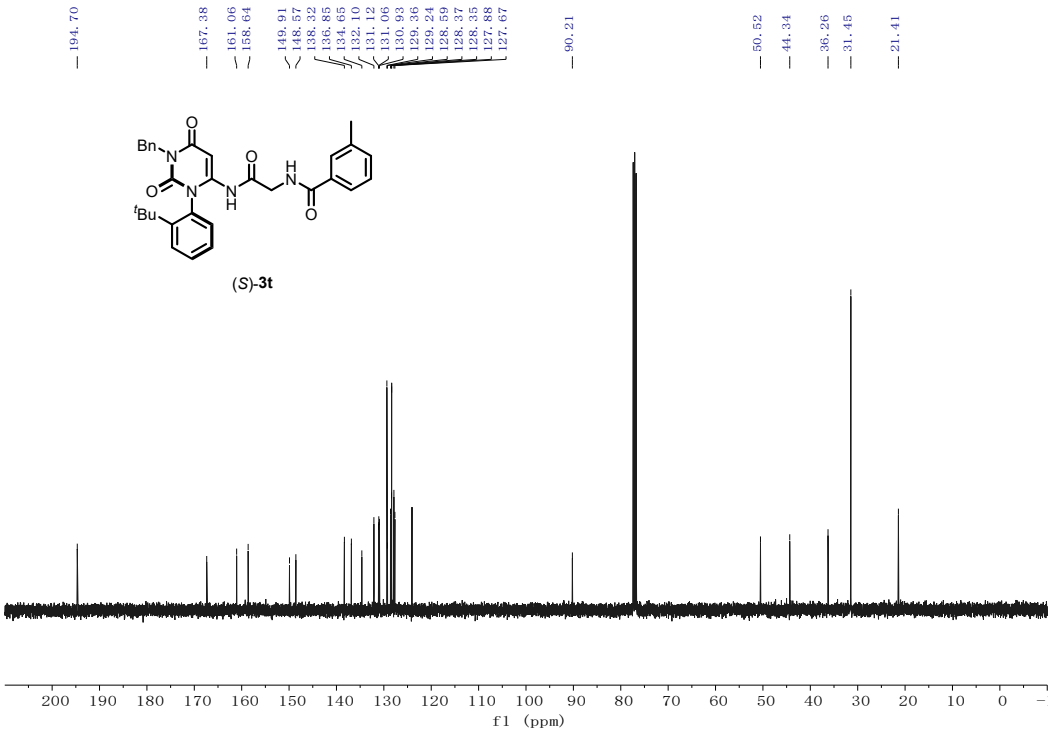

7.42
7.40
7.39
7.37
7.36
7.34
7.32
7.23
7.21
7.19
7.17
7.16
7.16
7.14
7.12
5.10
5.07
4.56
2.13
Bn
O
N
O
N
NH2
Me
(R)-1r
5.00
4.00
1.00
2.00
2.00
3.00
f1 (ppm)

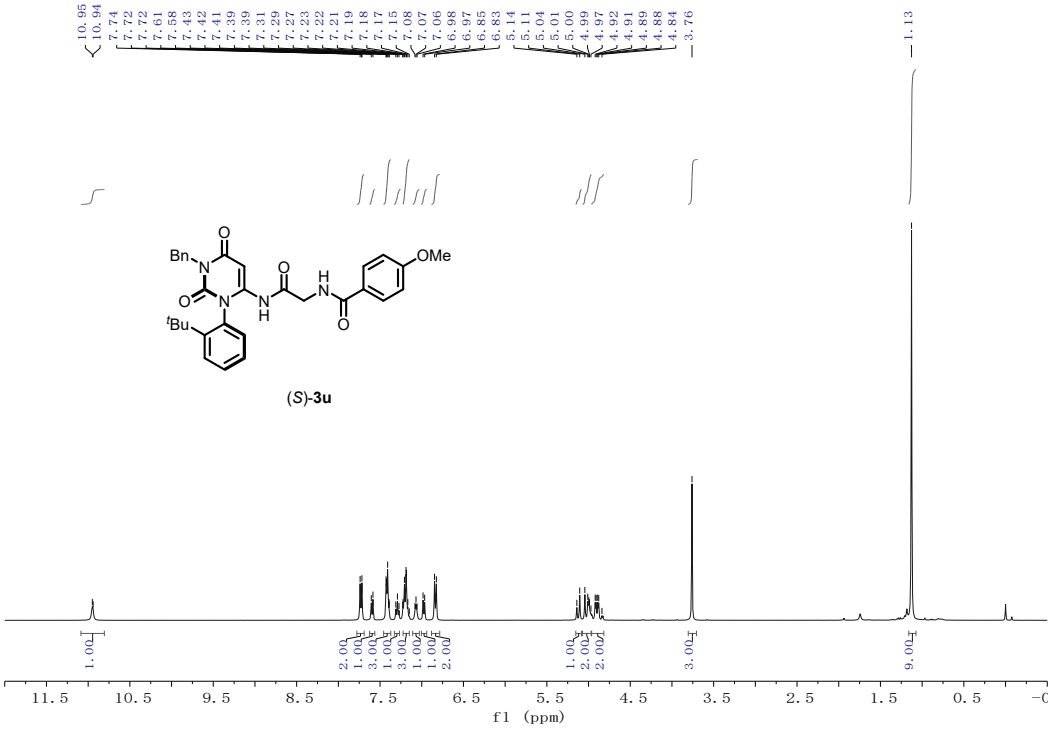

163.19
153.05
150.99
137.68
137.33
132.61
131.92
130.43
129.05
128.51
128.24
127.90
127.22
77.07
44.11
17.21
Bn
O
N
O
N
NH2
Me
(R)-1r
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

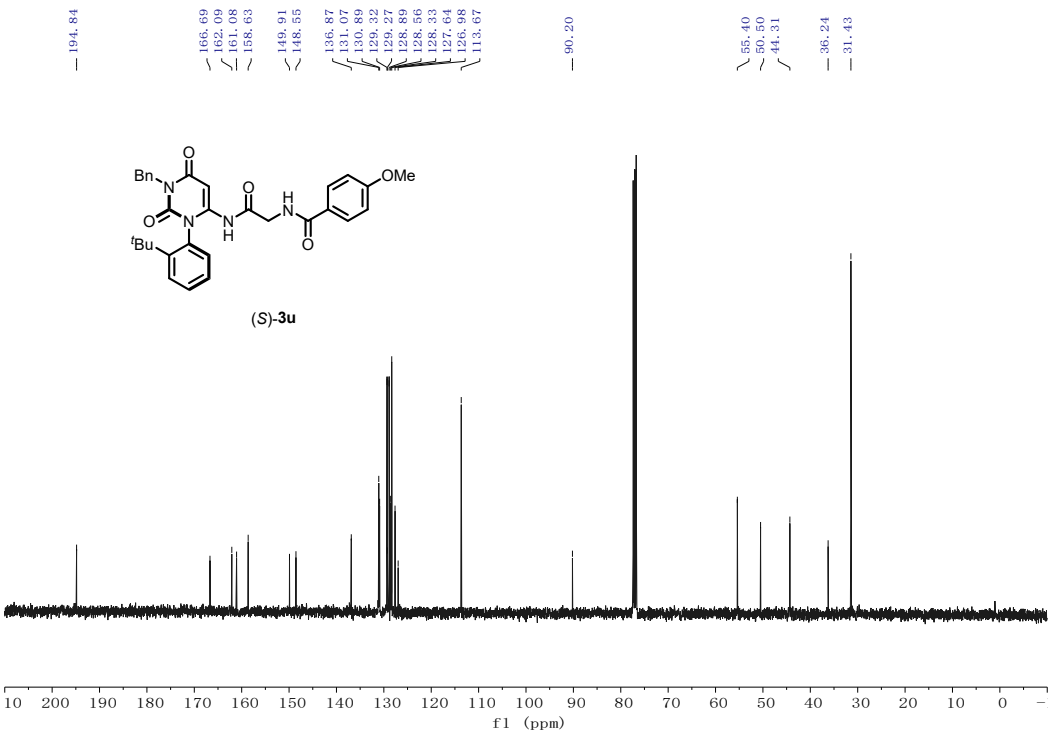

10.94
7.67
7.65
7.60
7.58
7.43
7.41
7.39
7.31
7.29
7.27
7.22
7.21
7.18
7.15
7.13
7.11
6.98
6.96
5.14
5.10
5.04
5.01
4.99
4.93
4.92
4.90
4.88
2.31
1.13
Bn
O
N
O
N
H
N
O
H
N
O
tBu
(S)-3s
1.00
2.00
1.00
3.00
1.00
6.00
1.00
1.00
2.00
2.00
3.00
9.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

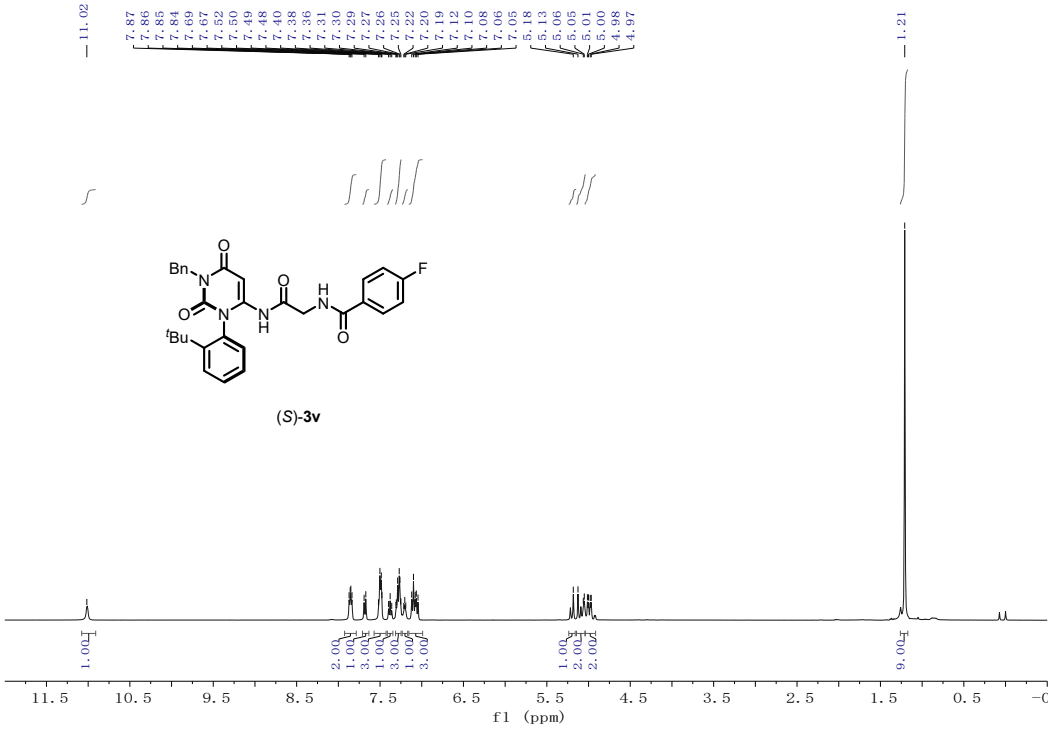

194.72
167.09
161.06
158.62
149.91
148.53
141.67
136.87
131.80
131.08
131.05
130.88
129.33
129.26
129.13
128.56
128.33
127.63
127.09
90.18
50.48
44.30
36.23
31.43
21.47
Bn
tBu
(S)-3s
f1 (ppm)

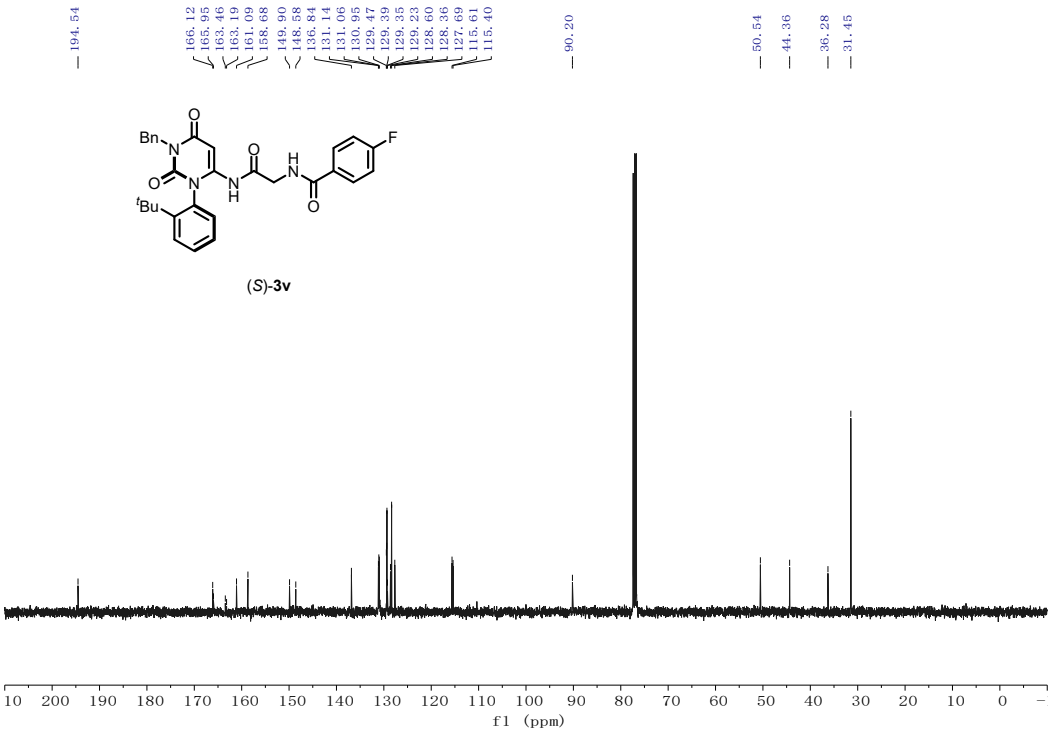

10.96
7.62
7.60
7.60
7.55
7.54
7.45
7.44
7.43
7.42
7.41
7.33
7.31
7.29
7.24
7.23
7.21
7.20
7.19
7.17
7.13
6.99
6.97
5.15
5.11
5.05
5.02
5.01
4.99
4.96
4.96
4.94
4.92
4.91
2.32
1.13
Bn
tBu
(S)-3t
1.00
2.00
1.00
3.00
1.00
5.00
1.00
1.00
1.00
2.00
2.00
3.00
9.00
f1 (ppm)


194.70
167.38
161.06
158.64
149.91
148.57
138.32
136.85
134.65
132.10
131.12
131.06
130.93
129.36
129.24
128.59
128.37
128.35
127.88
127.67
90.21
50.52
44.34
36.26
31.45
21.41
Bn
tBu
(S)-3t
f1 (ppm)

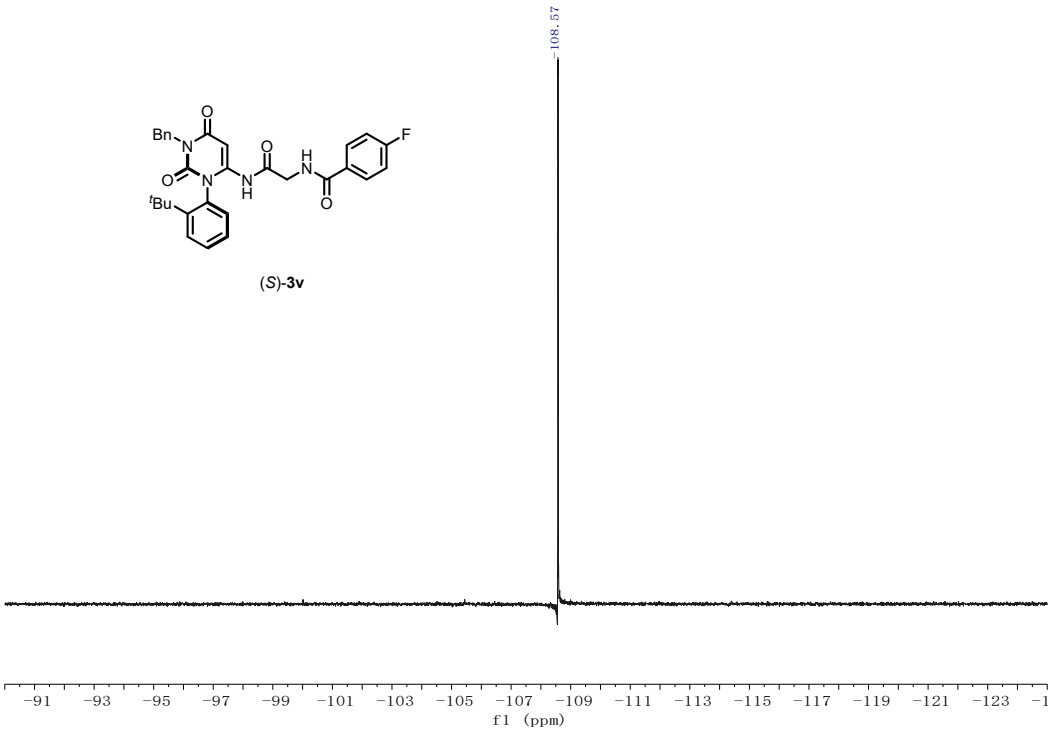

10.95
10.94
7.74
7.72
7.72
7.61
7.58
7.43
7.42
7.41
7.39
7.39
7.31
7.29
7.27
7.23
7.22
7.21
7.19
7.18
7.17
7.15
7.08
7.07
7.06
6.98
6.97
6.85
6.83
5.14
5.11
5.04
5.01
5.00
4.99
4.97
4.92
4.91
4.89
4.88
4.84
3.76
1.13
Bn
OMe
tBu
(S)-3u
1.00
2.00
1.00
3.00
1.00
3.00
1.00
1.00
2.00
1.00
2.00
2.00
3.00
9.00
f1 (ppm)


194.84
166.69
162.09
161.08
158.63
149.91
148.55
136.87
131.07
130.89
129.32
129.27
128.89
128.56
128.33
127.64
126.98
113.67
90.20
55.40
50.50
44.31
36.24
31.43
Bn
OMe
tBu
(S)-3u
f1 (ppm)

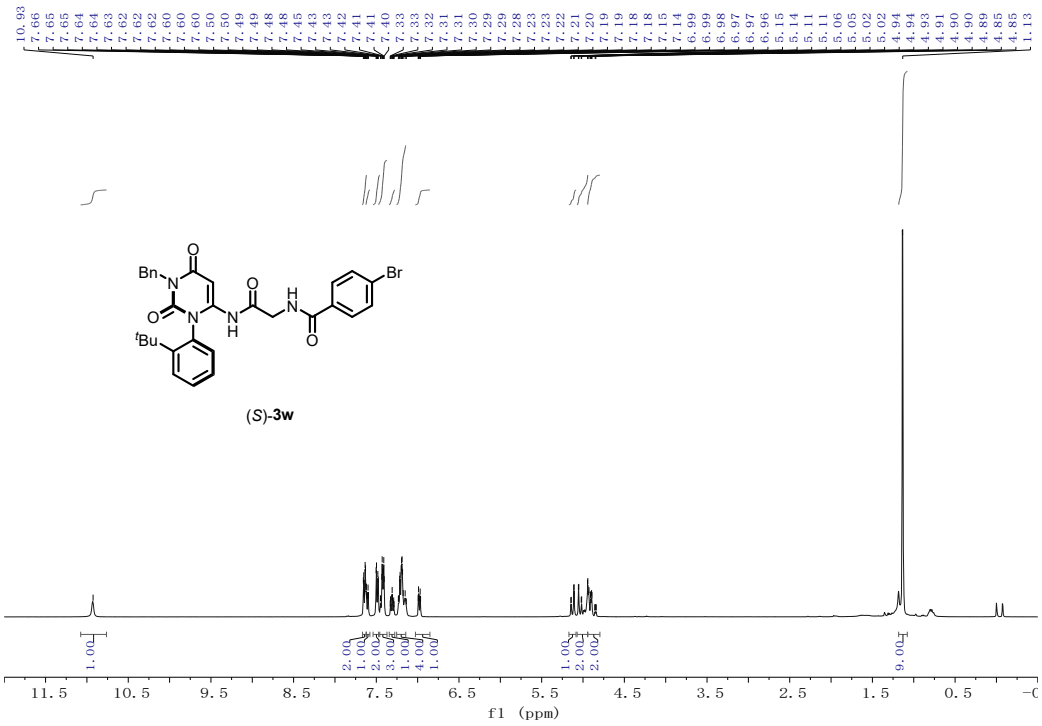

11.02
7.87
7.86
7.85
7.84
7.69
7.67
7.52
7.50
7.49
7.48
7.40
7.38
7.36
7.31
7.30
7.29
7.27
7.26
7.25
7.22
7.20
7.19
7.12
7.10
7.08
7.06
7.05
5.18
5.13
5.06
5.05
5.01
5.00
4.98
4.97
1.21
Bn
F
tBu
(S)-3v
1.00
2.00
1.00
3.00
1.00
3.00
1.00
3.00
1.00
2.00
2.00
9.00
f1 (ppm)

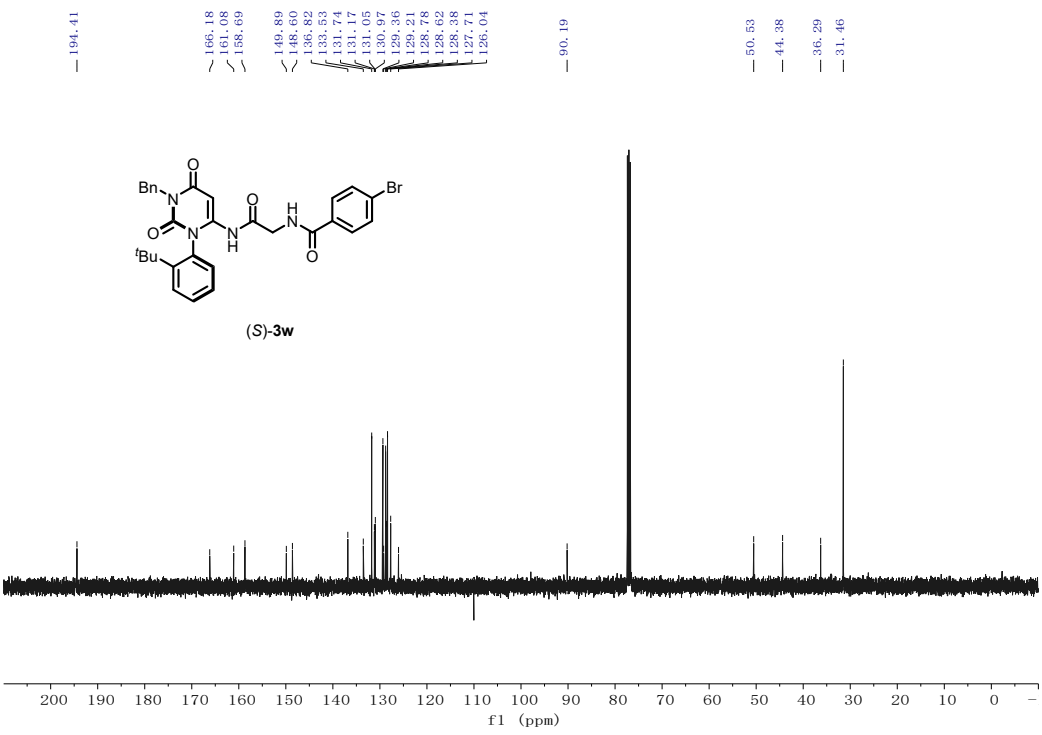

194.54
166.12
165.95
163.46
163.19
161.09
158.68
149.90
148.58
136.84
131.14
131.06
130.95
129.47
129.39
129.35
129.23
128.60
128.36
127.69
115.61
115.40
90.20
50.54
44.36
36.28
31.45
Bn
tBu
F
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

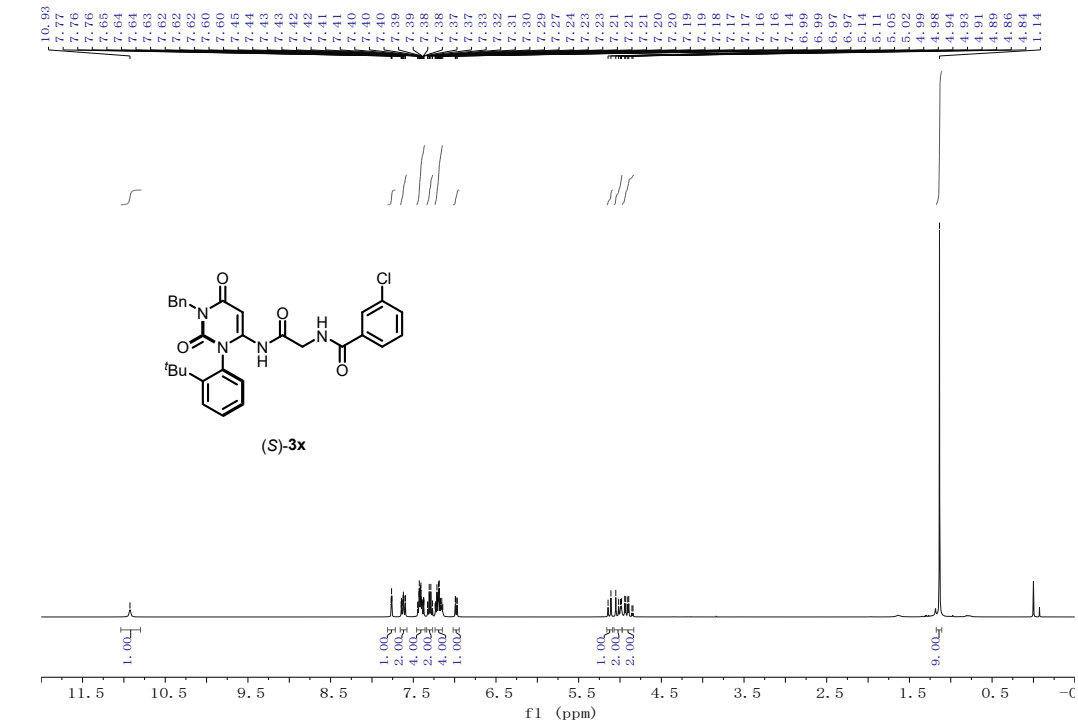
(*S*)-**3v**

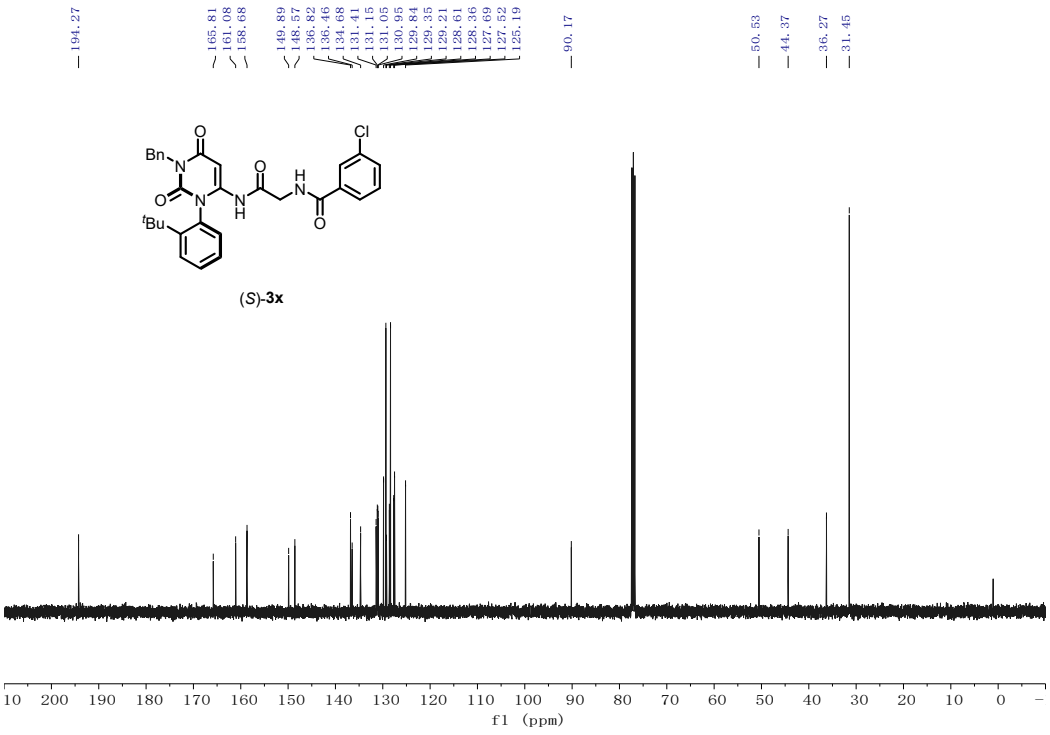

-108.57
Bn
tBu
F
−91 −93 −95 −97 −99 −101 −103 −105 −107 −109 −111 −113 −115 −117 −119 −121 −123
f1 (ppm)

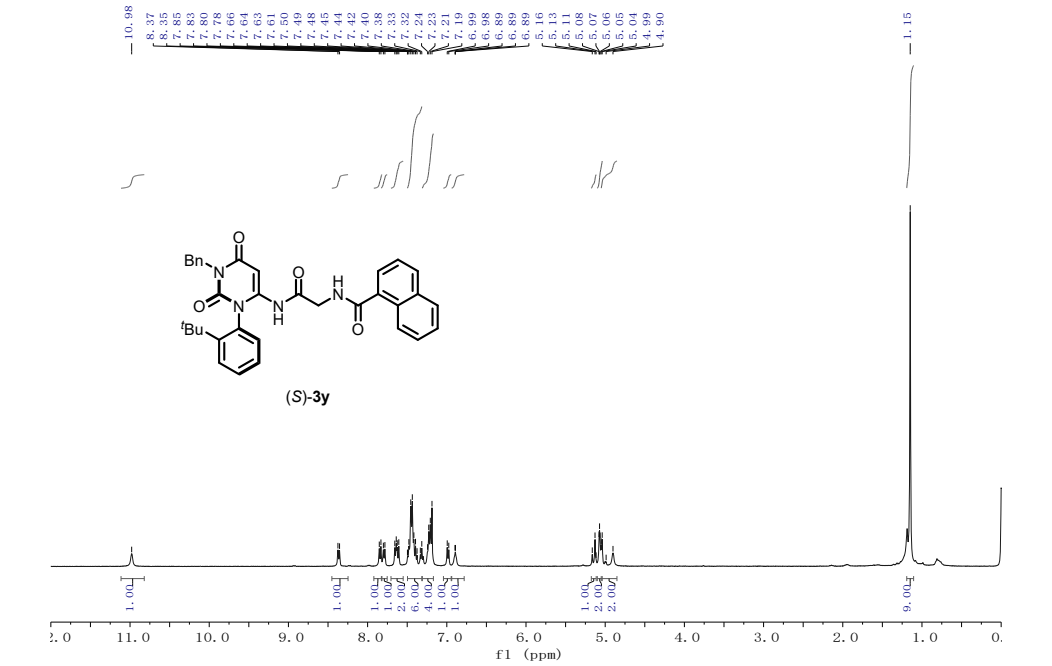
(*S*)-**3v**

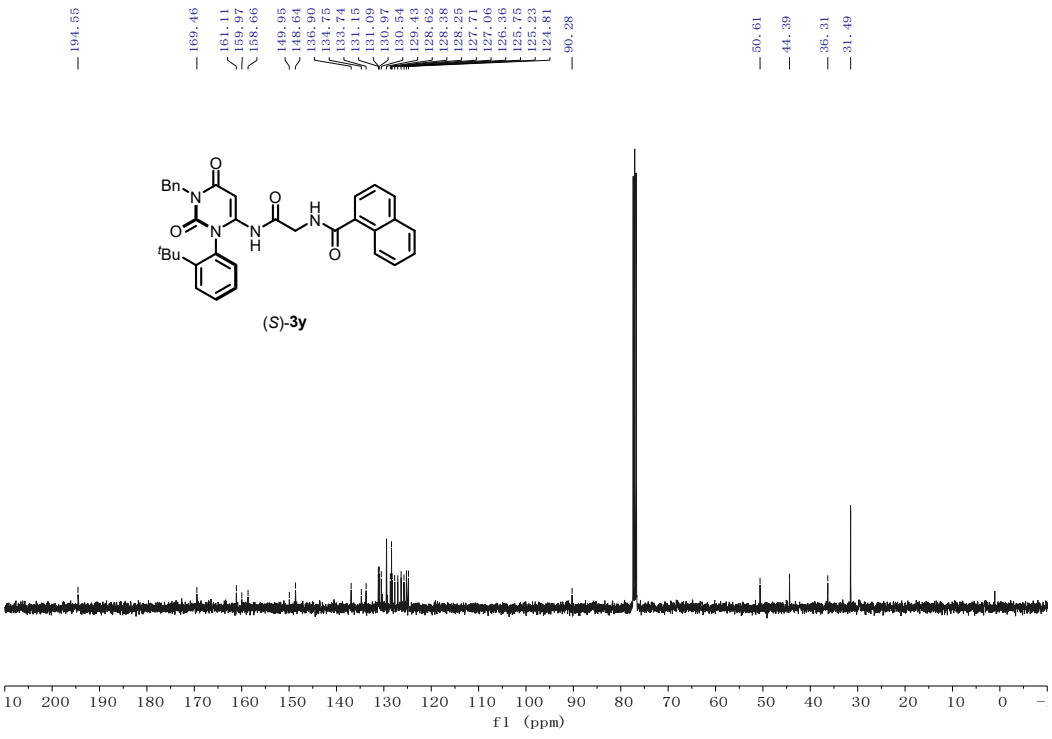

10.93
7.66 7.65 7.65 7.64 7.64 7.63 7.62 7.62 7.62 7.60 7.60 7.60 7.50 7.50 7.49 7.49 7.48 7.48 7.45 7.43 7.43 7.42 7.41 7.41 7.40 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.23 7.23 7.22 7.21 7.20 7.19 7.19 7.18 7.18 7.15 7.14 6.99 6.99 6.98 6.97 6.97 6.96 5.15 5.14 5.11 5.11 5.06 5.05 5.02 5.02 4.94 4.94 4.93 4.91 4.90 4.90 4.89 4.85 4.85 1.13
Bn
Br
tBu
(S)-3w
1.00 2.00 1.00 2.00 3.00 1.00 4.00 1.00 1.00 2.00 2.00 9.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

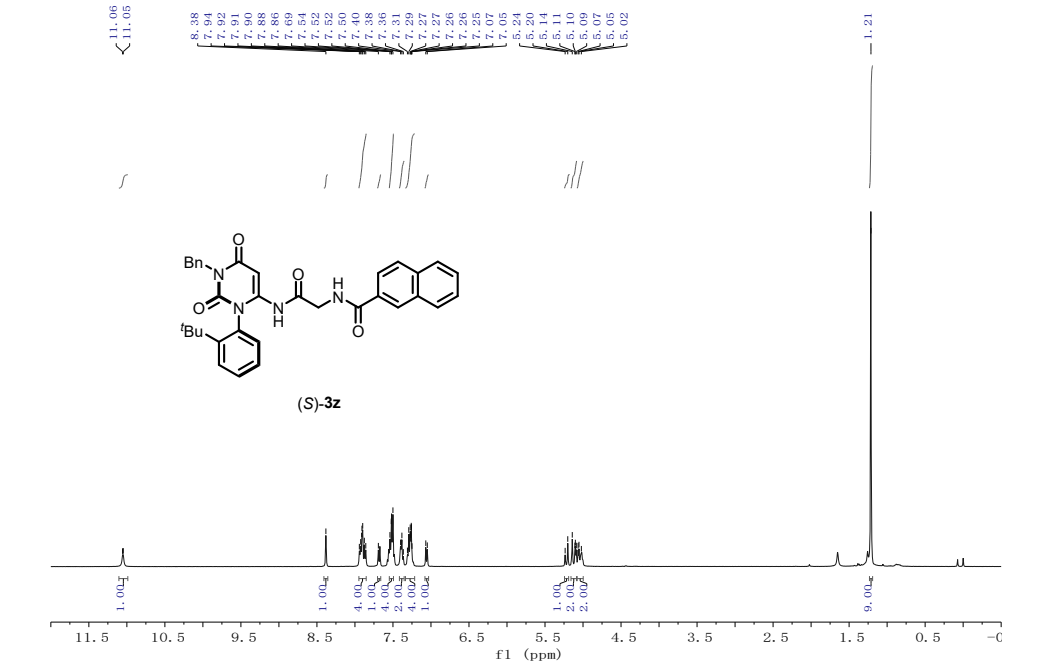

194.41
166.18 161.08 158.69 149.89 148.60 136.82 133.53 131.74 131.17 131.05 130.97 129.36 129.21 128.78 128.62 128.38 127.71 126.04
90.19
50.53 44.38 36.29 31.46
Bn
Br
tBu
(S)-3w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

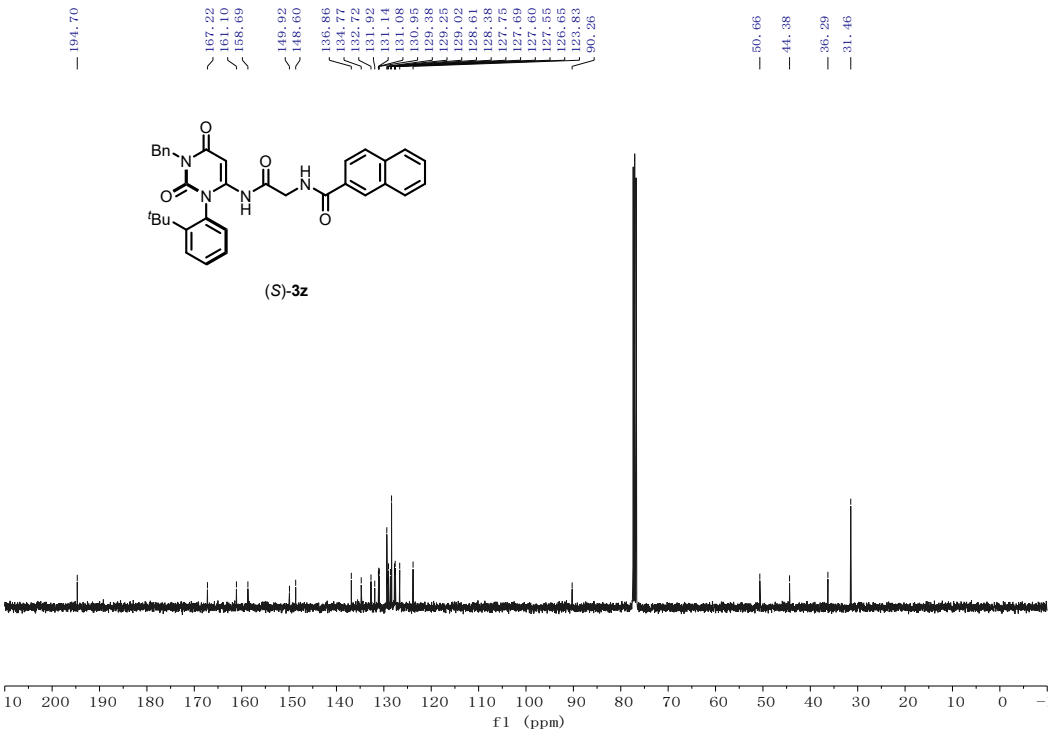

10.93
7.77
7.76
7.76
7.65
7.64
7.63
7.62
7.62
7.60
7.45
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.33
7.32
7.31
7.30
7.29
7.27
7.24
7.23
7.23
7.21
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.17
7.16
7.16
7.14
6.99
6.99
6.97
6.97
5.14
5.11
5.05
5.02
4.99
4.98
4.94
4.93
4.91
4.89
4.86
4.84
1.14
Bn
N
O
O
N
H
N
O
H
N
O
Cl
tBu
(S)-3x
1.00
1.00
2.00
4.00
2.00
4.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

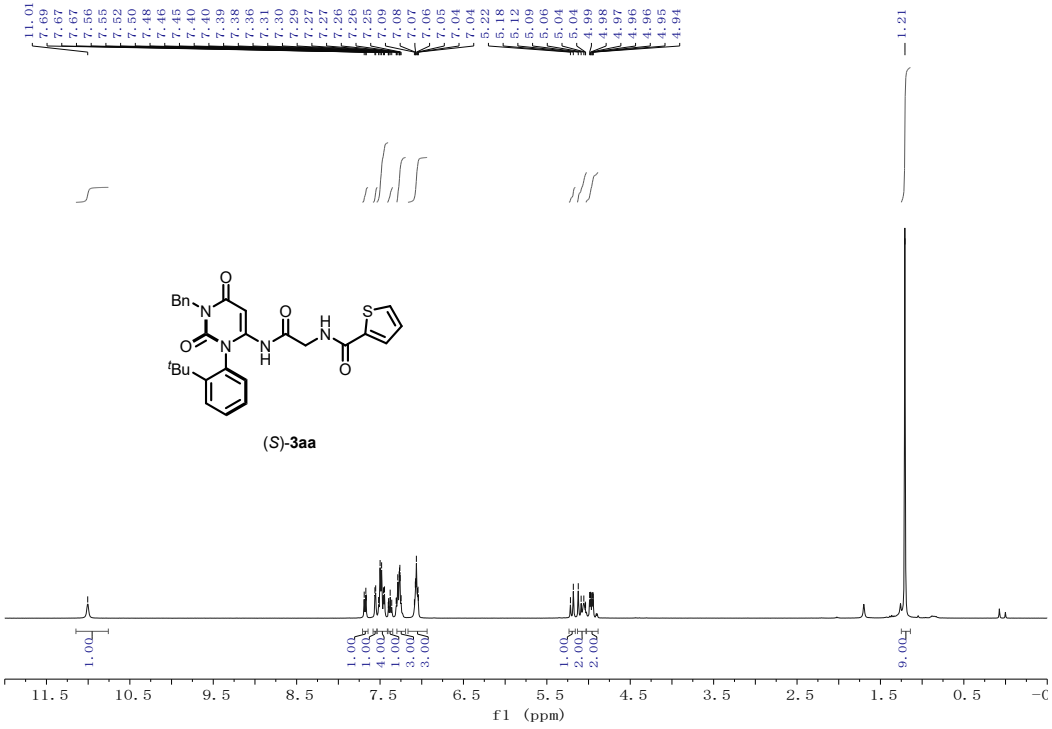

194.27
165.81
161.08
158.68
149.89
148.67
136.82
136.46
134.68
131.41
131.15
131.05
130.95
129.84
129.35
129.21
128.61
128.36
127.69
127.52
125.19
90.17
50.53
44.37
36.27
31.45
Bn
N
O
O
N
H
N
O
H
N
O
Cl
tBu
(S)-3x
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.98
8.37
8.35
7.85
7.83
7.80
7.78
7.66
7.64
7.63
7.61
7.50
7.49
7.48
7.45
7.44
7.42
7.40
7.38
7.33
7.32
7.24
7.23
7.21
7.19
6.99
6.98
6.89
6.89
6.89
5.16
5.13
5.11
5.08
5.07
5.06
5.05
5.04
4.99
4.90
1.15
Bn
tBu
(S)-3y
1.00
1.00
1.00
1.00
2.00
6.00
4.00
1.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

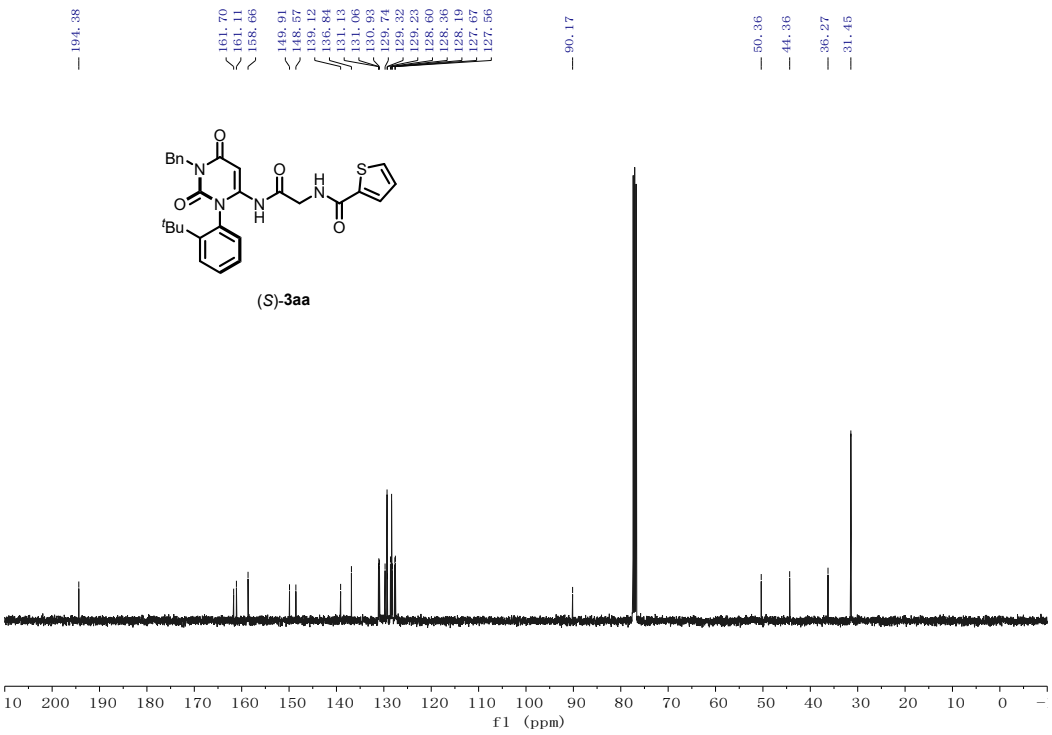

194.55
169.46
161.11
159.97
158.66
149.95
148.64
136.90
134.75
133.74
131.15
131.09
130.97
130.54
129.43
128.62
128.38
128.25
127.71
127.06
126.36
125.75
125.23
124.81
90.28
50.61
44.39
36.31
31.49
Bn
tBu
(S)-3y
f1 (ppm)


11.06
11.05
8.38
7.94
7.92
7.91
7.90
7.88
7.86
7.69
7.54
7.52
7.50
7.40
7.38
7.36
7.31
7.29
7.27
7.27
7.26
7.26
7.25
7.07
7.05
5.24
5.20
5.14
5.11
5.10
5.09
5.07
5.05
5.02
1.21
Bn
tBu
(S)-3z
1.00
1.00
4.00
1.00
4.00
2.00
4.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

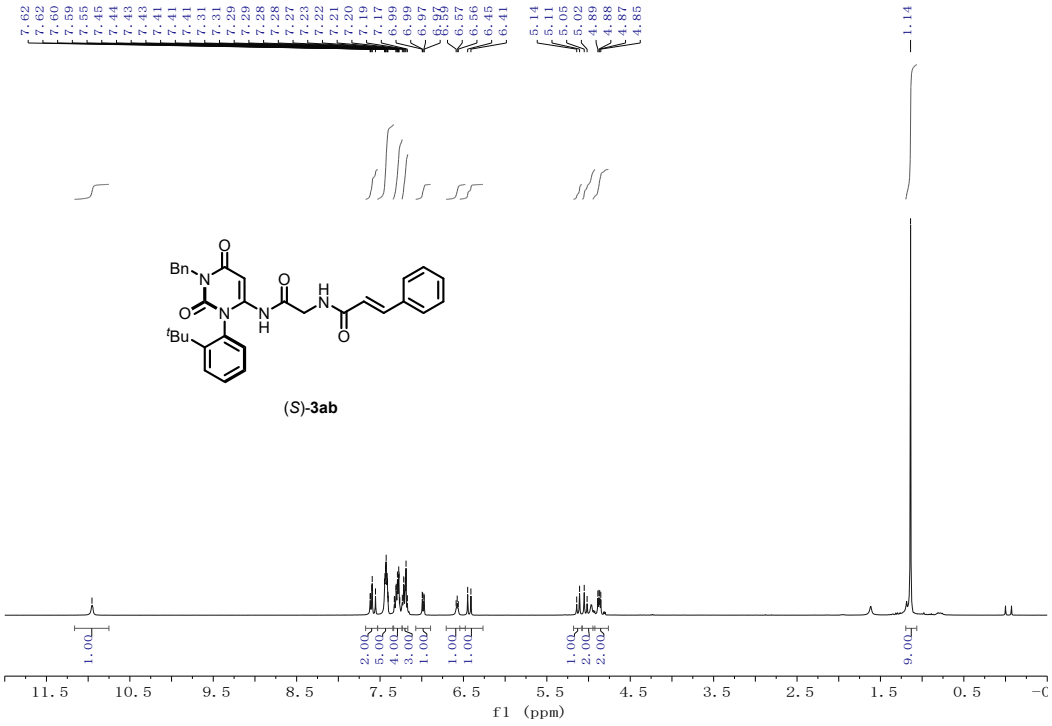

194.70
167.22
161.10
158.69
149.92
148.60
136.86
134.77
132.72
131.92
131.14
131.08
130.95
129.38
129.25
129.02
128.61
128.38
127.75
127.69
127.60
127.55
126.65
123.83
90.26
50.66
44.38
36.29
31.46
Bn
tBu
(S)-3z
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.01
7.69
7.67
7.67
7.56
7.55
7.52
7.50
7.48
7.46
7.45
7.40
7.40
7.39
7.38
7.36
7.31
7.30
7.29
7.27
7.27
7.26
7.26
7.25
7.09
7.08
7.07
7.06
7.05
7.04
7.04
5.22
5.18
5.12
5.09
5.06
5.04
5.04
4.99
4.98
4.97
4.96
4.96
4.95
4.94
1.21
Bn
O
N
O
N
H
N
H
O
S
O
tBu
1.00
1.00
1.00
4.00
1.00
3.00
3.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

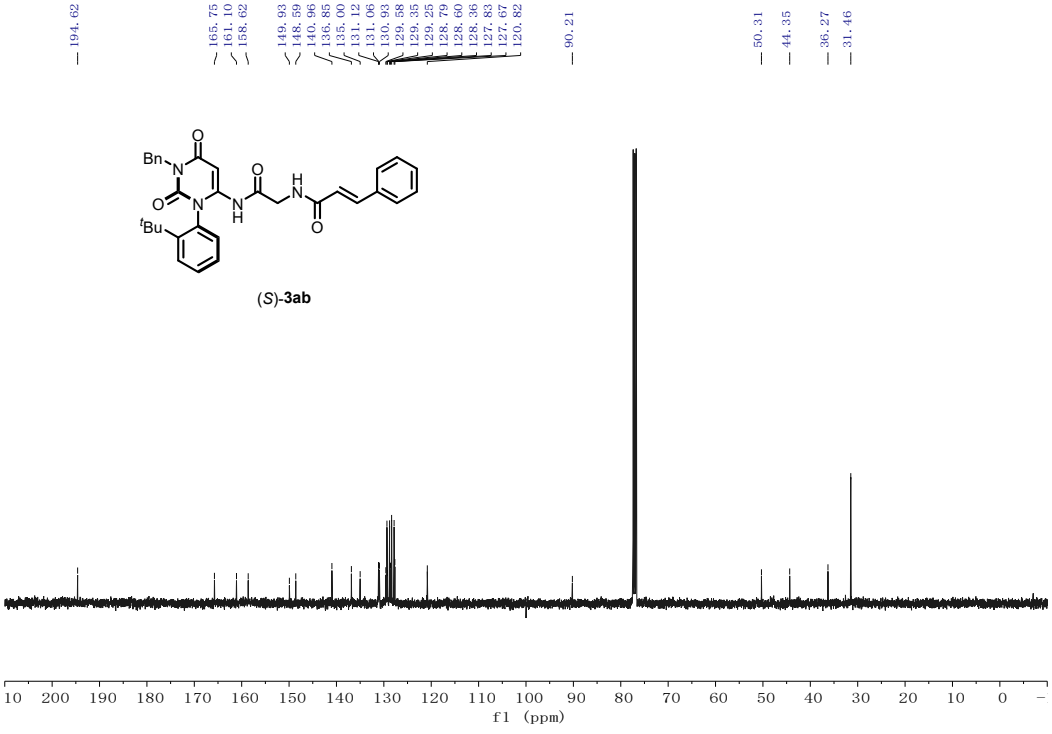
(*S*)-**3aa**


194.38
161.70
161.11
158.66
149.91
148.57
139.12
136.84
131.13
131.06
130.93
129.74
129.32
129.23
128.60
128.36
128.19
127.67
127.56
90.17
50.36
44.36
36.27
31.45
Bn
O
N
O
N
H
N
H
O
S
O
tBu
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

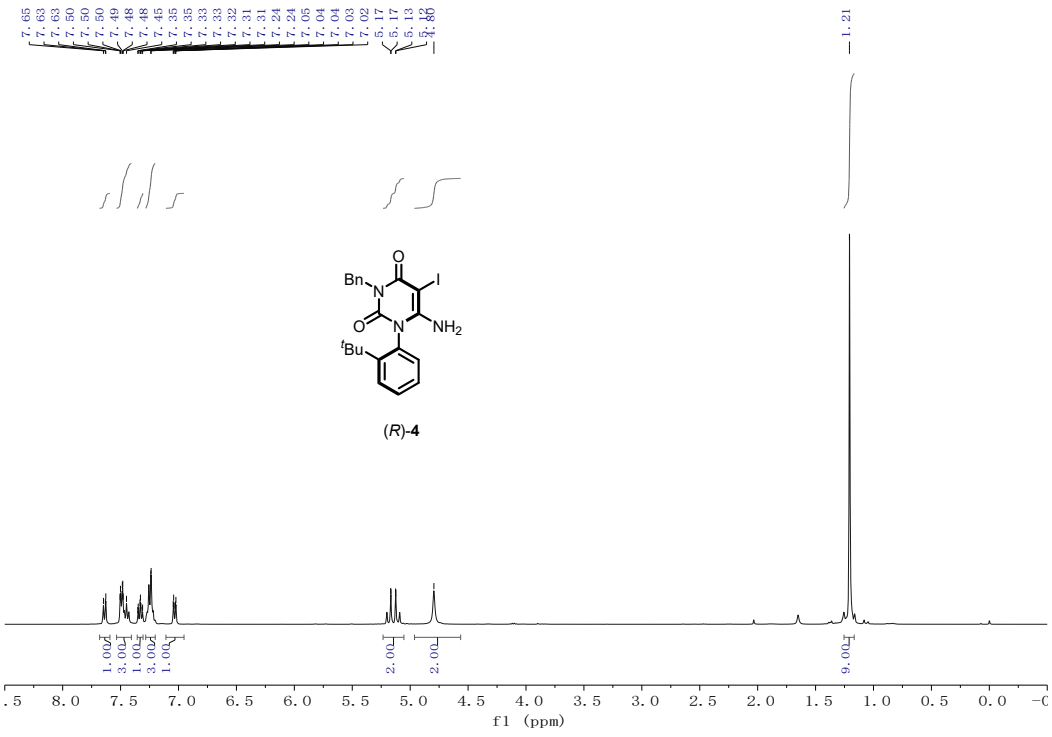
(*S*)-**3aa**


7.62
7.62
7.60
7.59
7.55
7.45
7.44
7.43
7.43
7.41
7.41
7.41
7.31
7.29
7.29
7.28
7.27
7.23
7.22
7.21
7.20
7.19
7.17
6.99
6.99
6.97
6.57
6.56
6.45
6.41
5.14
5.11
5.05
5.02
4.89
4.88
4.87
4.85
1.14
Bn
tBu
1.00
2.00
5.00
4.00
3.00
1.00
1.00
1.00
1.00
2.00
2.00
9.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

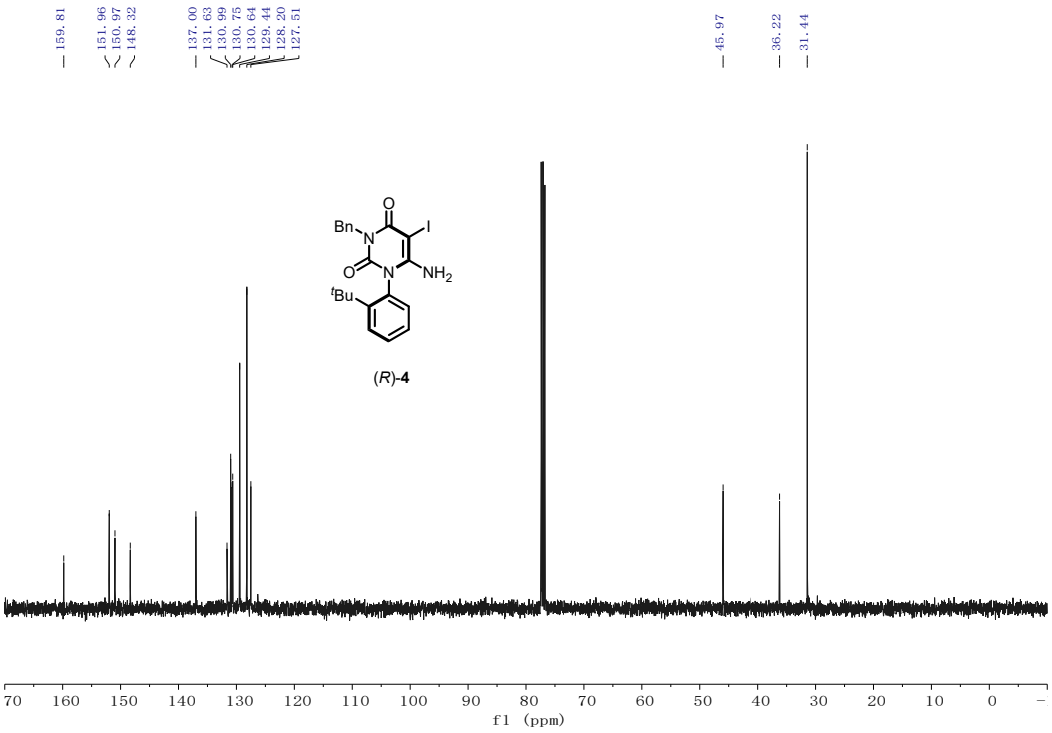
(*S*)-**3ab**


194.62
165.75
161.10
158.62
149.93
148.59
140.96
136.85
135.00
131.12
131.06
130.93
129.58
129.35
129.25
128.79
128.60
128.36
127.83
127.67
120.82
90.21
50.31
44.35
36.27
31.46
Bn
tBu
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

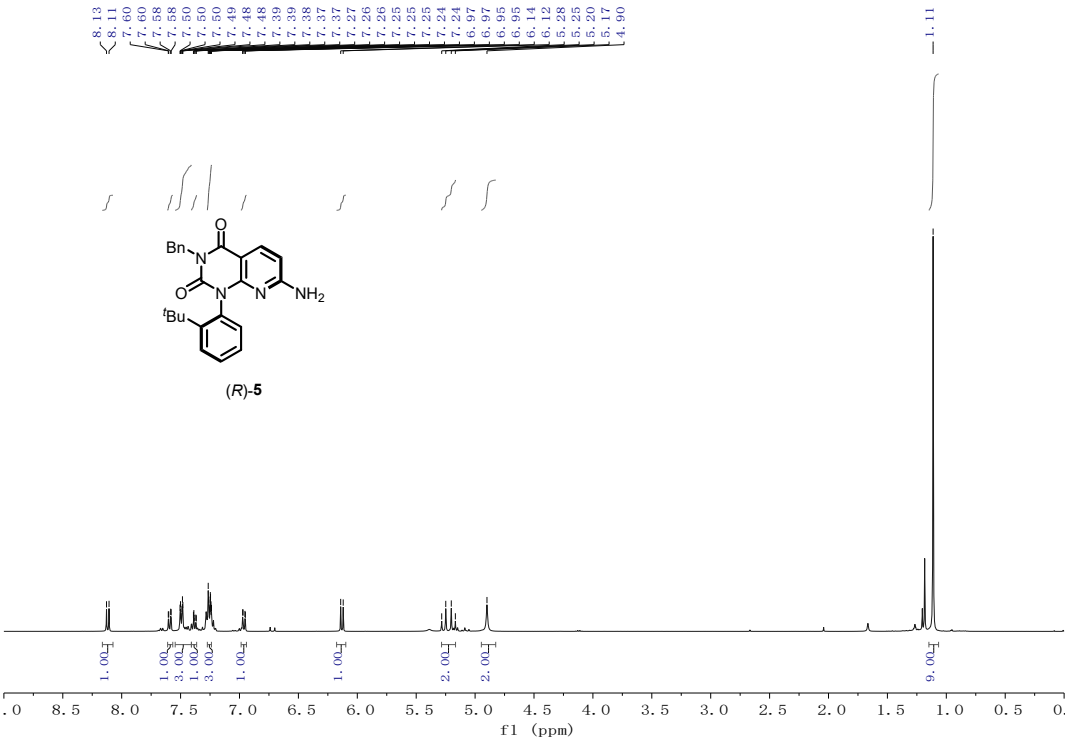
(*S*)-**3ab**


7.65
7.63
7.63
7.50
7.50
7.50
7.49
7.48
7.48
7.45
7.35
7.33
7.32
7.31
7.31
7.24
7.24
7.05
7.04
7.04
7.03
7.02
5.17
5.17
5.13
1.21
Bn
I
NH2
tBu
1.00
3.00
1.00
3.00
1.00
2.00
2.00
9.00
f1 (ppm)

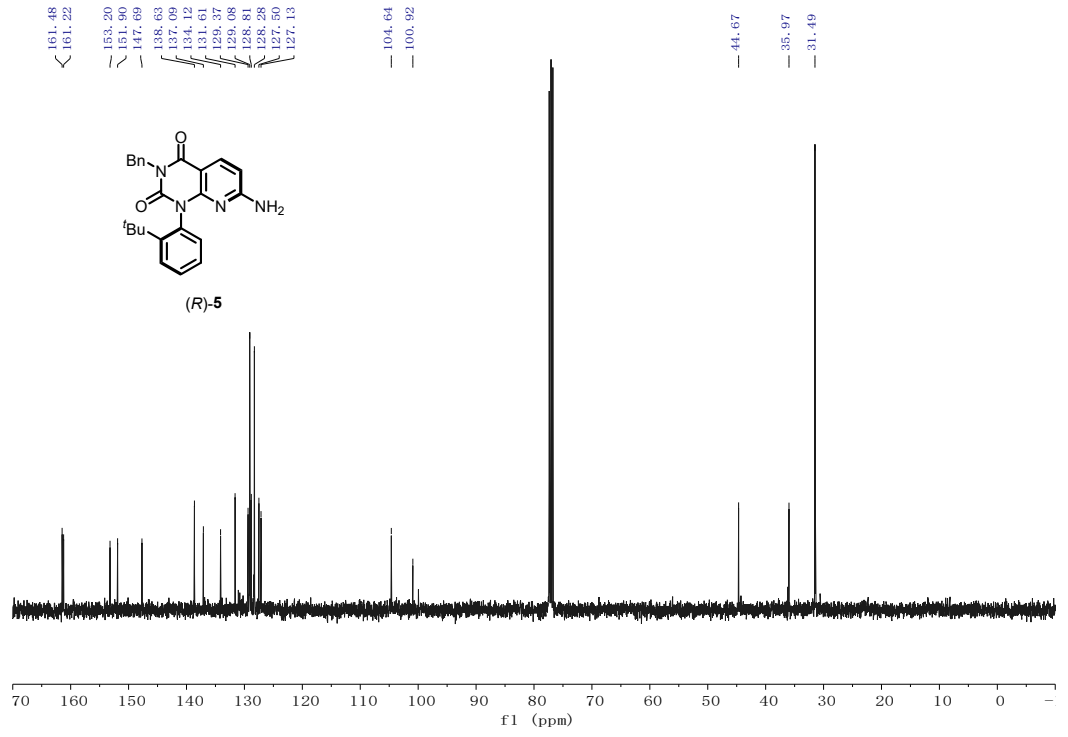
(*R*)-**4**


159.81
151.96
150.97
148.32
137.00
131.63
130.99
130.75
130.64
129.44
128.20
127.51
45.97
36.22
31.44
Bn
I
NH2
tBu
f1 (ppm)

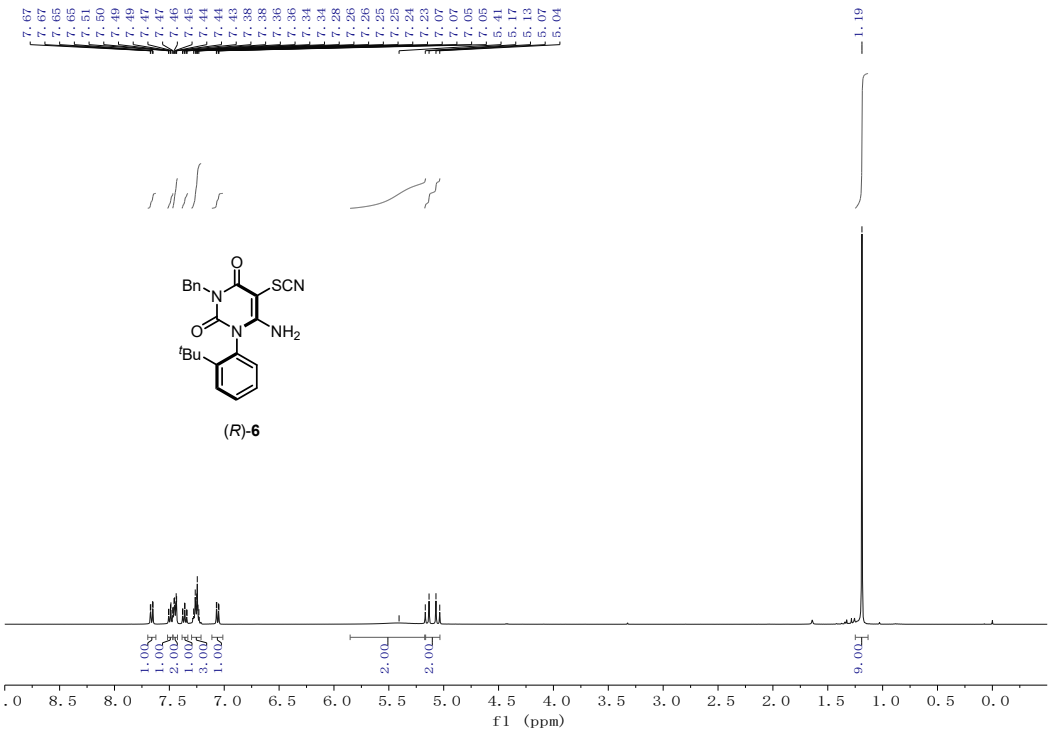
(*R*)-**4**


8.13
8.11
7.60
7.60
7.58
7.58
7.50
7.50
7.50
7.49
7.48
7.48
7.39
7.39
7.38
7.37
7.37
7.27
7.26
7.26
7.25
7.25
7.25
7.24
7.24
6.97
6.97
6.95
6.95
6.14
6.12
5.28
5.25
5.20
5.17
4.90
1.11
Bn
N
O
O
N
N
NH2
tBu
1.00
1.00
3.00
1.00
3.00
1.00
1.00
2.00
2.00
9.00
f1 (ppm)

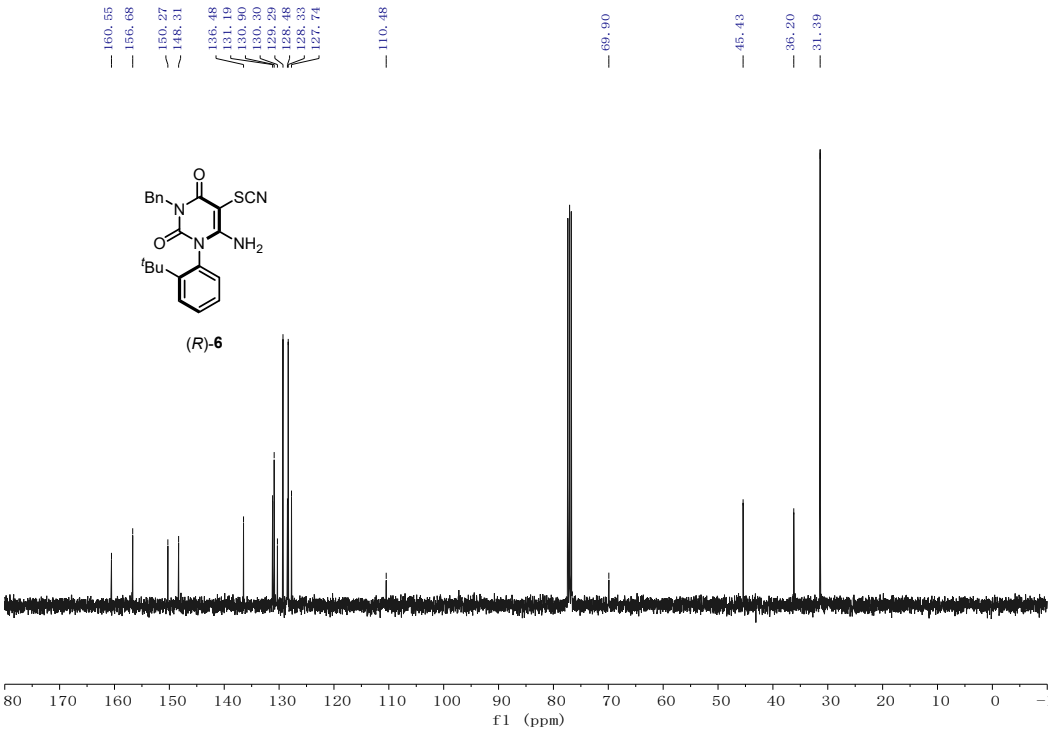
(*R*)-**5**


161.48
161.22
153.20
151.90
147.69
138.63
137.09
134.12
131.61
129.37
129.08
128.81
128.28
127.50
127.13
104.64
100.92
44.67
35.97
31.49
Bn
N
O
O
N
N
NH2
tBu
f1 (ppm)

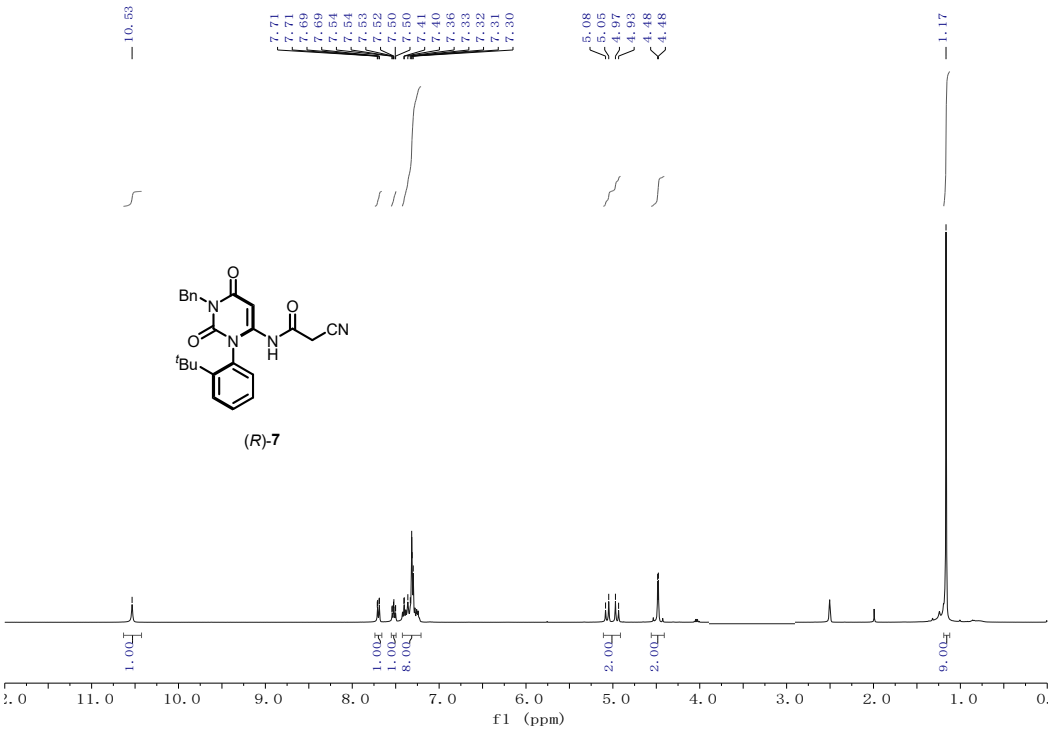
(*R*)-**5**


7.67
7.67
7.65
7.65
7.51
7.50
7.49
7.49
7.47
7.47
7.46
7.45
7.44
7.44
7.43
7.38
7.38
7.36
7.36
7.34
7.34
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.07
7.07
7.05
5.41
5.17
5.13
5.07
5.04
1.19
Bn
N
O
O
N
SCN
NH2
tBu
1.00
1.00
2.00
1.00
3.00
1.00
2.00
2.00
9.00
f1 (ppm)

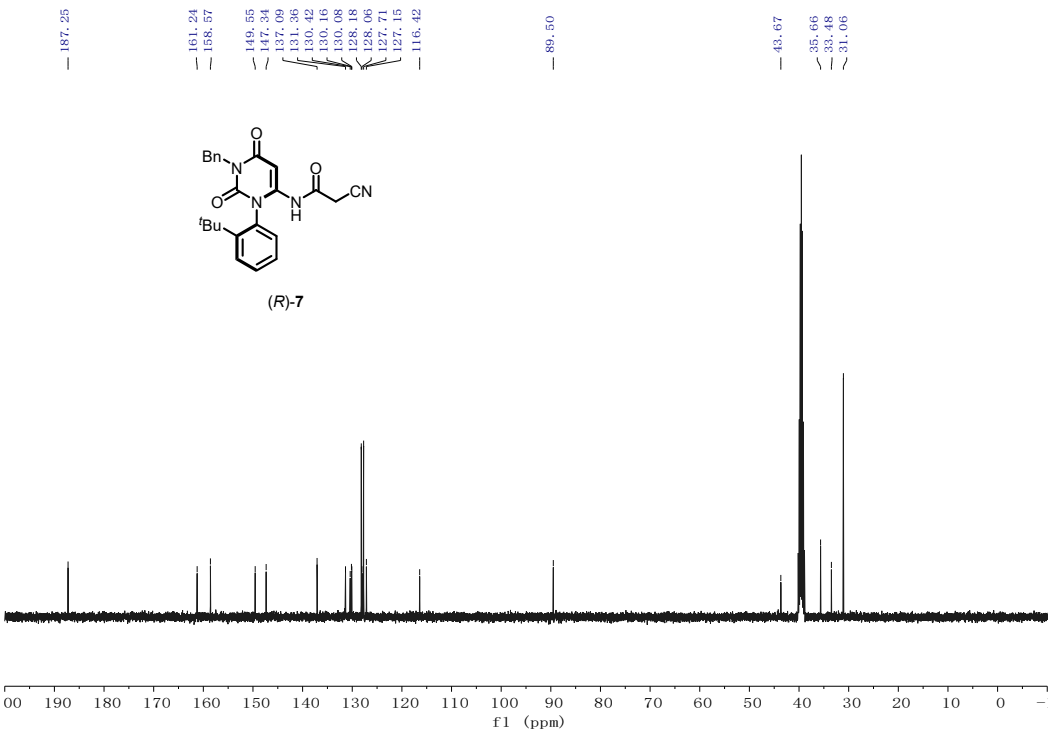
(*R*)-**6**


160.55
156.68
150.27
148.31
136.48
131.19
130.90
130.30
129.29
128.48
128.33
127.74
110.48
69.90
45.43
36.20
31.39
Bn
N
O
O
N
SCN
NH2
tBu
f1 (ppm)

(*R*)-**6**

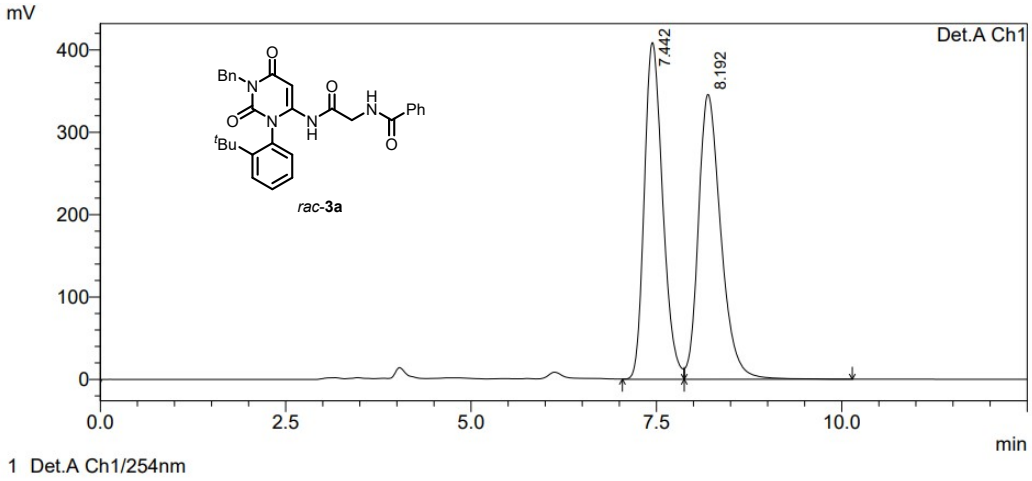

10.53
7.71
7.71
7.69
7.69
7.54
7.54
7.53
7.52
7.50
7.50
7.41
7.40
7.36
7.33
7.32
7.31
7.30
5.08
5.05
4.97
4.93
4.48
4.48
1.17
Bn
N
O
O
N
H
O
CN
tBu
1.00
1.00
1.00
8.00
2.00
2.00
9.00
f1 (ppm)

(*R*)-**7**


187.25
161.24
158.57
149.55
147.34
137.09
131.36
130.42
130.16
130.08
128.18
128.06
127.71
127.15
116.42
89.50
43.67
35.66
33.48
31.06
Bn
N
O
O
N
H
O
CN
tBu
f1 (ppm)

(*R*)-**7**

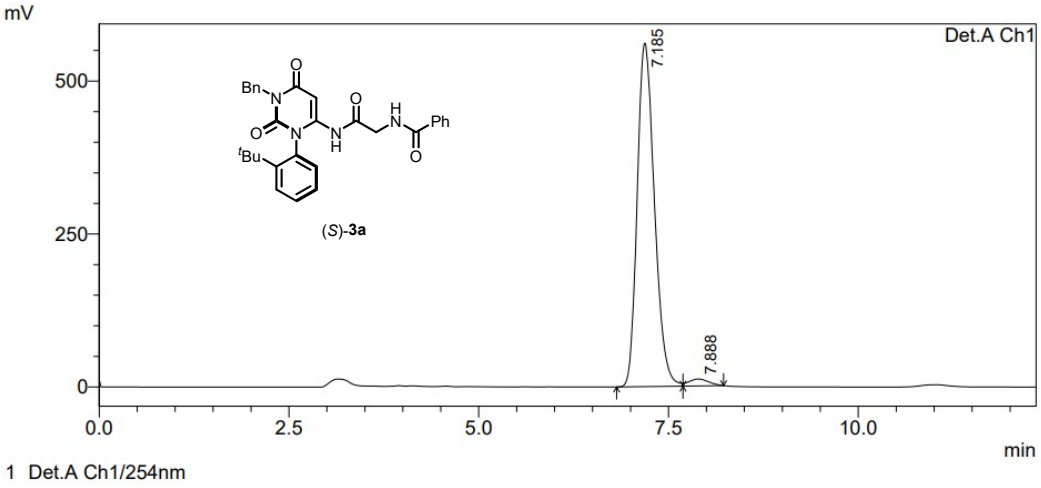
13. HPLC spectra



PeakTable

Detector A Ch1 254nm

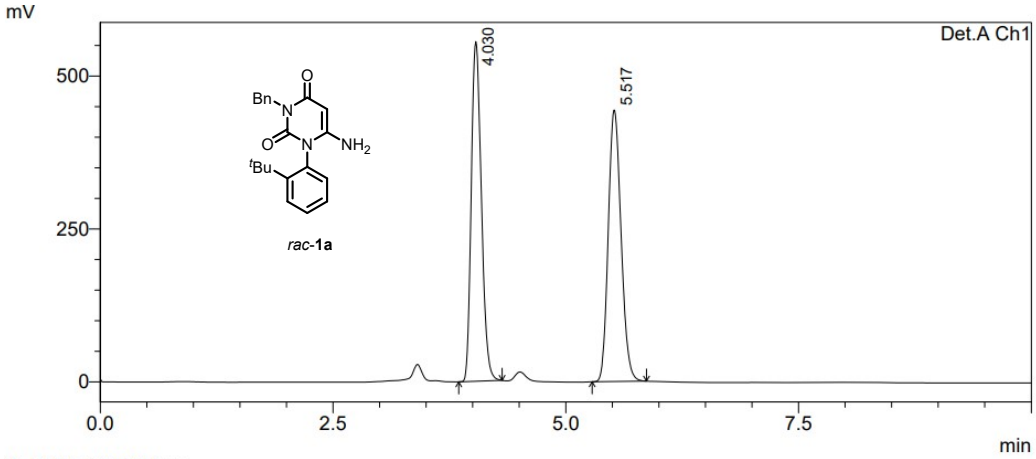
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.442	7056821	407746	49.162	54.158
2	8.192	7297477	345130	50.838	45.842
Total		14354299	752876	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.185	8862201	561310	97.739	98.022
2	7.888	205015	11324	2.261	1.978
Total		9067216	572635	100.000	100.000

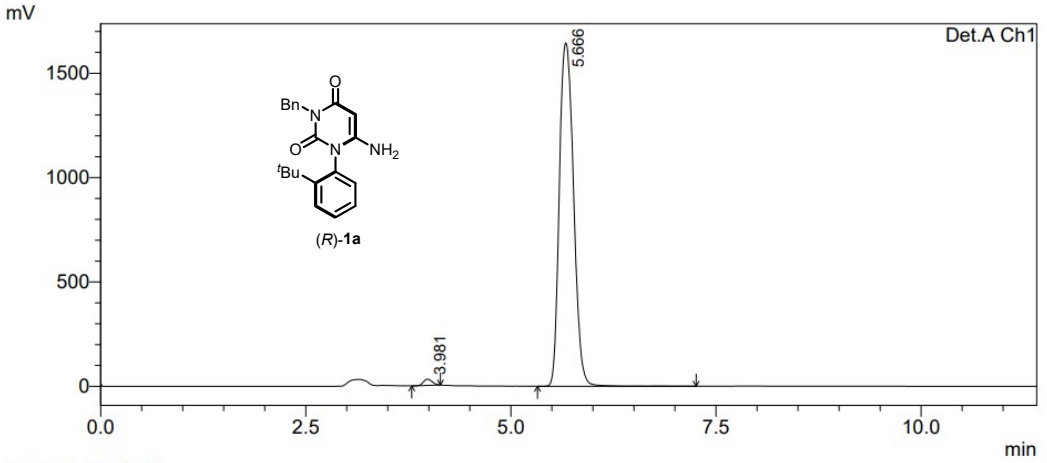


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.030	4189222	551620	49.702	55.626
2	5.517	4239401	440036	50.298	44.374
Total		8428623	991656	100.000	100.000

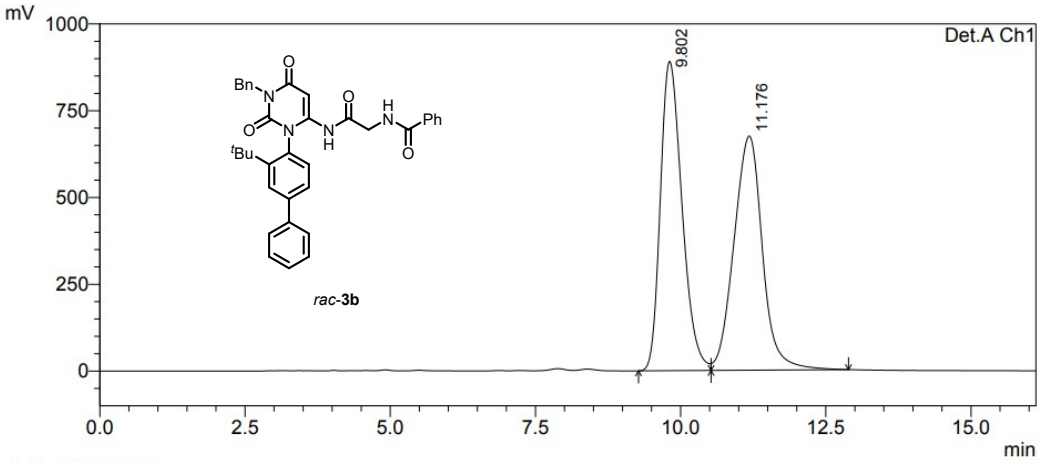


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.981	224021	29891	1.118	1.786
2	5.666	19819569	1643900	98.882	98.214
Total		20043589	1673790	100.000	100.000

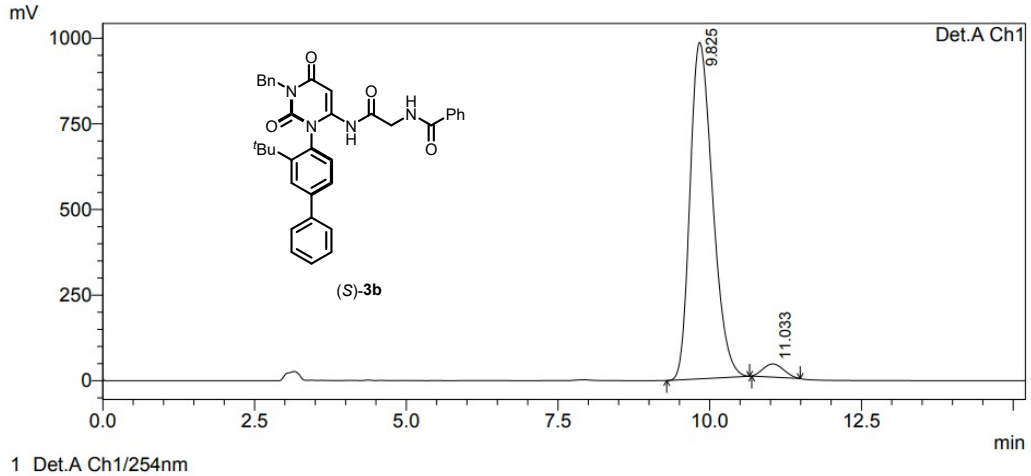


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.802	23132199	889732	50.141	56.901
2	11.176	23002327	673906	49.859	43.099
Total		46134526	1563638	100.000	100.000

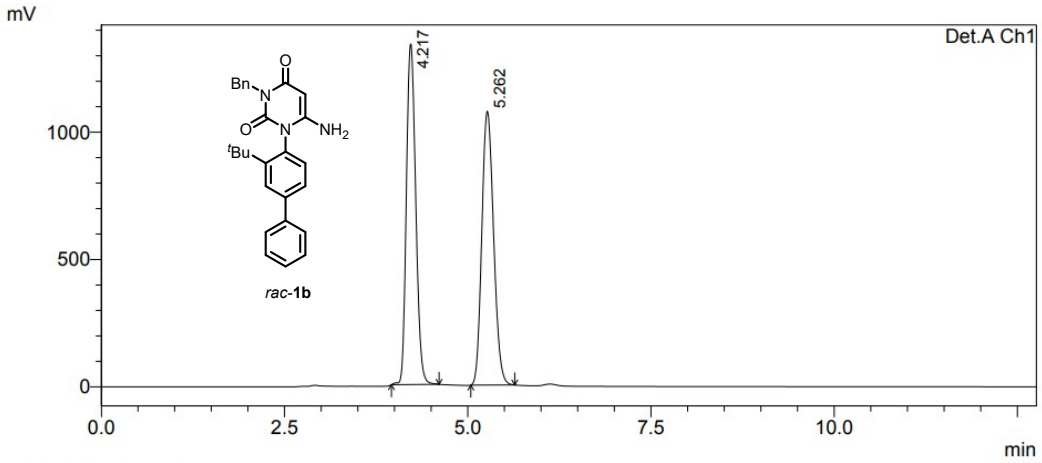


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.825	25442166	979207	96.558	96.237
2	11.033	906824	38284	3.442	3.763
Total		26348990	1017491	100.000	100.000

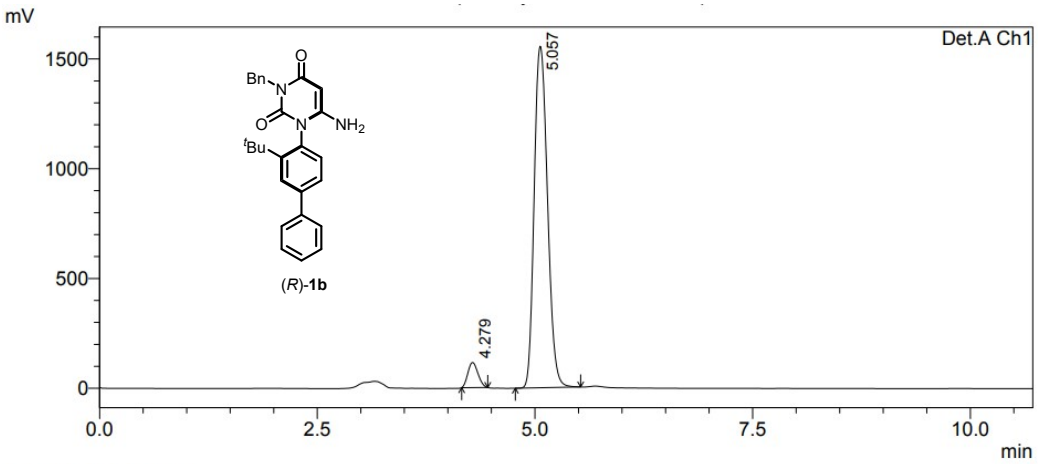


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.217	11882595	1336256	49.693	55.493
2	5.262	12029291	1071706	50.307	44.507
Total		23911887	2407962	100.000	100.000

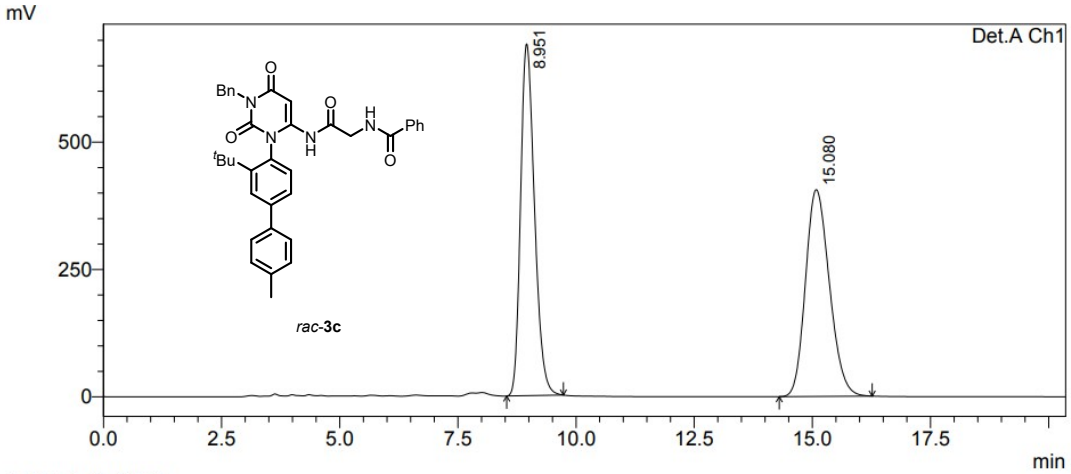


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.279	923249	113960	5.286	6.854
2	5.057	16541272	1548716	94.714	93.146
Total		17464521	1662676	100.000	100.000

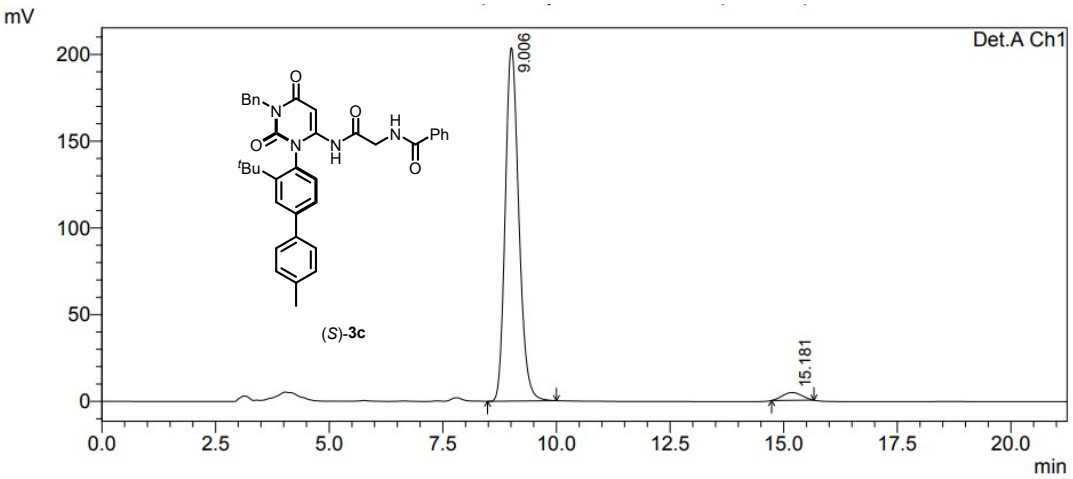


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.951	14176784	689586	49.768	62.965
2	15.080	14309107	405612	50.232	37.035
Total		28485891	1095198	100.000	100.000

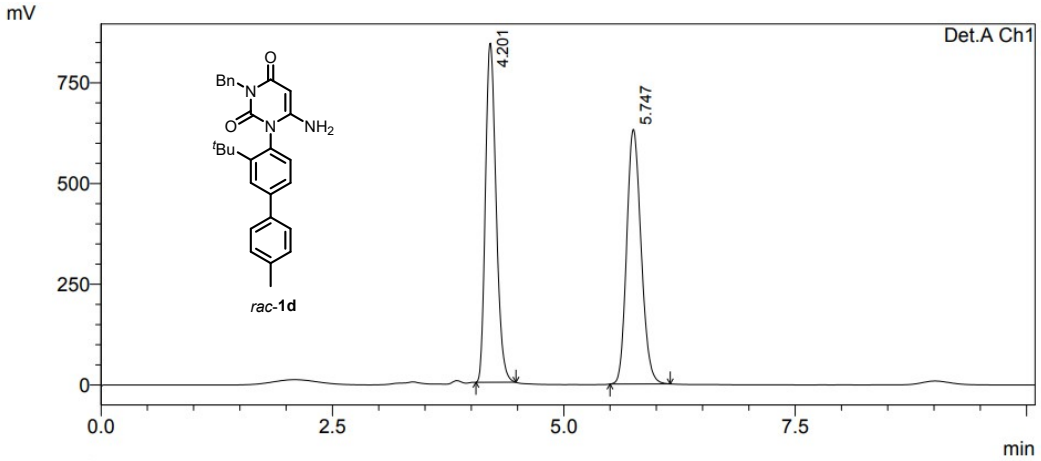


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.006	4226971	203686	96.965	97.851
2	15.181	132298	4474	3.035	2.149
Total		4359269	208160	100.000	100.000

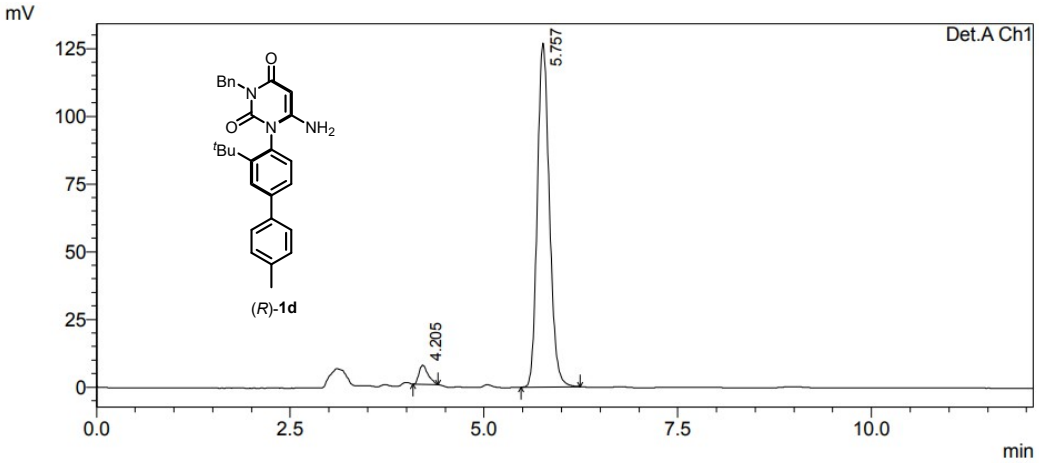


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.201	6730675	832641	49.598	56.953
2	5.747	6839881	629335	50.402	43.047
Total		13570556	1461976	100.000	100.000

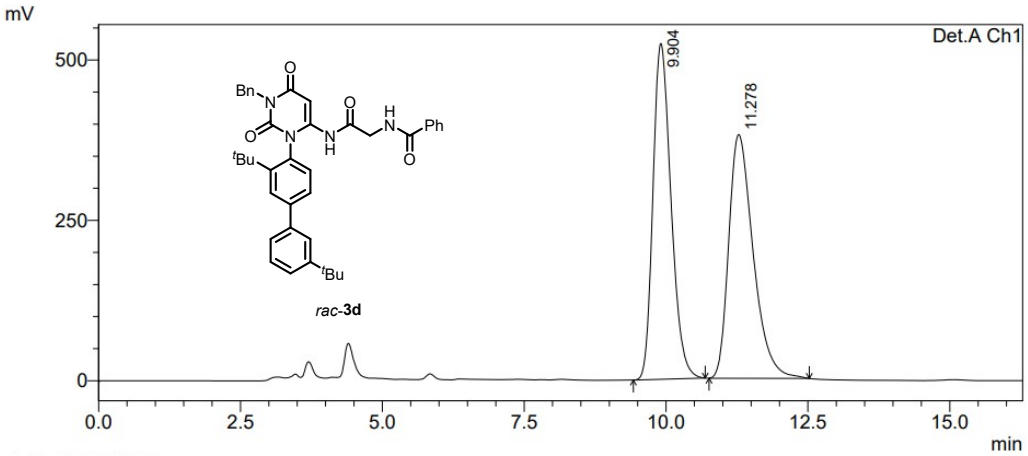


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

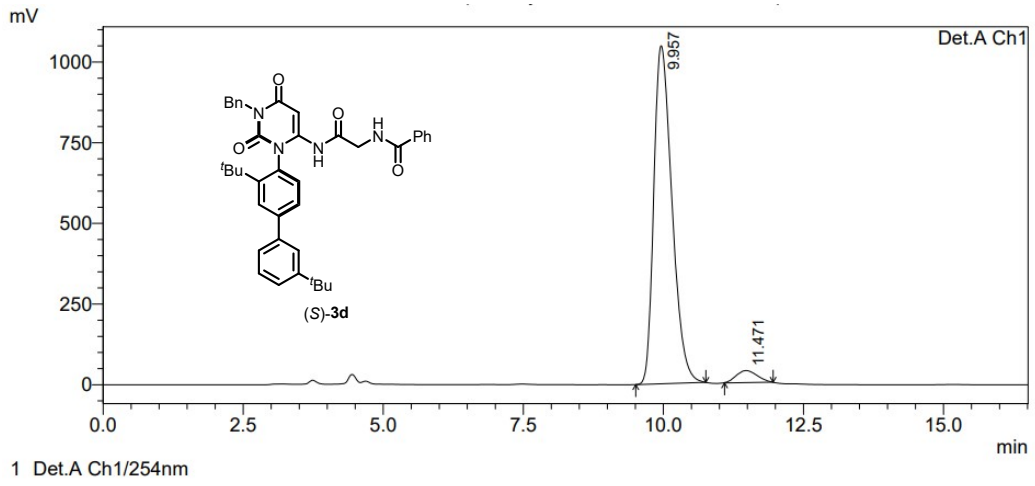
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.205	57936	7103	4.048	5.297
2	5.757	1373328	126993	95.952	94.703
Total		1431264	134097	100.000	100.000



PeakTable

Detector A Ch1 254nm

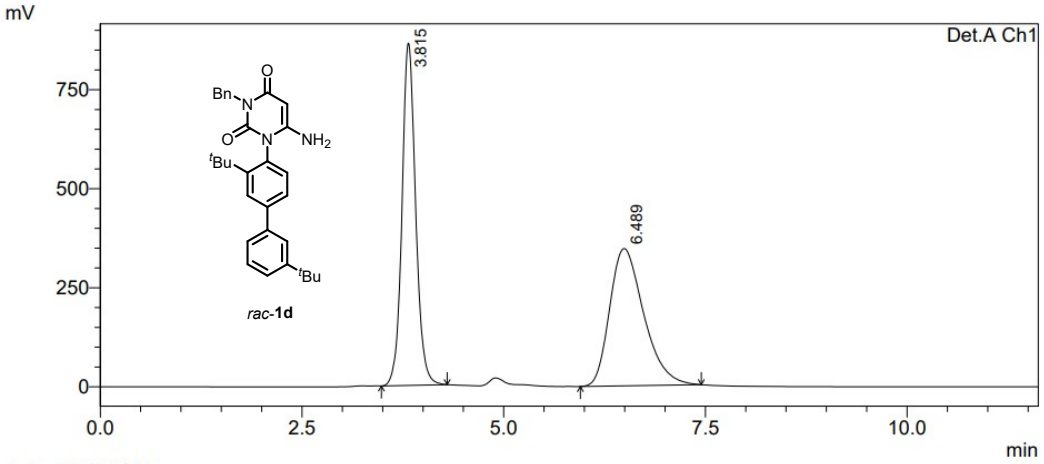
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.904	11586310	523158	50.441	57.950
2	11.278	11383494	379620	49.559	42.050
Total		22969804	902779	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.957	23589641	1046270	96.049	96.564
2	11.471	970269	37224	3.951	3.436
Total		24559910	1083494	100.000	100.000

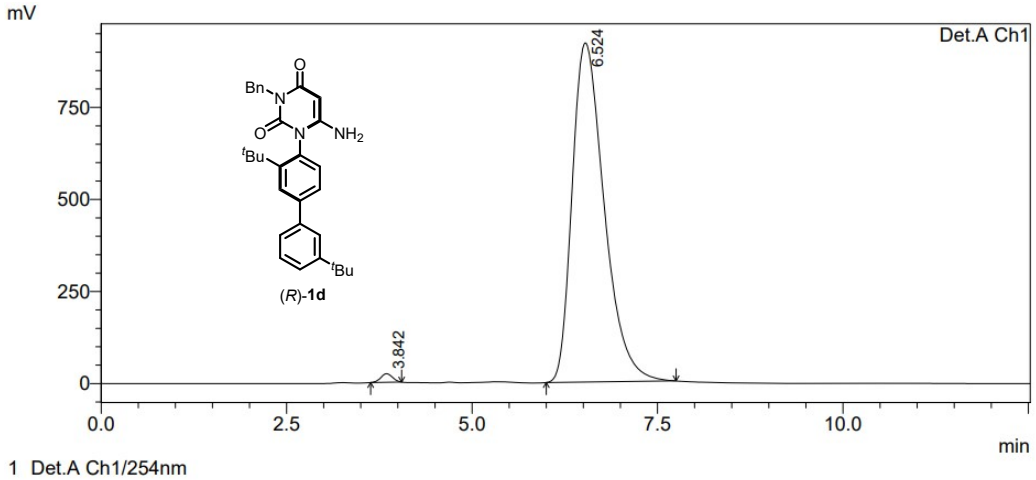


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.815	10145876	860168	49.915	71.339
2	6.489	10180404	345572	50.085	28.661
Total		20326280	1205740	100.000	100.000

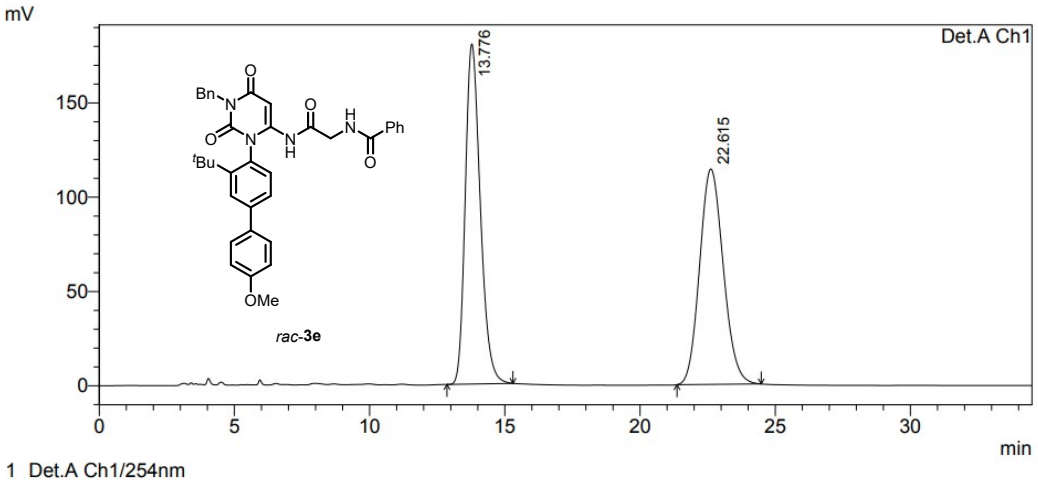


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.842	254330	23361	0.910	2.479
2	6.524	27693693	919165	99.090	97.521
Total		27948022	942526	100.000	100.000

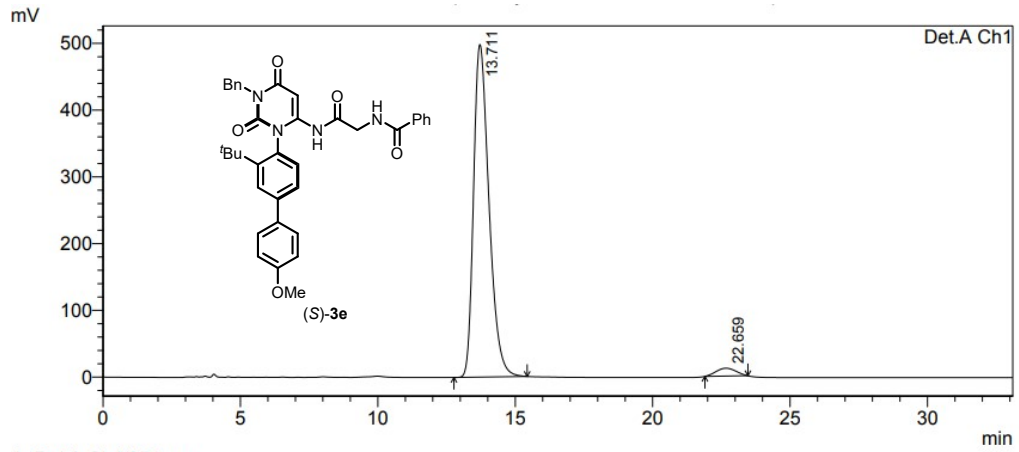


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.776	6978964	180358	50.104	61.242
2	22.615	6949959	114142	49.896	38.758
Total		13928923	294500	100.000	100.000

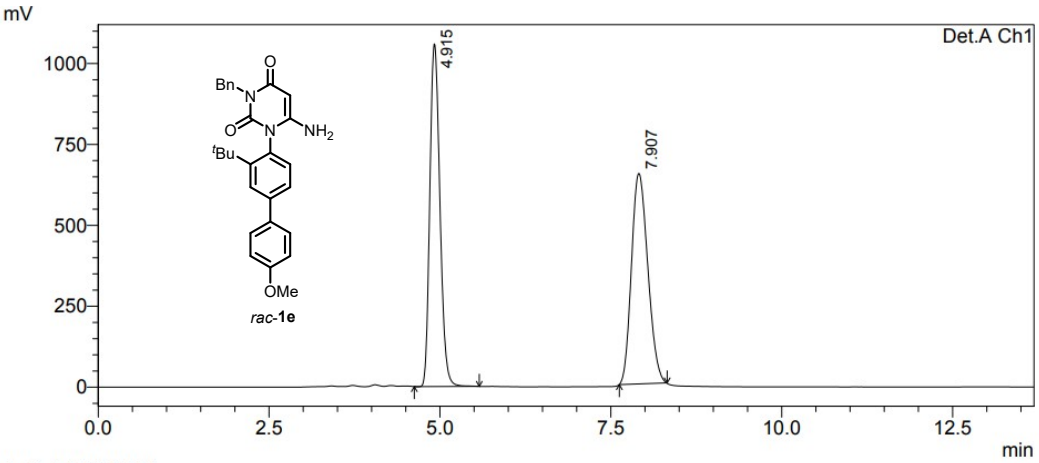


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.711	19429762	497822	97.067	97.699
2	22.659	587057	11727	2.933	2.301
Total		20016818	509549	100.000	100.000

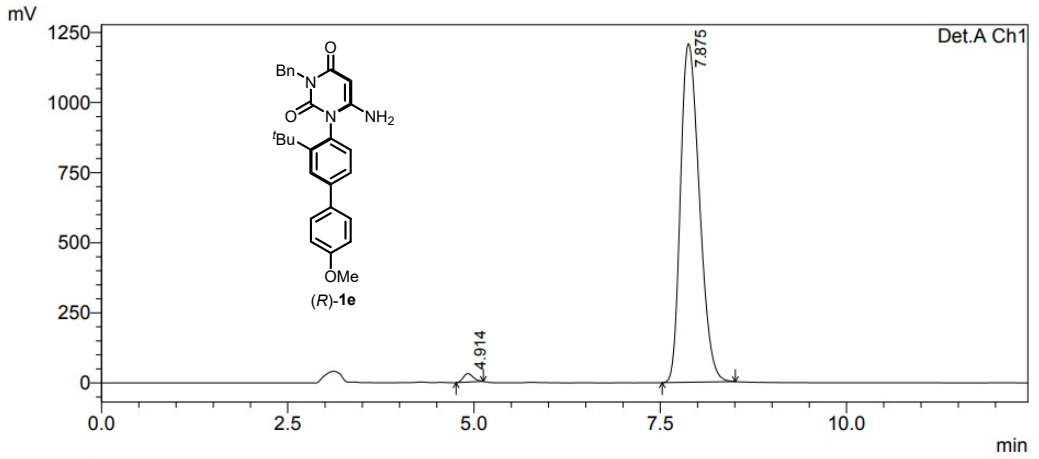


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.915	10862790	1057177	50.115	61.989
2	7.907	10813093	648251	49.885	38.011
Total		21675883	1705428	100.000	100.000

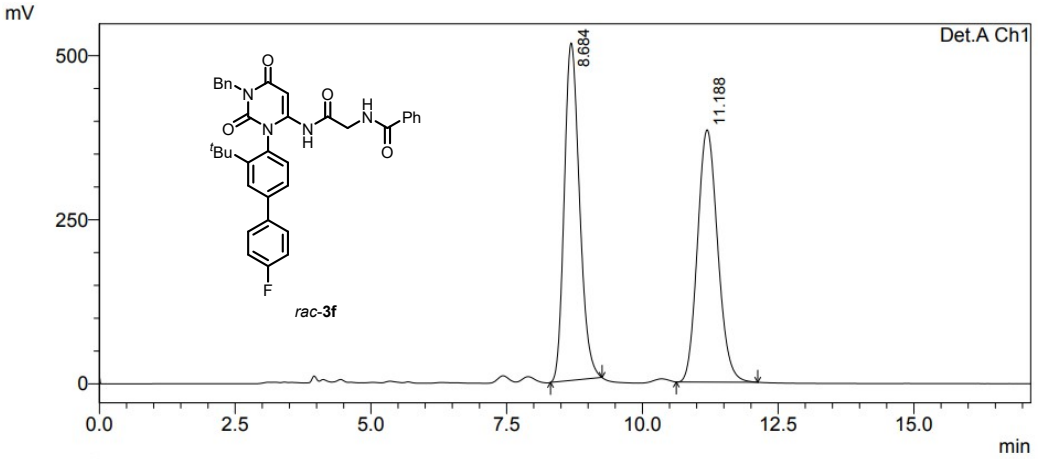


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.914	286068	30367	1.324	2.458
2	7.875	21320168	1205063	98.676	97.542
Total		21606236	1235430	100.000	100.000

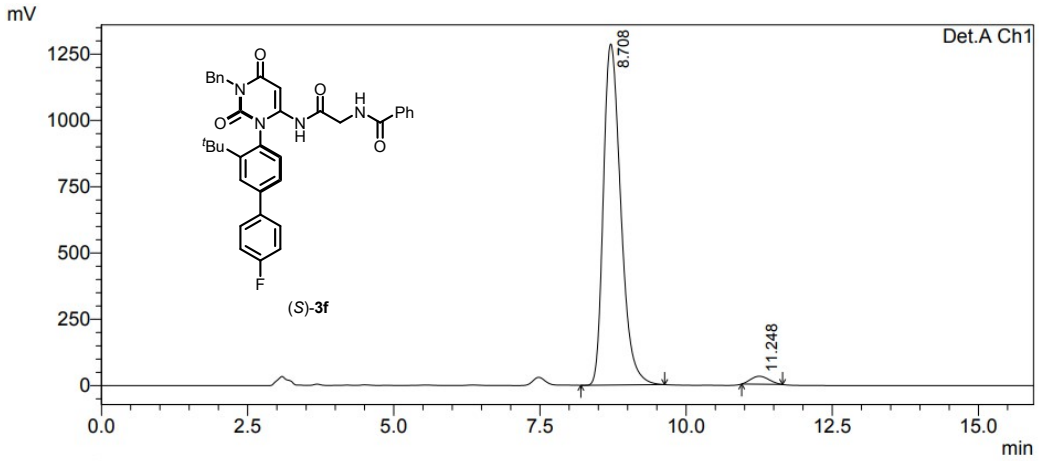


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.684	10056112	514129	50.299	57.238
2	11.188	9936660	384094	49.701	42.762
Total		19992772	898222	100.000	100.000

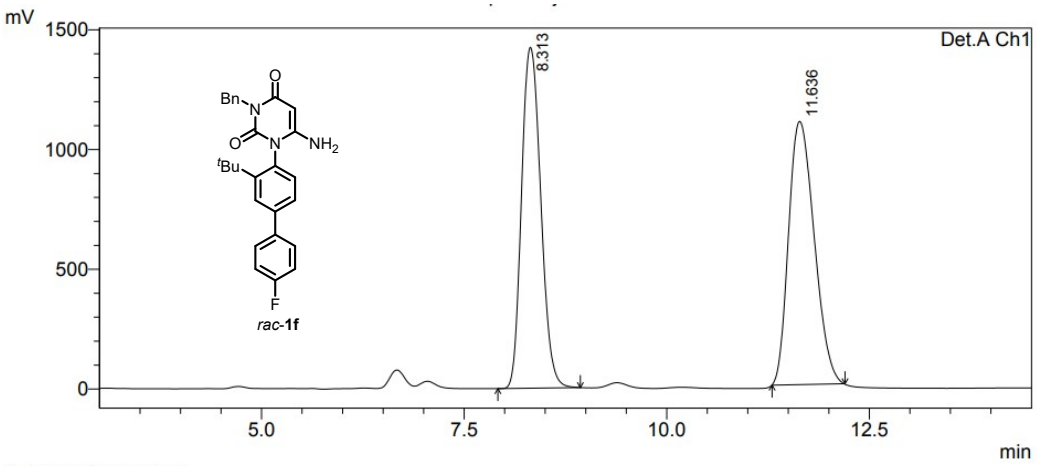


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.708	26682660	1286346	97.633	97.729
2	11.248	646916	29895	2.367	2.271
Total		27329576	1316241	100.000	100.000

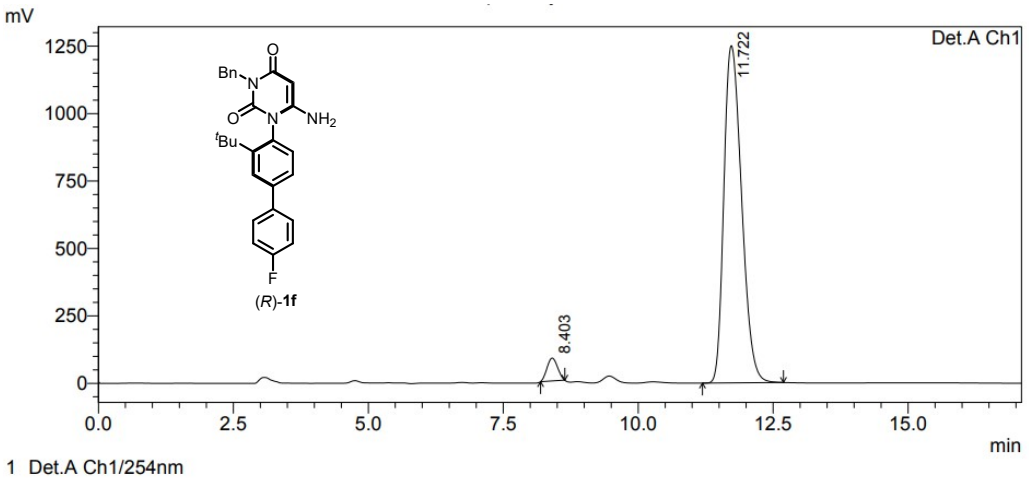


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.313	23502468	1422245	49.274	56.419
2	11.636	24195295	1098610	50.726	43.581
Total		47697763	2520856	100.000	100.000

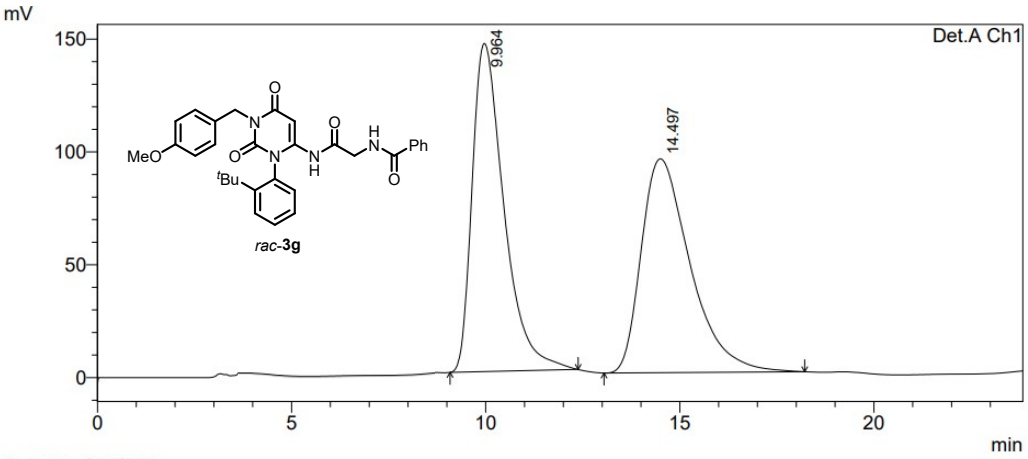


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.403	1150507	84687	3.870	6.348
2	11.722	28579568	1249440	96.130	93.652
Total		29730075	1334127	100.000	100.000

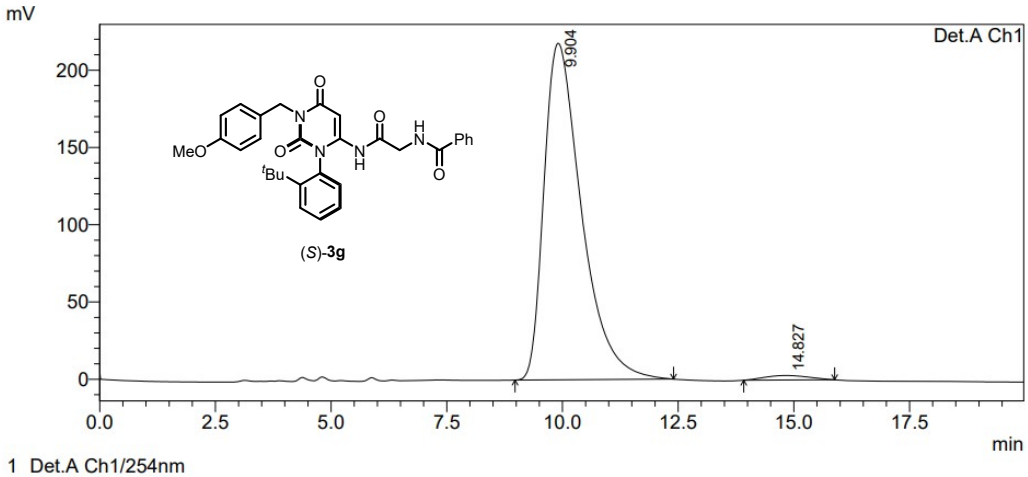


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.964	8275674	145401	49.952	60.558
2	14.497	8291522	94700	50.048	39.442
Total		16567195	240101	100.000	100.000

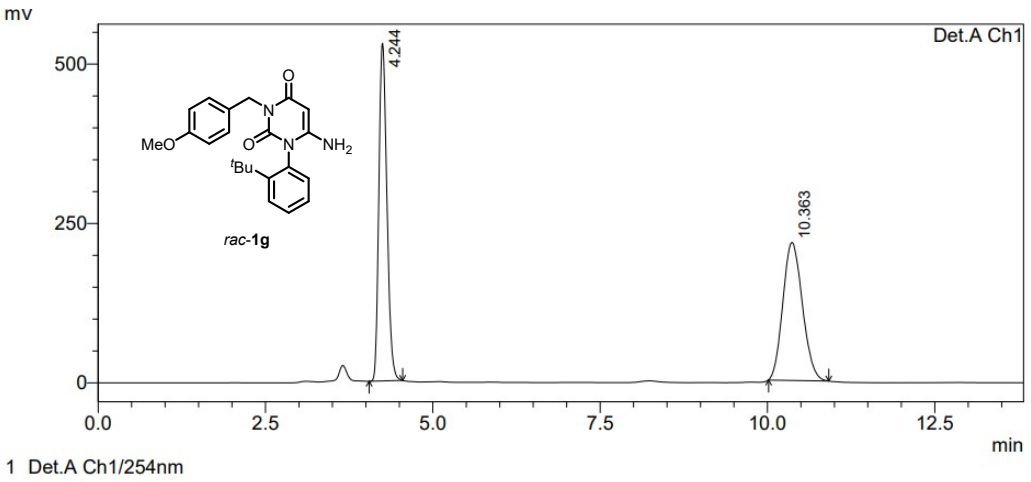


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

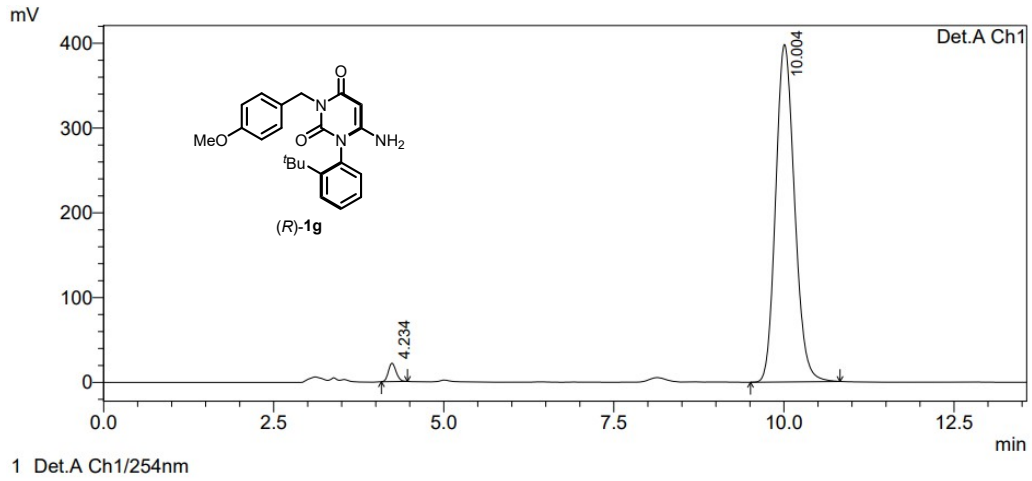
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.904	12276067	217715	98.444	98.671
2	14.827	193985	2932	1.556	1.329
Total		12470052	220646	100.000	100.000



PeakTable

Detector A Ch1 254nm

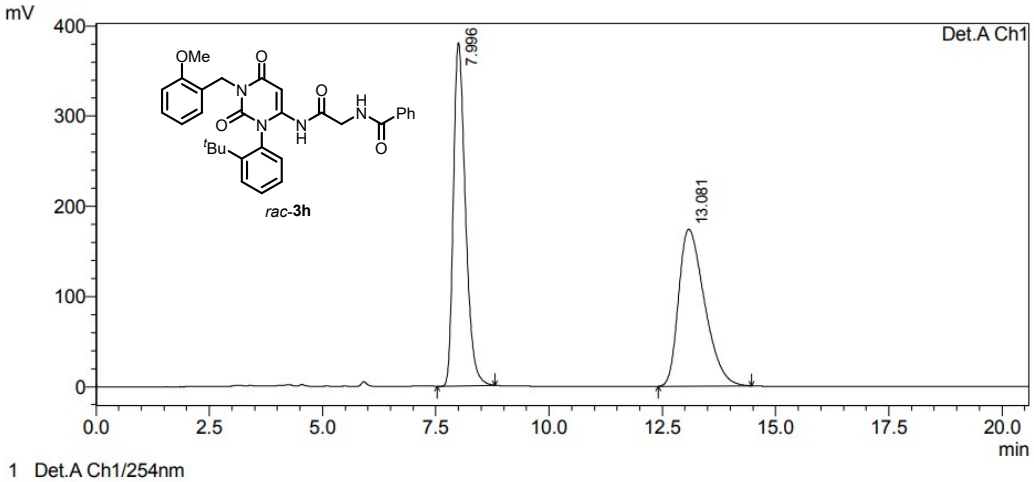
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.244	4435861	528719	50.174	70.952
2	10.363	4405140	216459	49.826	29.048
Total		8841001	745178	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.234	170573	21583	2.173	5.147
2	10.004	7678970	397752	97.827	94.853
Total		7849542	419334	100.000	100.000

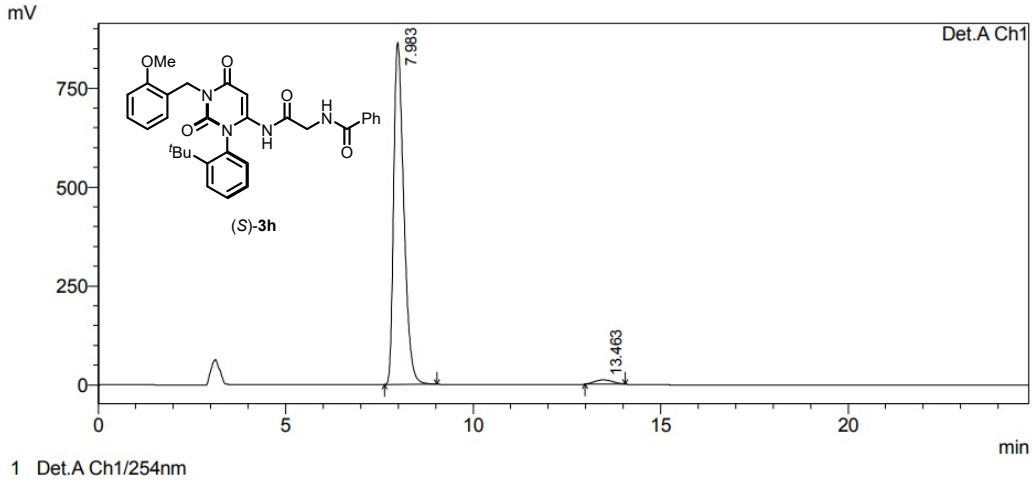


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.996	7009412	379854	50.208	68.606
2	13.081	6951211	173817	49.792	31.394
Total		13960623	553671	100.000	100.000

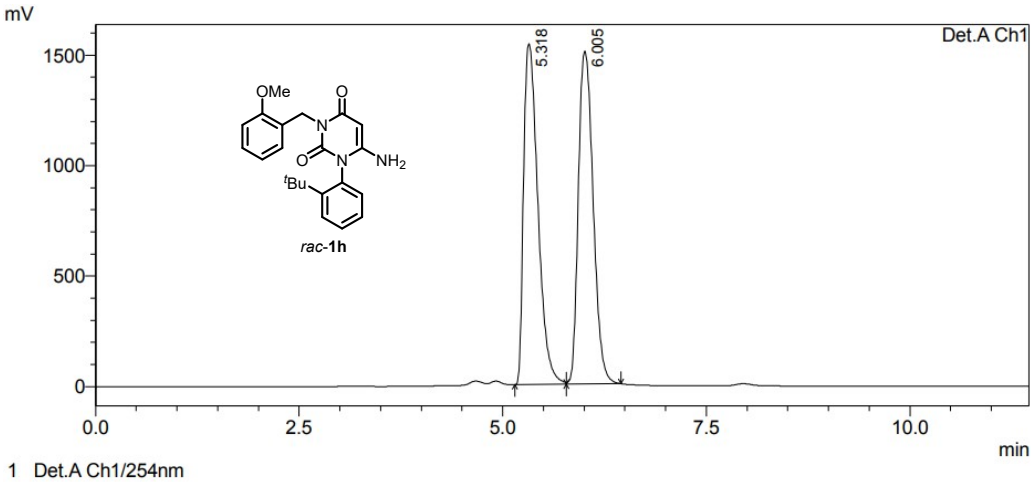


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.983	16276205	862546	97.844	98.788
2	13.463	358598	10579	2.156	1.212
Total		16634803	873125	100.000	100.000

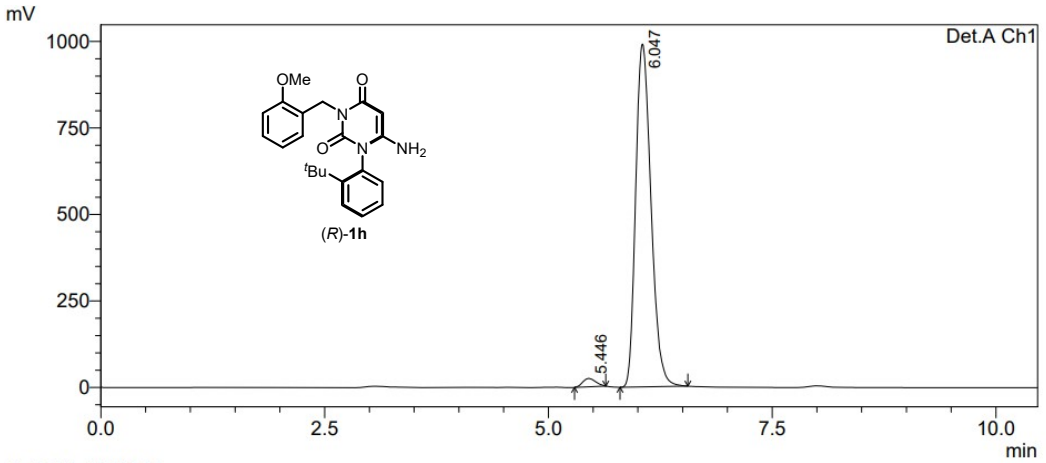


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.318	18869427	1536372	49.753	50.518
2	6.005	19057038	1504870	50.247	49.482
Total		37926465	3041242	100.000	100.000

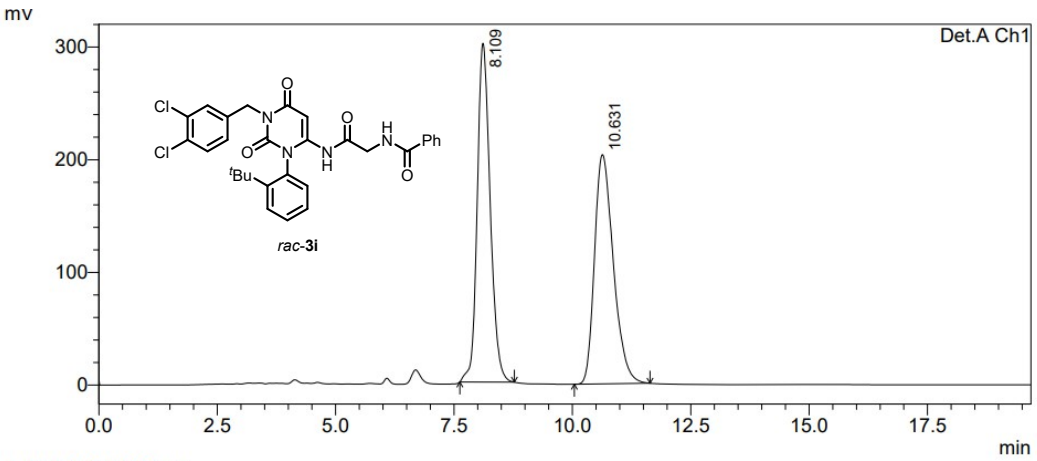


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.446	244561	24174	2.030	2.381
2	6.047	11800451	991170	97.970	97.619
Total		12045012	1015343	100.000	100.000

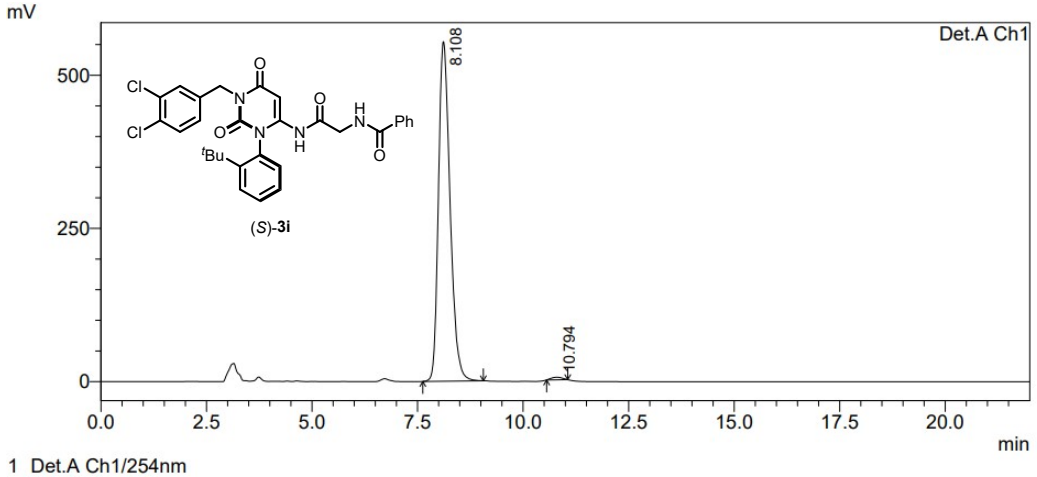


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.109	5736119	297284	50.512	59.410
2	10.631	5619761	203109	49.488	40.590
Total		11355880	500393	100.000	100.000

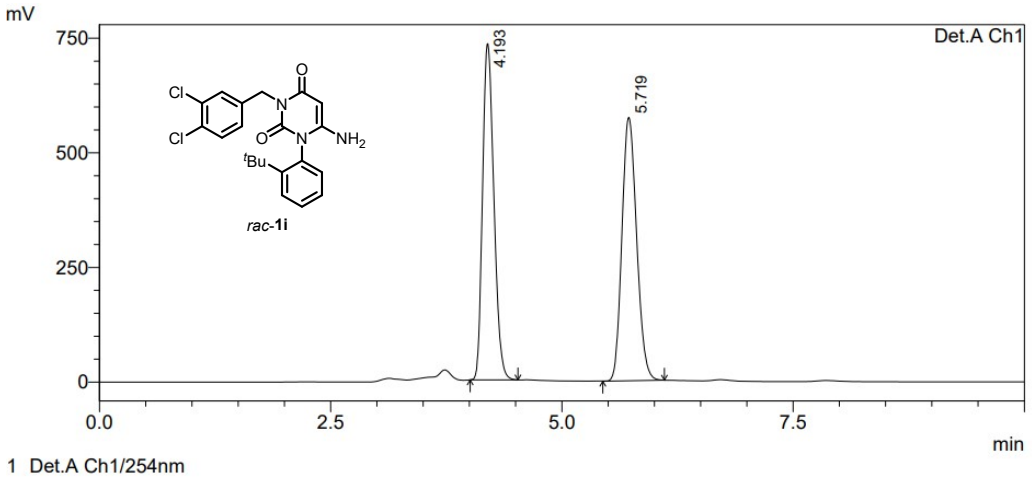


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.108	10603799	552952	99.285	99.247
2	10.794	76345	4194	0.715	0.753
Total		10680144	557146	100.000	100.000

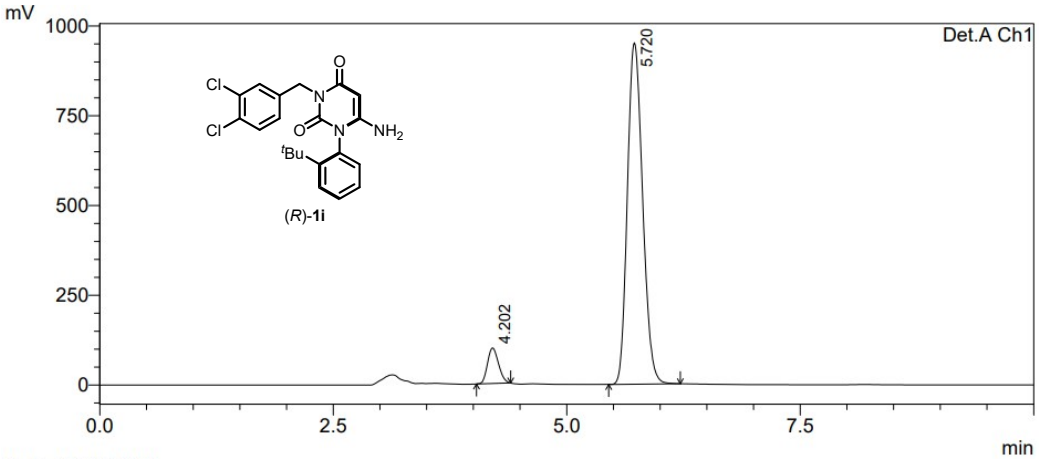


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.193	6248815	726771	49.637	55.897
2	5.719	6340161	573425	50.363	44.103
Total		12588976	1300196	100.000	100.000

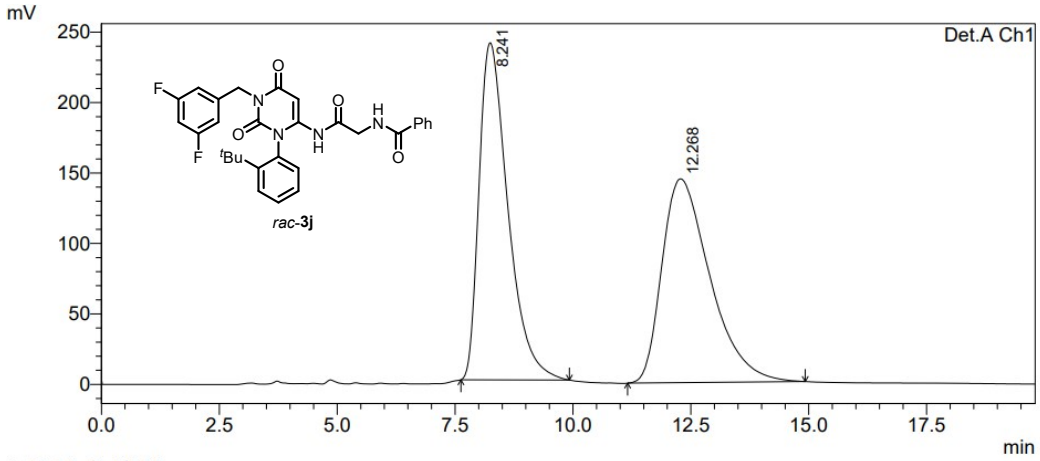


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.202	811296	97972	6.997	9.368
2	5.720	10782792	947826	93.003	90.632
Total		11594088	1045798	100.000	100.000

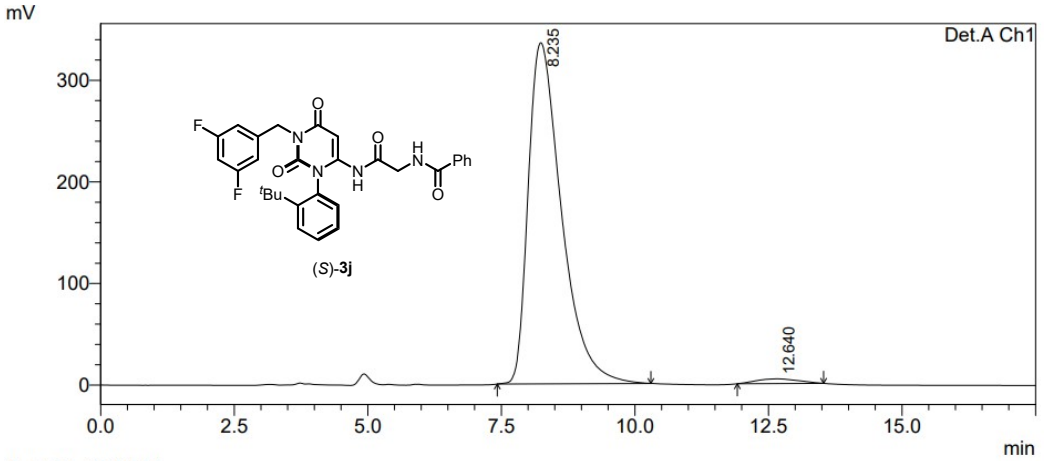


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.241	10191567	239106	49.850	62.337
2	12.268	10252827	144467	50.150	37.663
Total		20444393	383573	100.000	100.000

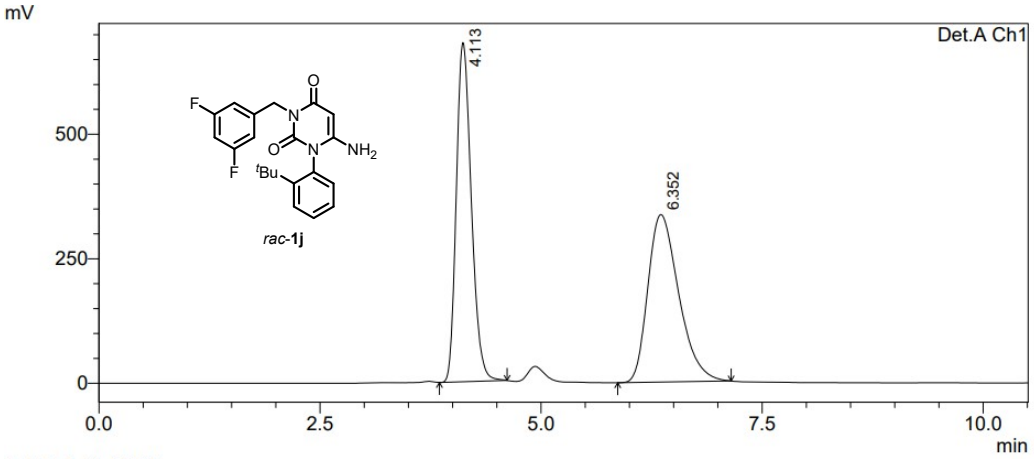


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.235	14528918	335666	98.283	98.633
2	12.640	253852	4651	1.717	1.367
Total		14782770	340318	100.000	100.000

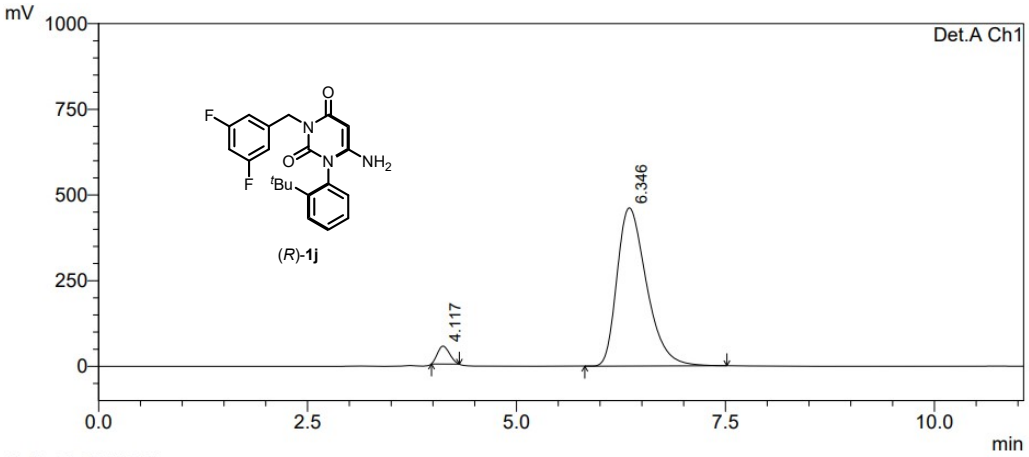


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.113	8037468	678957	49.613	66.904
2	6.352	8162805	335866	50.387	33.096
Total		16200273	1014823	100.000	100.000

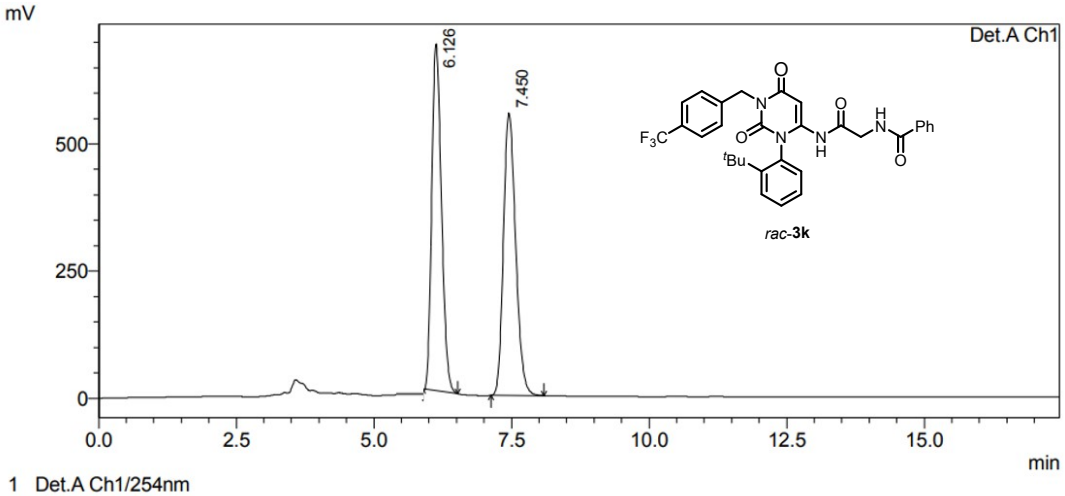


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.117	525063	51790	4.418	10.088
2	6.346	11359330	461606	95.582	89.912
Total		11884393	513395	100.000	100.000

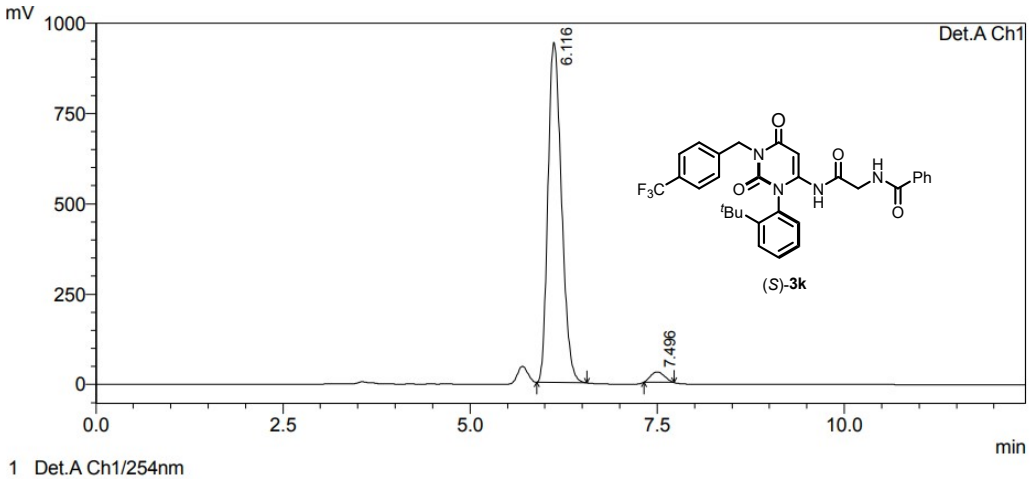


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.126	8324529	664628	49.249	54.642
2	7.450	8578299	551710	50.751	45.358
Total		16902829	1216338	100.000	100.000

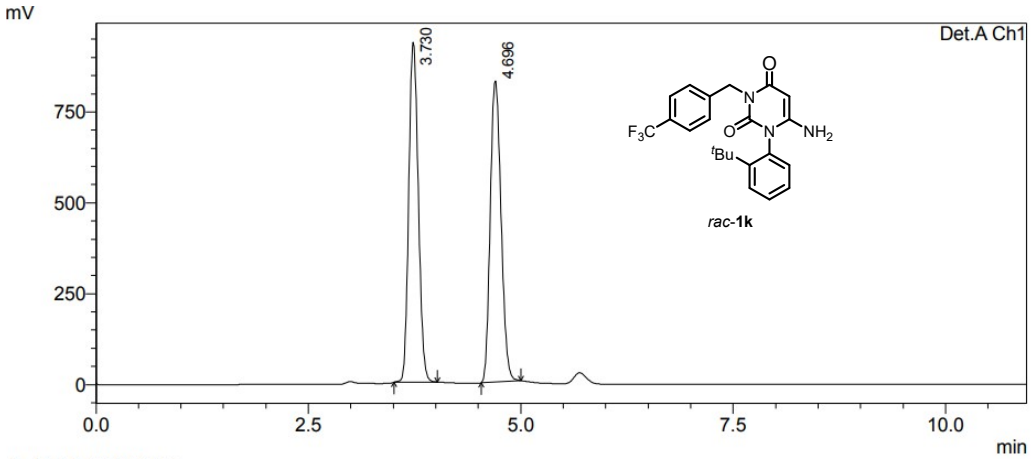


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.116	11855326	940423	96.991	97.041
2	7.496	367817	28679	3.009	2.959
Total		12223143	969101	100.000	100.000

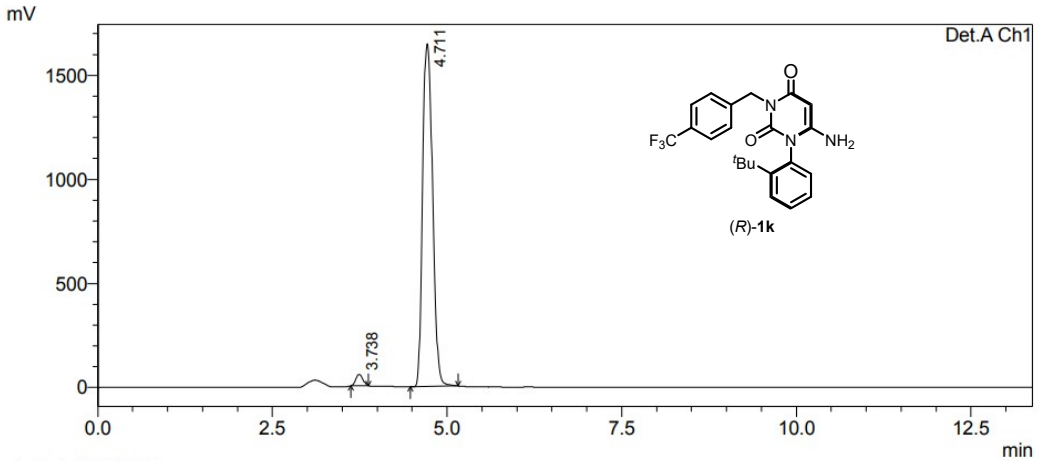


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.730	7316157	928882	50.224	52.937
2	4.696	7250988	825798	49.776	47.063
Total		14567145	1754680	100.000	100.000

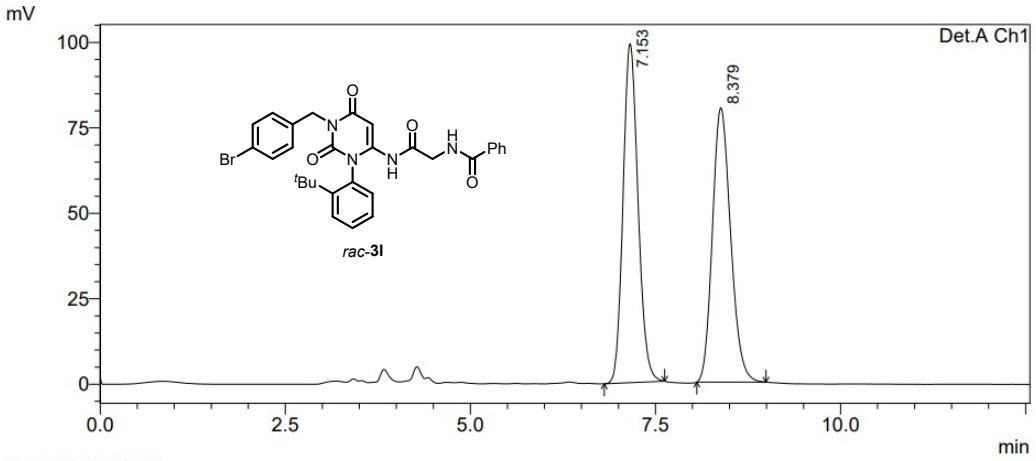


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

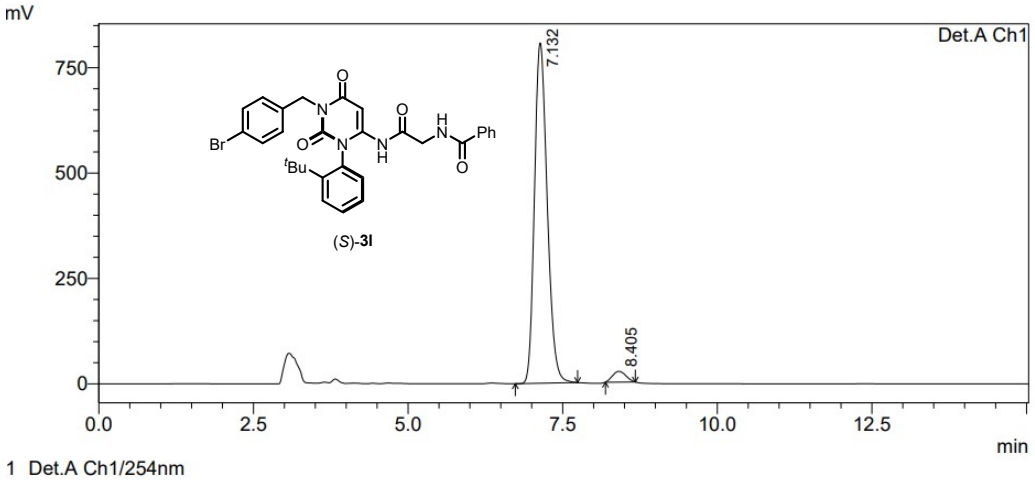
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.738	379893	53084	2.261	3.134
2	4.711	16421029	1640552	97.739	96.866
Total		16800921	1693636	100.000	100.000



PeakTable

Detector A Ch1 254nm

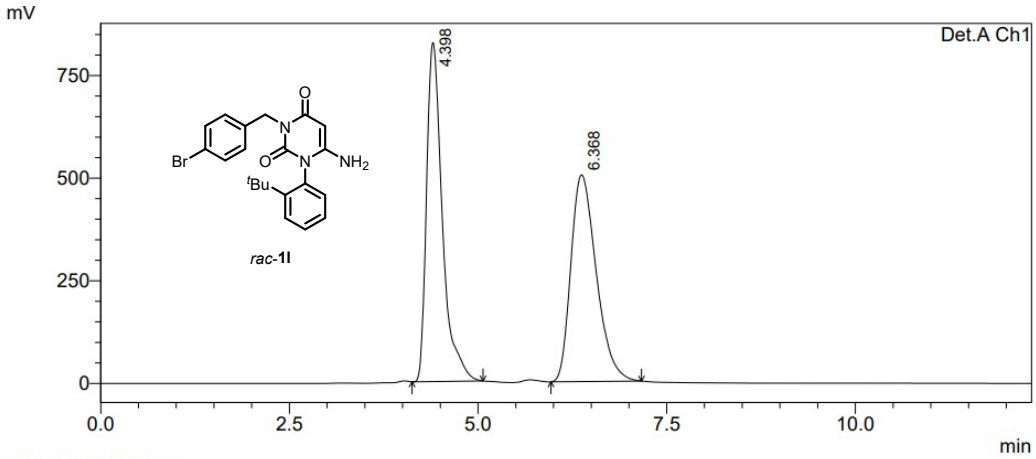
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.153	1392110	99110	50.293	55.290
2	8.379	1375883	80144	49.707	44.710
Total		2767993	179254	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.132	11575369	806886	96.787	96.909
2	8.405	384241	25739	3.213	3.091
Total		11959610	832624	100.000	100.000

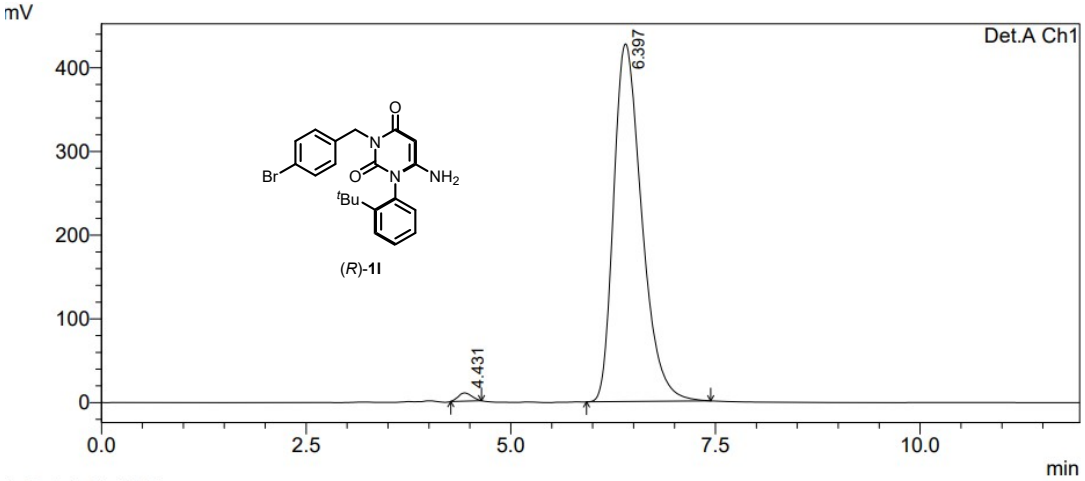


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.398	12000478	826201	50.440	62.156
2	6.368	11791231	503047	49.560	37.844
Total		23791709	1329248	100.000	100.000

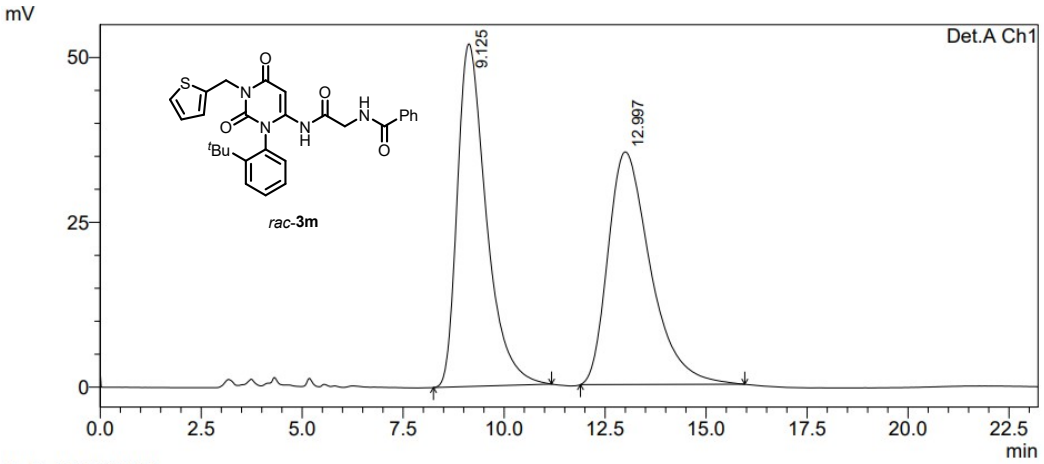


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

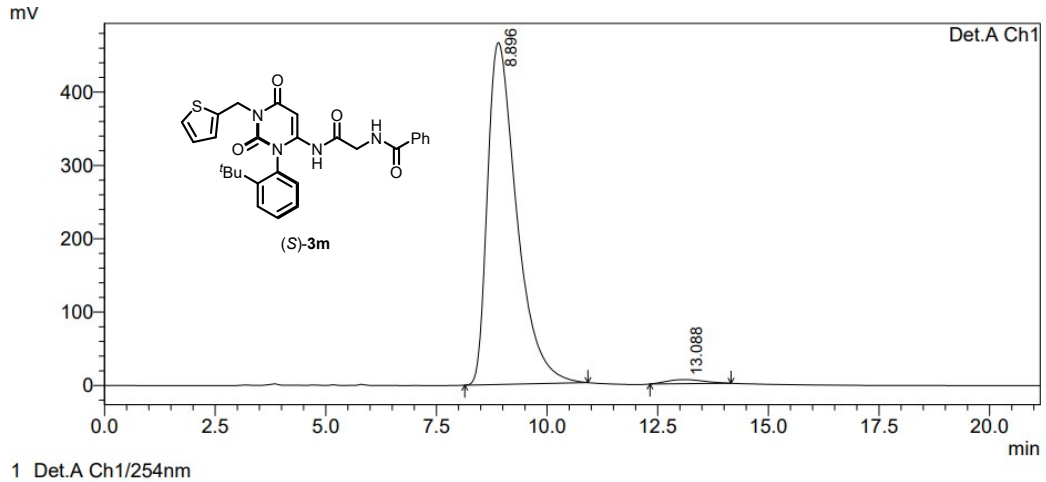
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.431	114062	9837	1.106	2.251
2	6.397	10201773	427119	98.894	97.749
Total		10315835	436956	100.000	100.000



PeakTable

Detector A Ch1 254nm

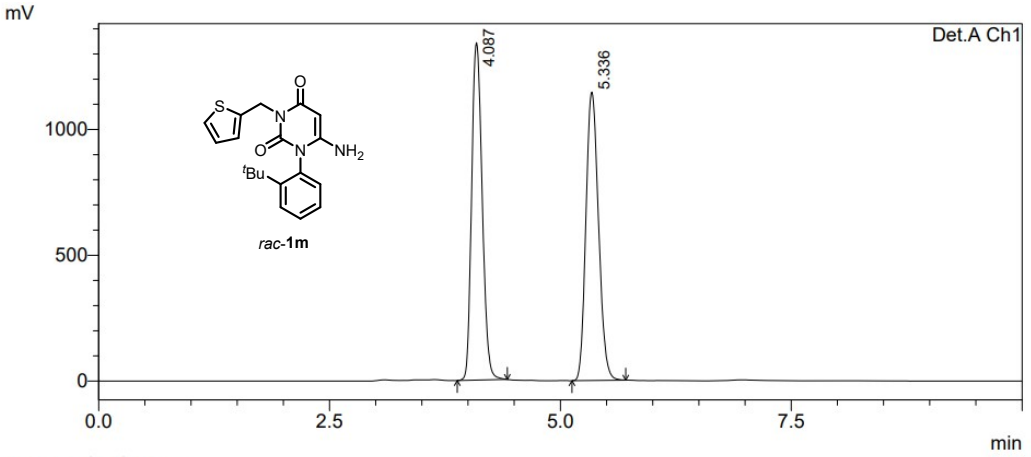
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.125	2588706	51945	50.108	59.571
2	12.997	2577531	35254	49.892	40.429
Total		5166237	87199	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.896	21415357	465622	98.498	98.799
2	13.088	326525	5662	1.502	1.201
Total		21741882	471284	100.000	100.000

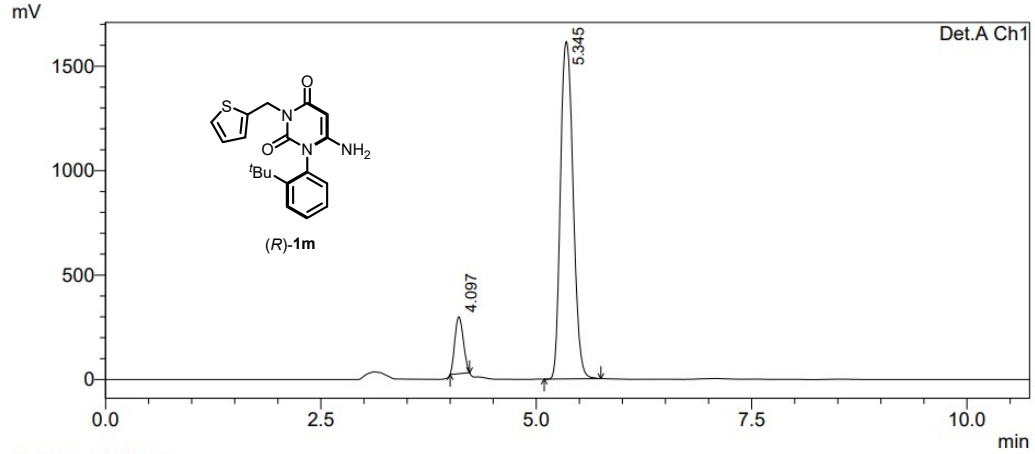


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.087	10655026	1341748	49.492	53.927
2	5.336	10873670	1146355	50.508	46.073
Total		21528696	2488104	100.000	100.000

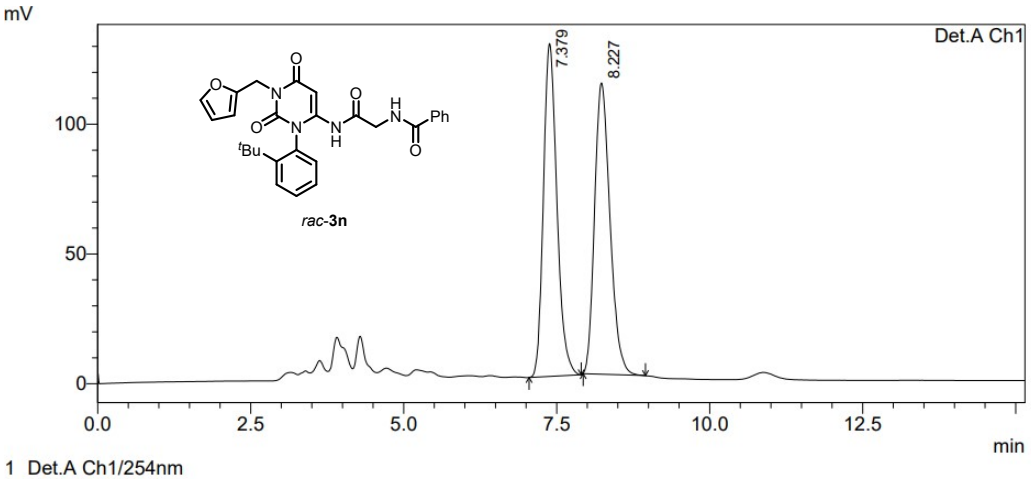


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.097	1855978	273040	10.102	14.452
2	5.345	16515772	1616260	89.898	85.548
Total		18371750	1889299	100.000	100.000

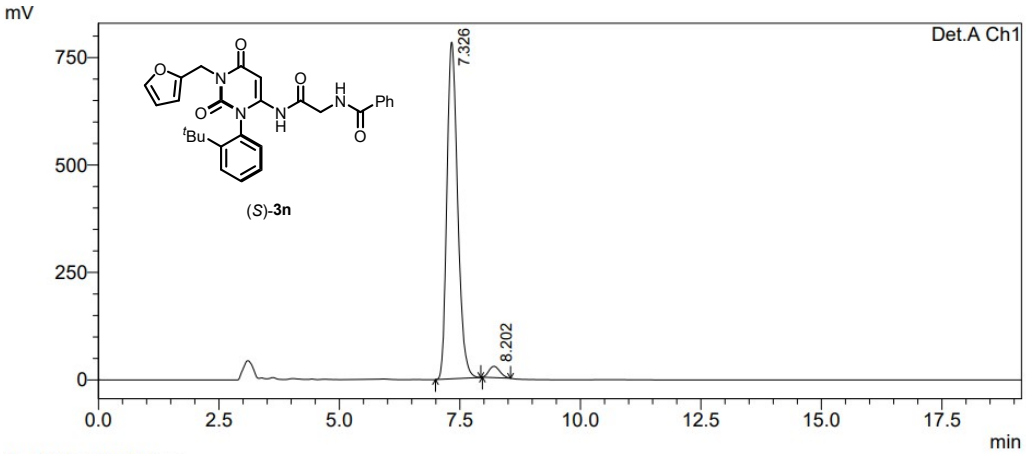


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.379	1961919	128056	49.922	53.306
2	8.227	1968078	112172	50.078	46.694
Total		3929998	240228	100.000	100.000

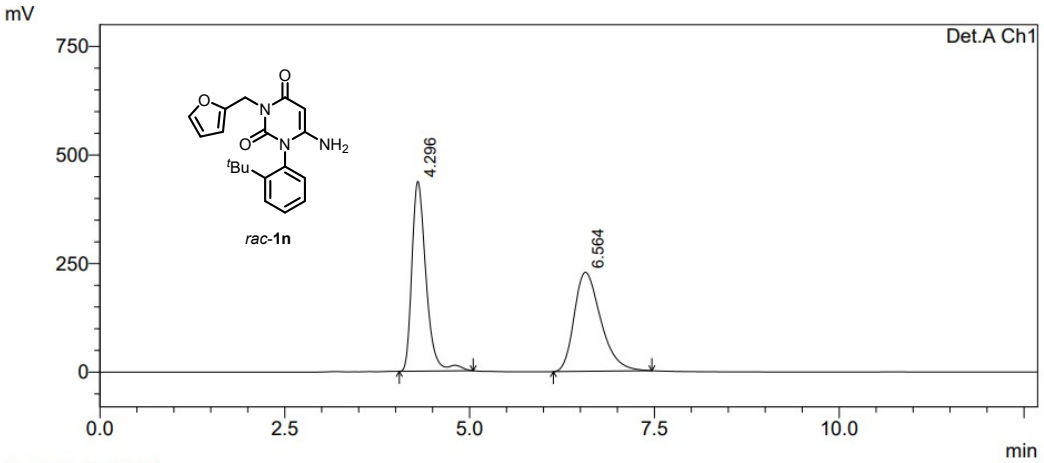


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.326	12122132	783487	96.630	96.726
2	8.202	422793	26519	3.370	3.274
Total		12544925	810006	100.000	100.000

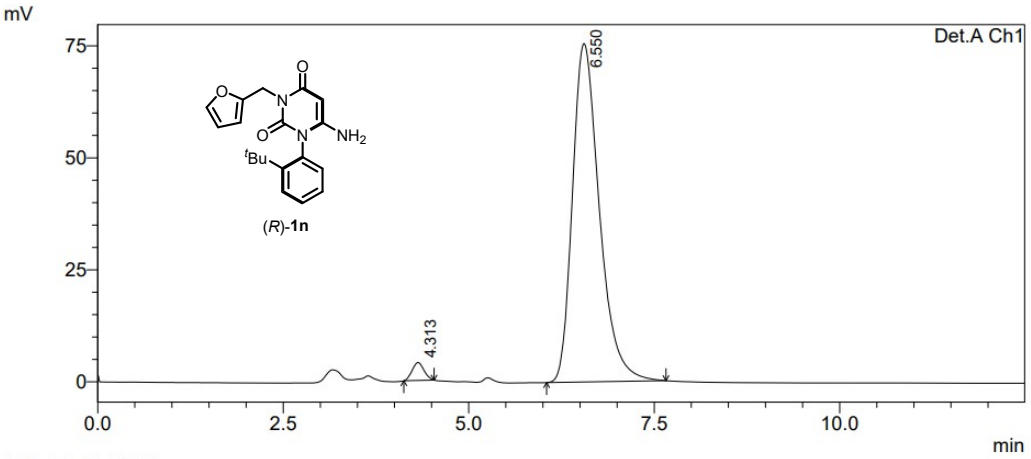


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.296	5831009	437184	50.580	65.743
2	6.564	5697187	227800	49.420	34.257
Total		11528195	664984	100.000	100.000

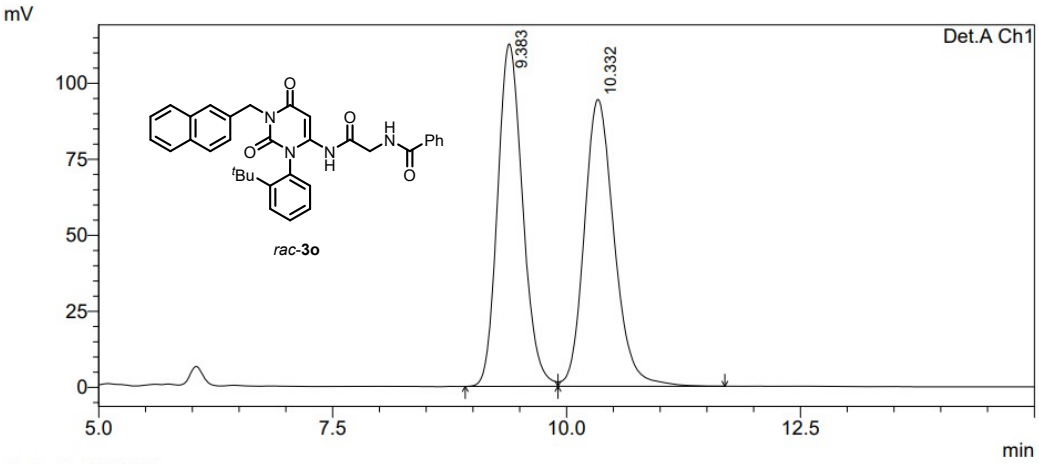


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.313	44504	4008	2.285	5.039
2	6.550	1903446	75537	97.715	94.961
Total		1947950	79545	100.000	100.000

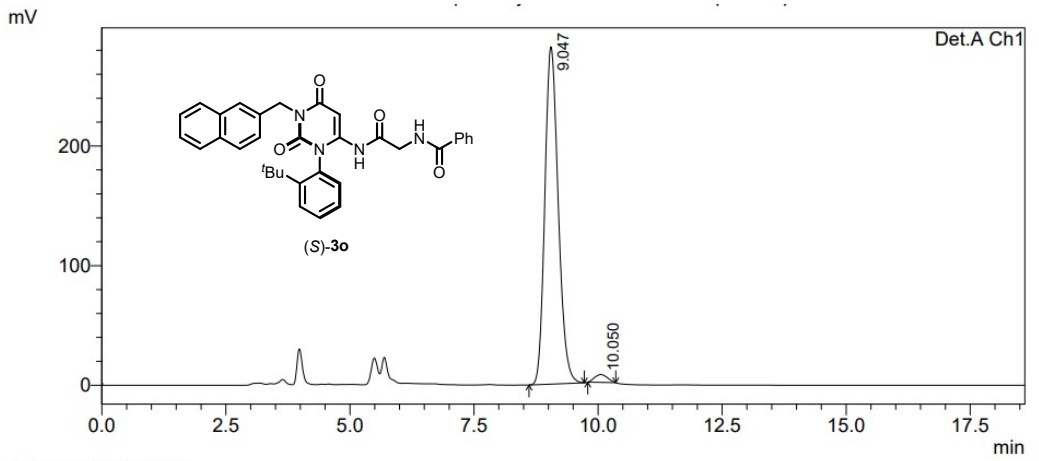


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.383	2093952	112599	49.975	54.415
2	10.332	2096058	94326	50.025	45.585
Total		4190009	206925	100.000	100.000

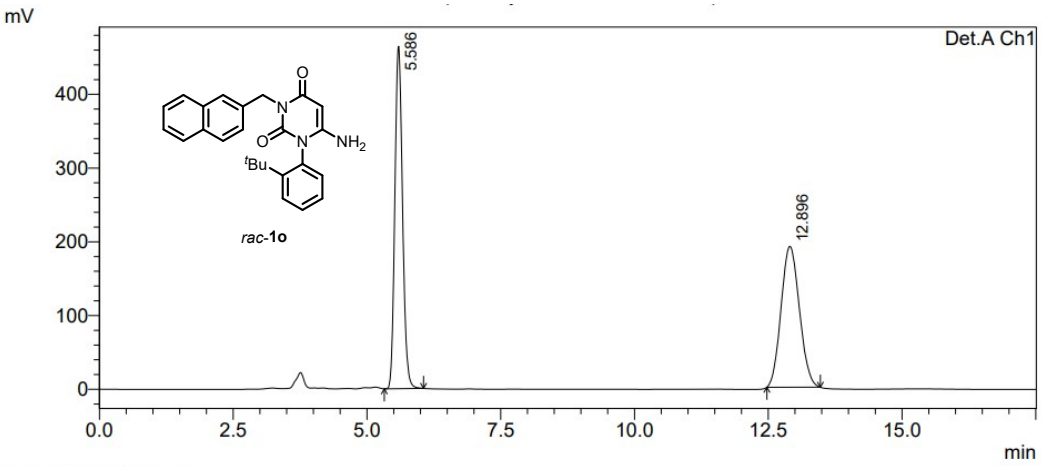


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.047	5296793	281748	97.793	97.722
2	10.050	119540	6567	2.207	2.278
Total		5416332	288315	100.000	100.000

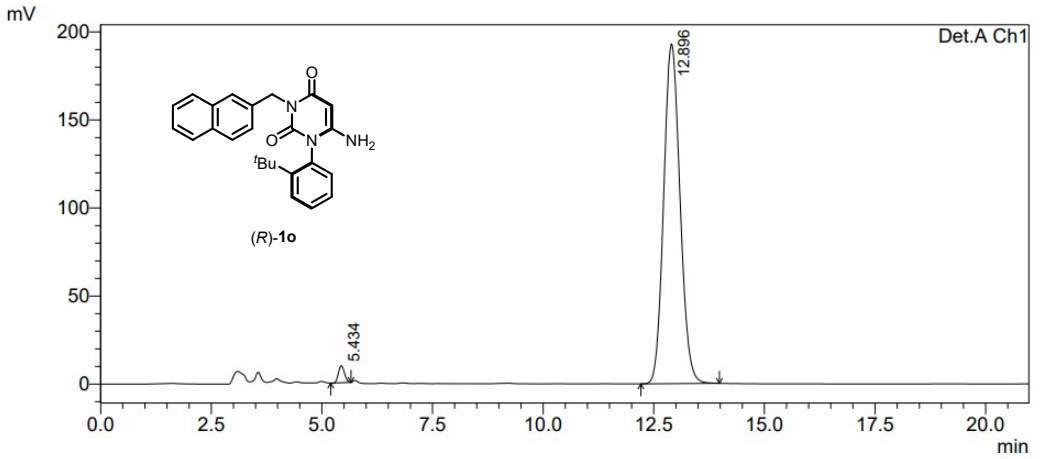


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.586	4631295	463311	50.507	70.858
2	12.896	4538373	190547	49.493	29.142
Total		9169667	653858	100.000	100.000

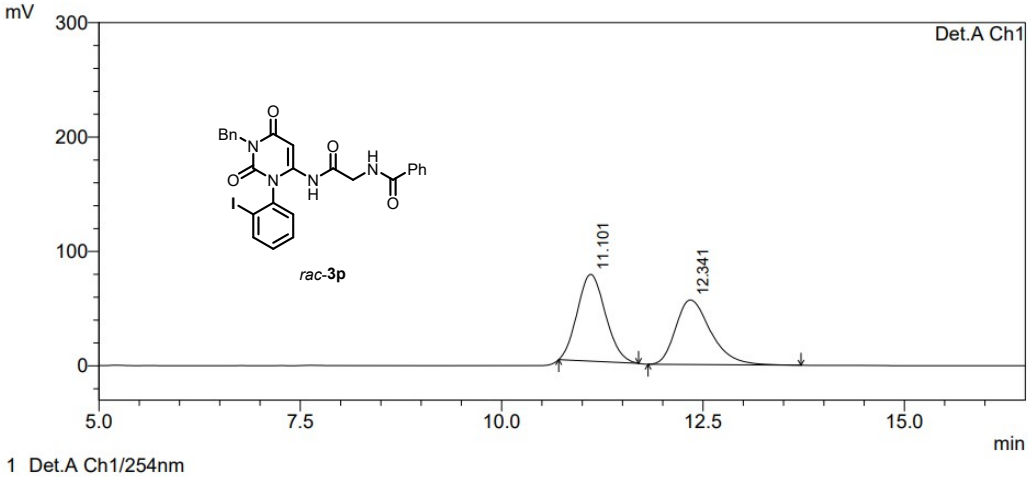


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.434	91753	9679	1.819	4.778
2	12.896	4953434	192921	98.181	95.222
Total		5045187	202600	100.000	100.000

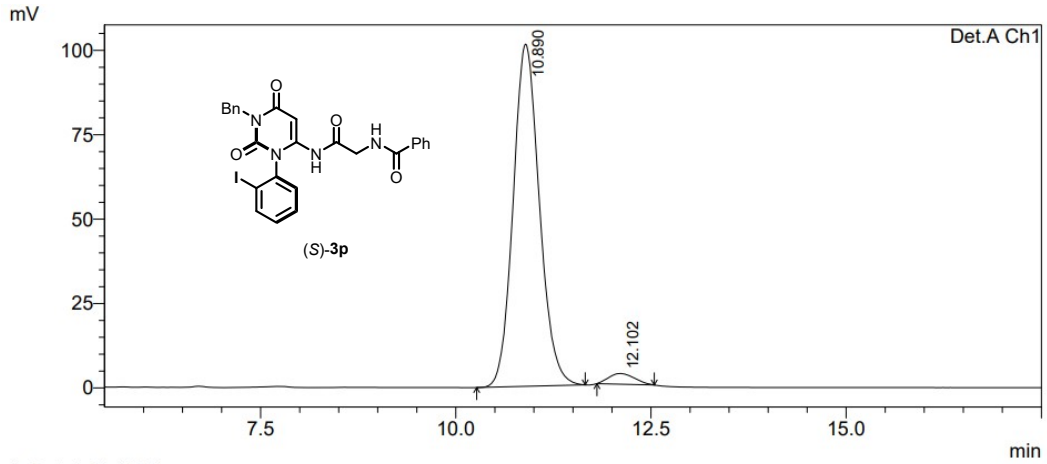


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.101	1845326	75800	51.854	57.283
2	12.341	1713347	56527	48.146	42.717
Total		3558673	132327	100.000	100.000

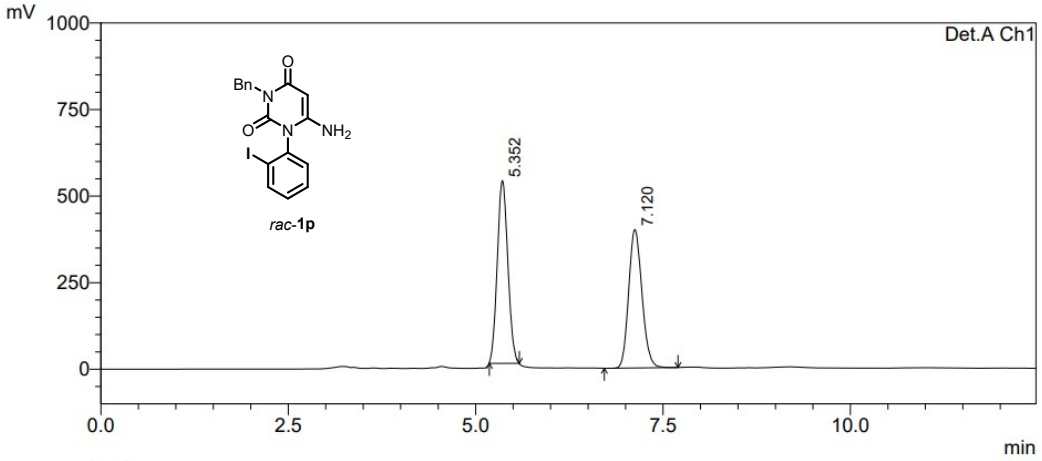


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.890	2371288	101270	97.013	96.958
2	12.102	73014	3177	2.987	3.042
Total		2444301	104447	100.000	100.000



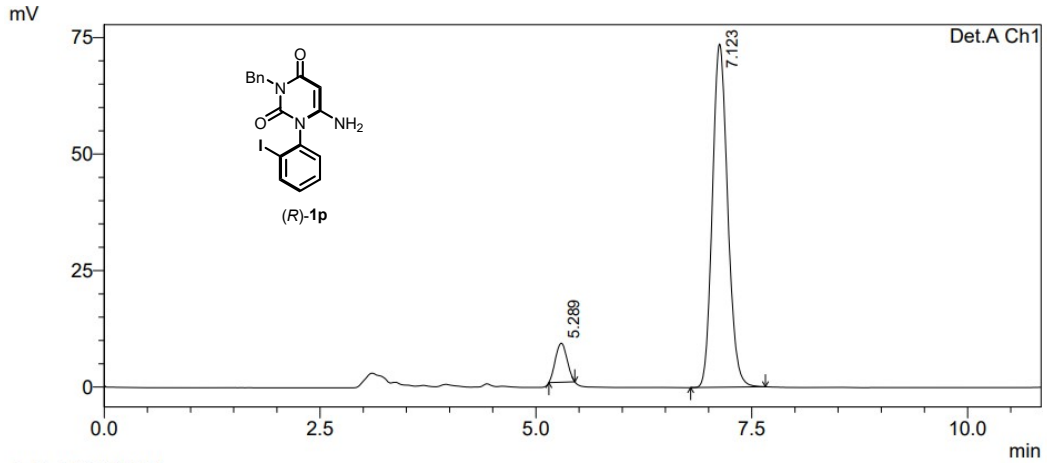
rac-**1p**

1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.352	5169189	524988	51.183	56.822
2	7.120	4930234	398922	48.817	43.178
Total		10099422	923910	100.000	100.000



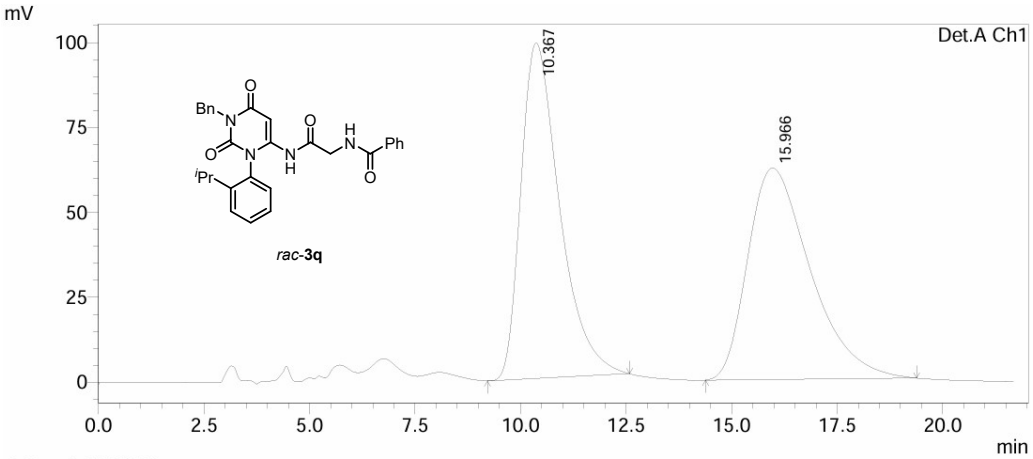
(*R*)-**1p**

1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.289	77691	8403	7.895	10.236
2	7.123	906356	73694	92.105	89.764
Total		984047	82098	100.000	100.000

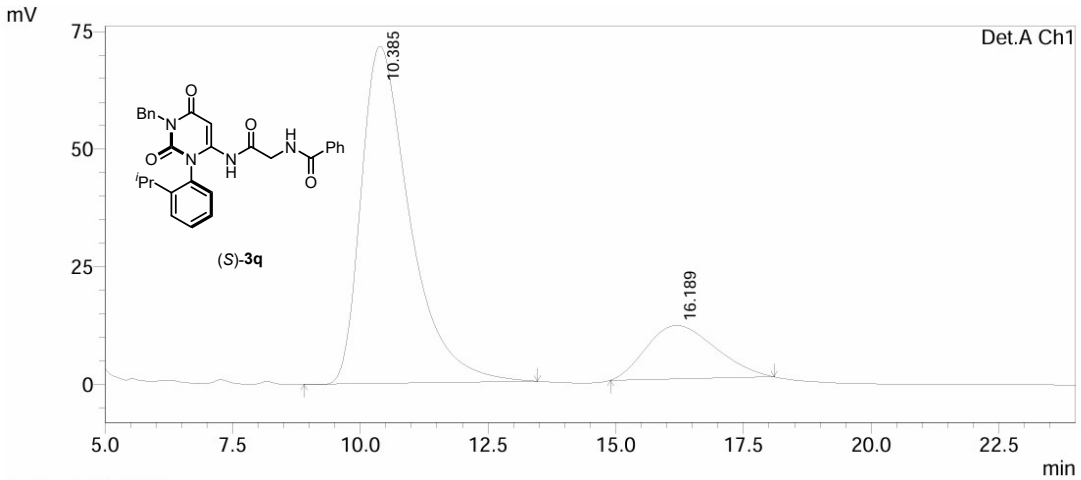


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.367	6293080	98715	49.512	61.334
2	15.966	6417259	62232	50.488	38.666
Total		12710340	160947	100.000	100.000

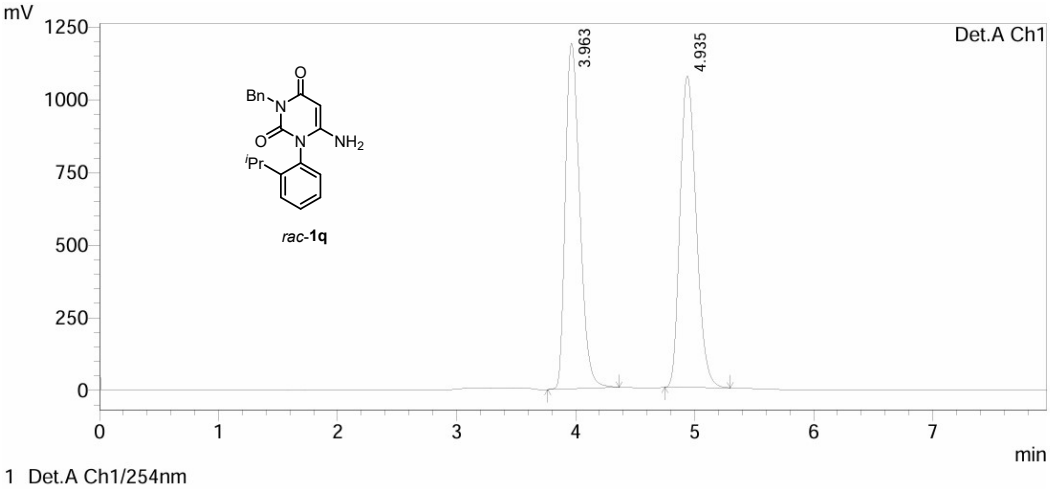


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.385	4747956	71596	81.688	86.330
2	16.189	1064335	11337	18.312	13.670
Total		5812291	82934	100.000	100.000

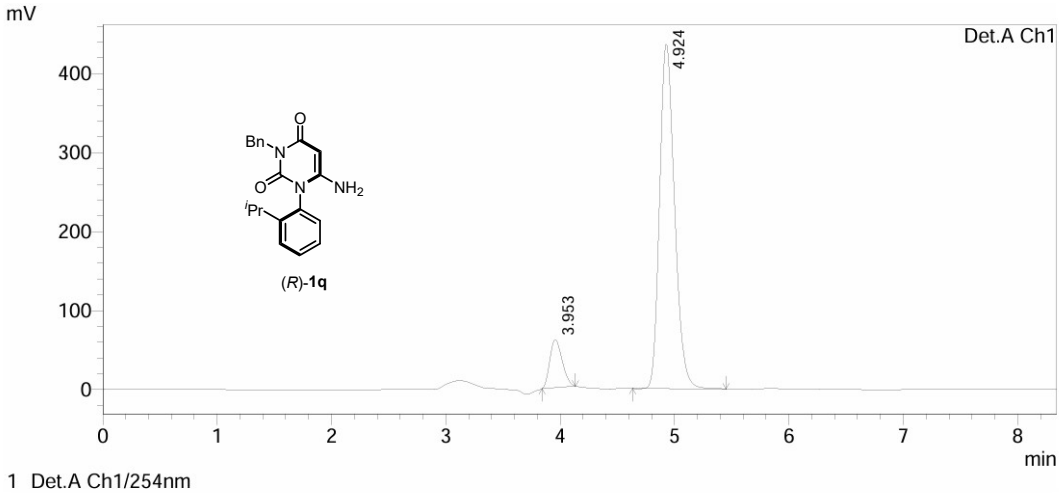


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.963	9987732	1184872	49.607	52.656
2	4.935	10145895	1065357	50.393	47.344
Total		20133627	2250229	100.000	100.000

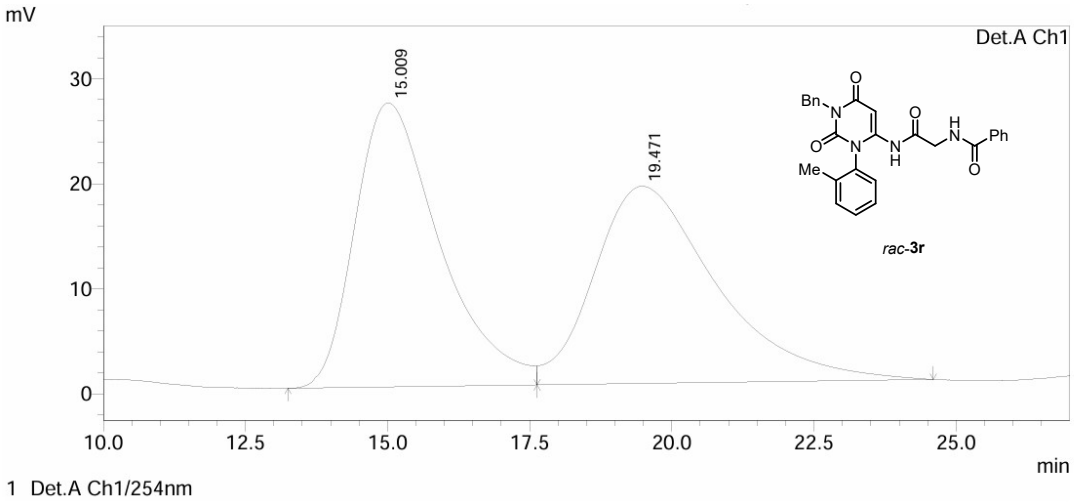


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

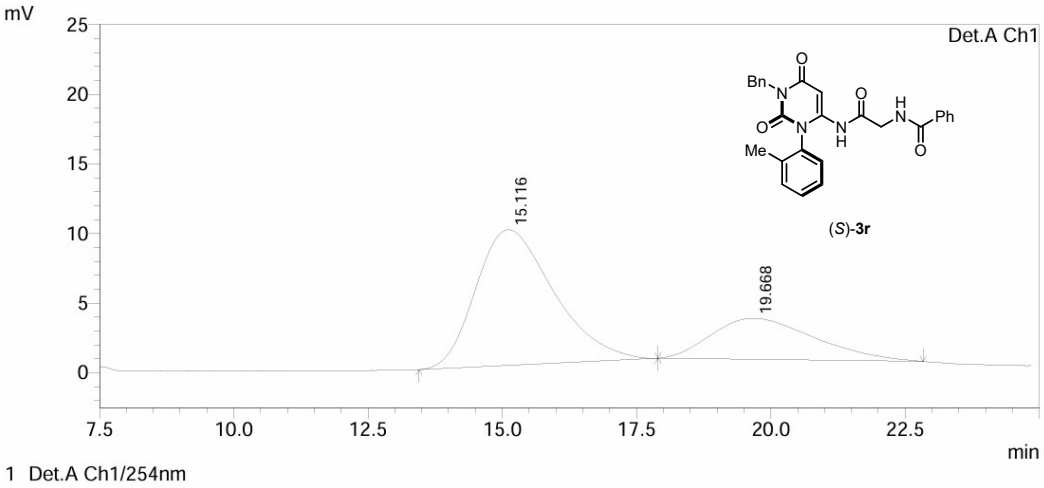
Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.953	456349	60765	10.298	12.244
2	4.924	3975234	435529	89.702	87.756
Total		4431583	496294	100.000	100.000



PeakTable

Detector A Ch1 254nm

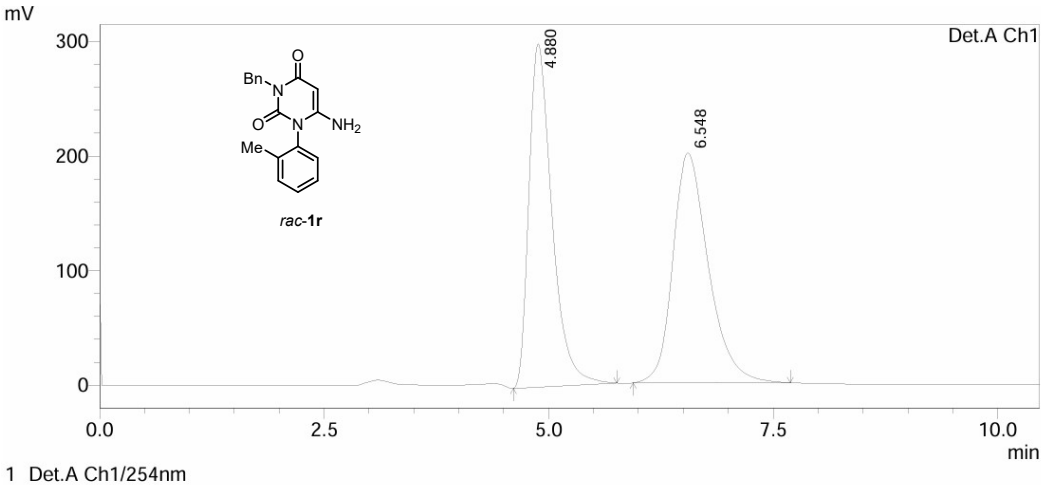
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.009	2799431	27029	49.903	59.028
2	19.471	2810262	18761	50.097	40.972
Total		5609693	45790	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.116	980299	9736	71.435	76.824
2	19.668	391996	2937	28.565	23.176
Total		1372294	12673	100.000	100.000

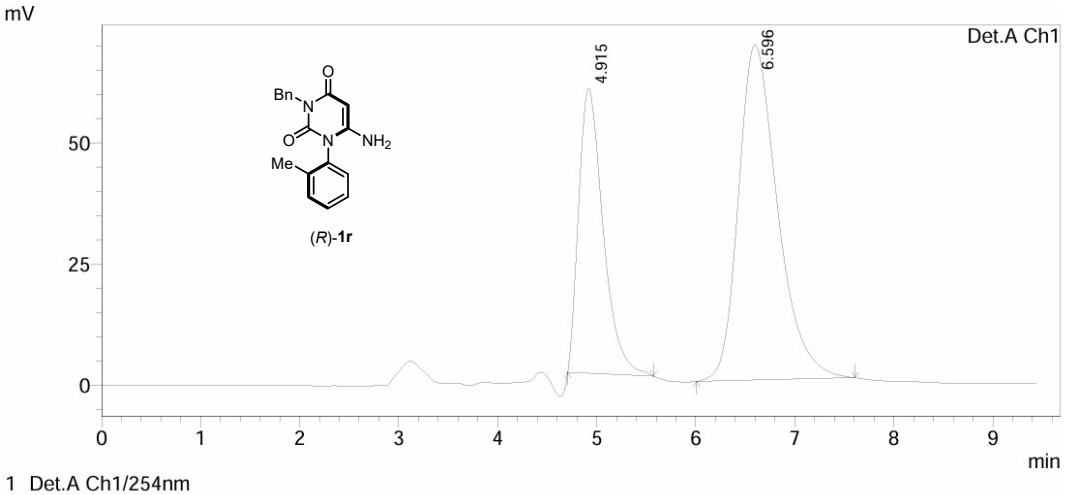


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.880	5348319	299372	49.232	59.917
2	6.548	5515251	200270	50.768	40.083
Total		10863570	499641	100.000	100.000

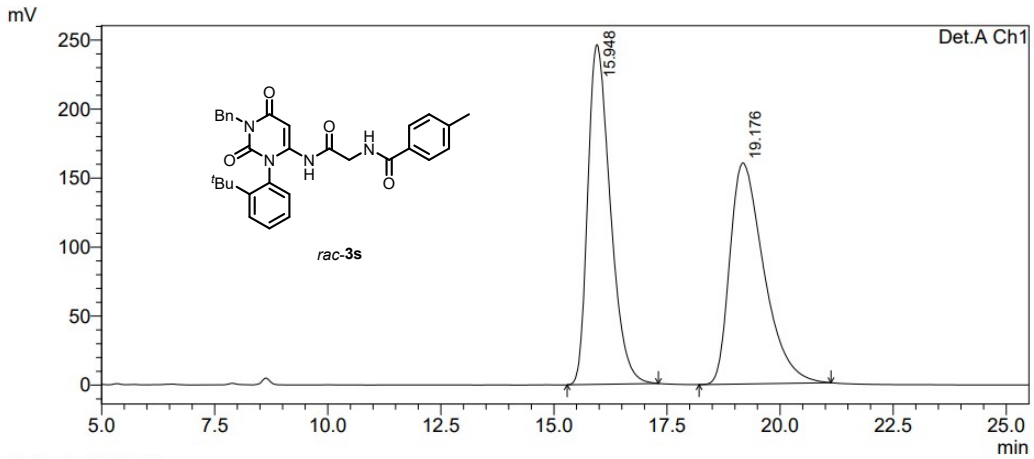


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

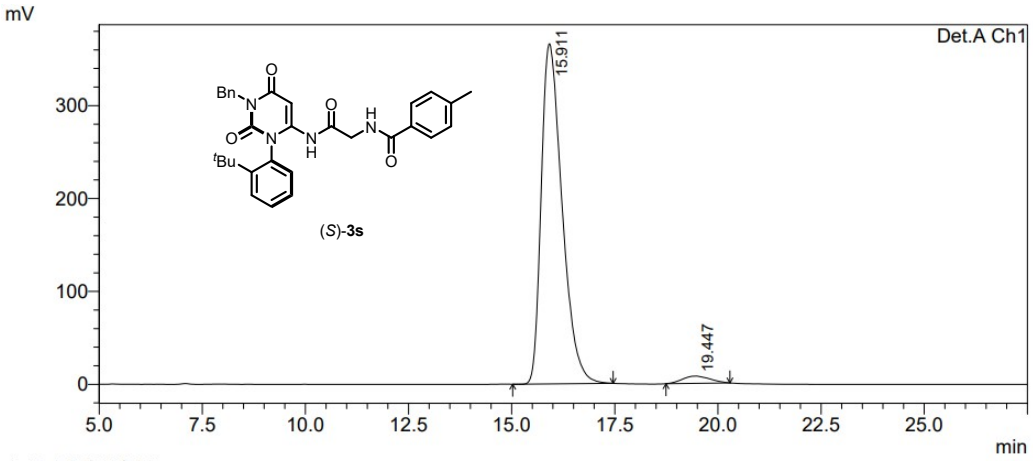
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.915	1006168	58743	34.617	45.944
2	6.596	1900373	69114	65.383	54.056
Total		2906541	127858	100.000	100.000



PeakTable

Detector A Ch1 254nm

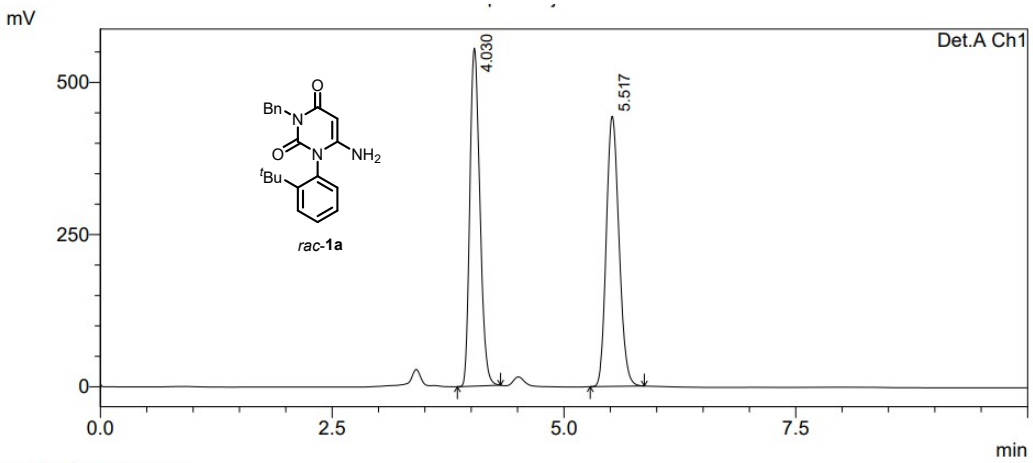
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.948	8518565	246116	50.408	60.583
2	19.176	8380802	160130	49.592	39.417
Total		16899367	406245	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.911	12843256	366051	97.282	97.911
2	19.447	358835	7809	2.718	2.089
Total		13202090	373860	100.000	100.000

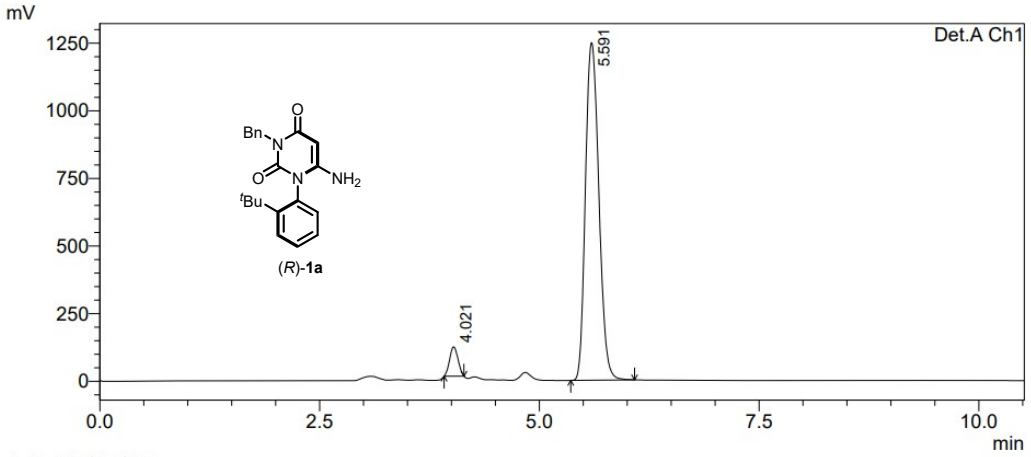


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.030	4189222	551620	49.702	55.626
2	5.517	4239401	440036	50.298	44.374
Total		8428623	991656	100.000	100.000

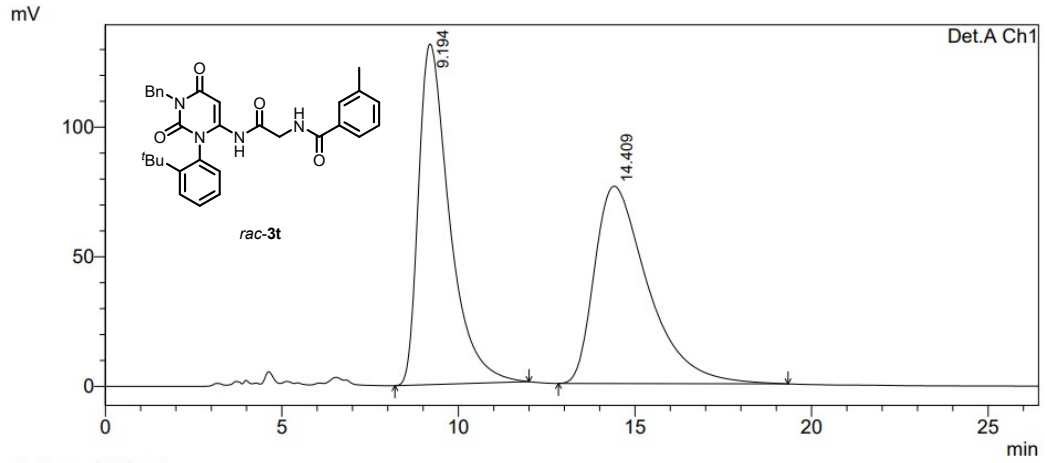


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.021	711751	108449	5.101	7.993
2	5.591	13240088	1248363	94.899	92.007
Total		13951838	1356812	100.000	100.000

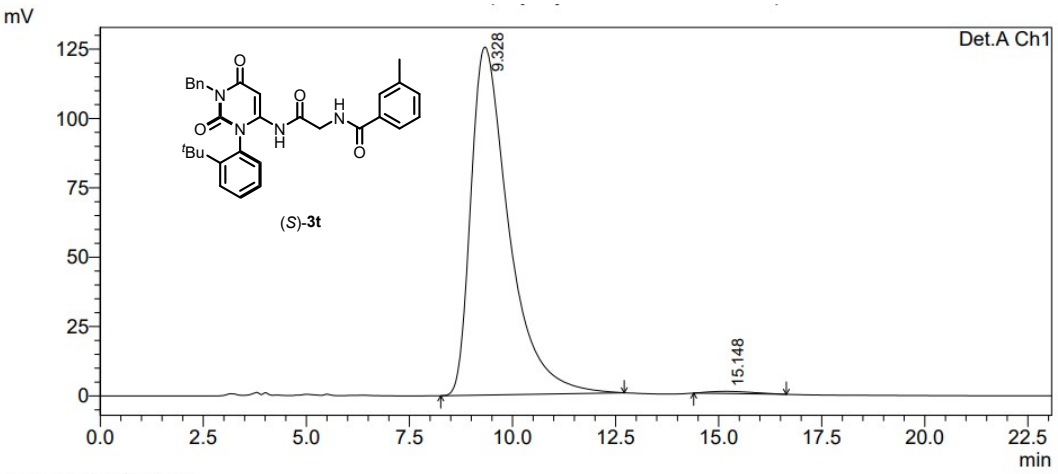


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.194	8027536	131405	49.974	63.340
2	14.409	8035878	76055	50.026	36.660
Total		16063414	207460	100.000	100.000

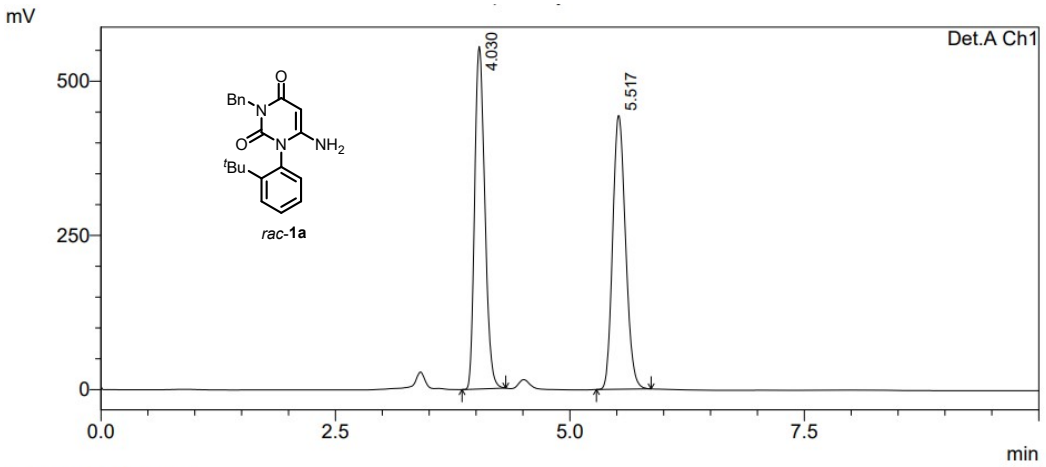


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.328	8047370	125456	99.269	99.394
2	15.148	59264	765	0.731	0.606
Total		8106634	126221	100.000	100.000

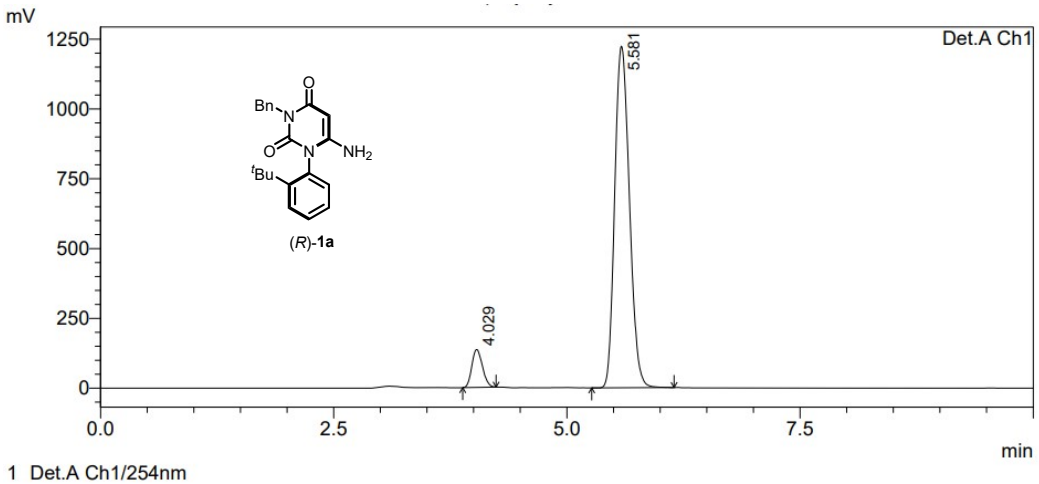


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.030	4189222	551620	49.702	55.626
2	5.517	4239401	440036	50.298	44.374
Total		8428623	991656	100.000	100.000

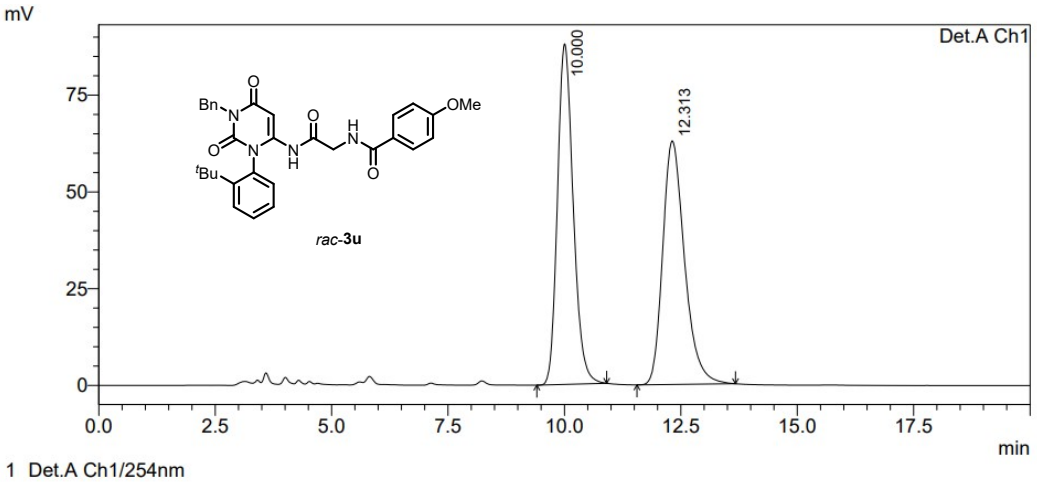


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.029	1072188	136065	7.406	10.006
2	5.581	13404162	1223763	92.594	89.994
Total		14476350	1359828	100.000	100.000

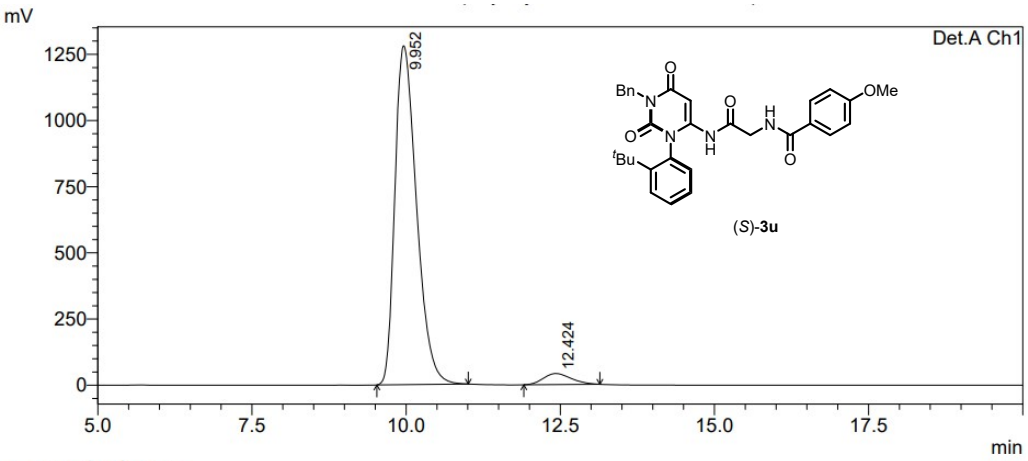


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.000	2072531	87982	50.292	58.371
2	12.313	2048452	62747	49.708	41.629
Total		4120983	150729	100.000	100.000

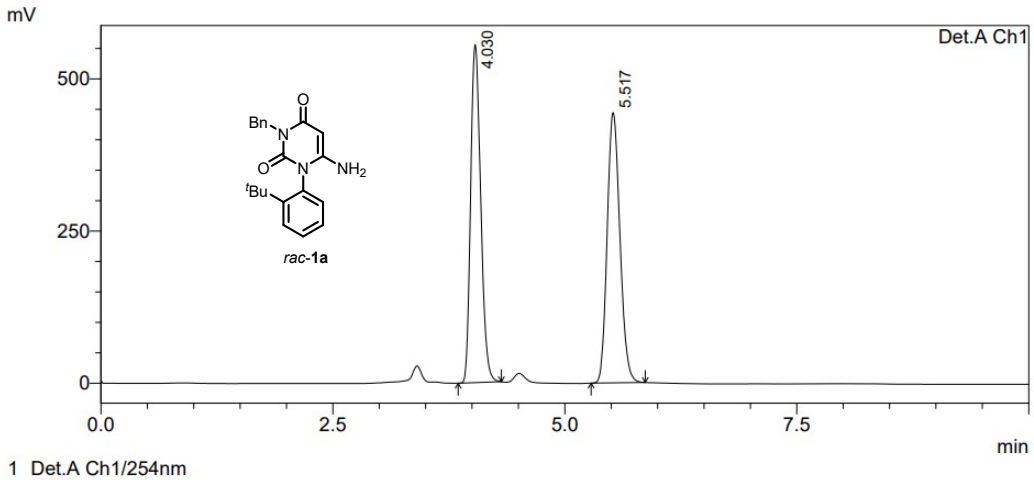


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.952	31217645	1278185	95.956	96.841
2	12.424	1315631	41694	4.044	3.159
Total		32533275	1319879	100.000	100.000

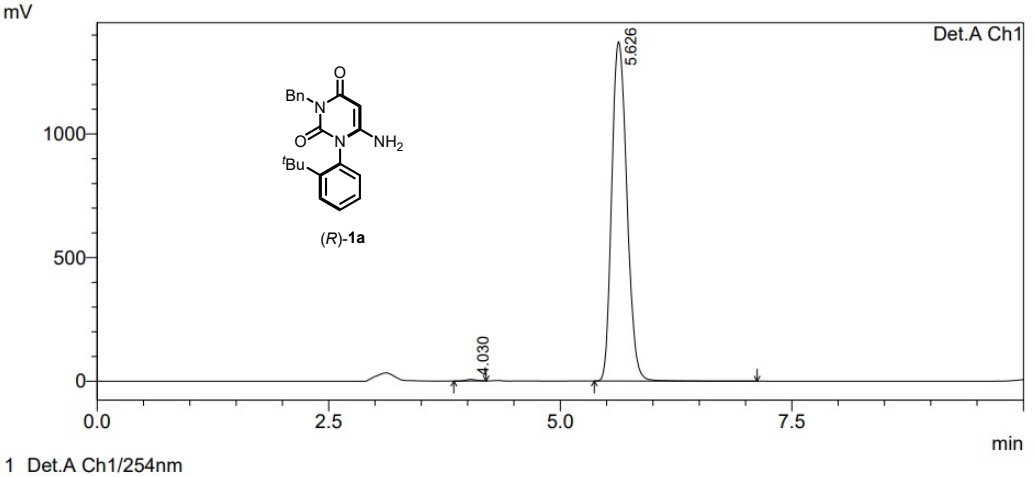


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.030	4189222	551620	49.702	55.626
2	5.517	4239401	440036	50.298	44.374
Total		8428623	991656	100.000	100.000

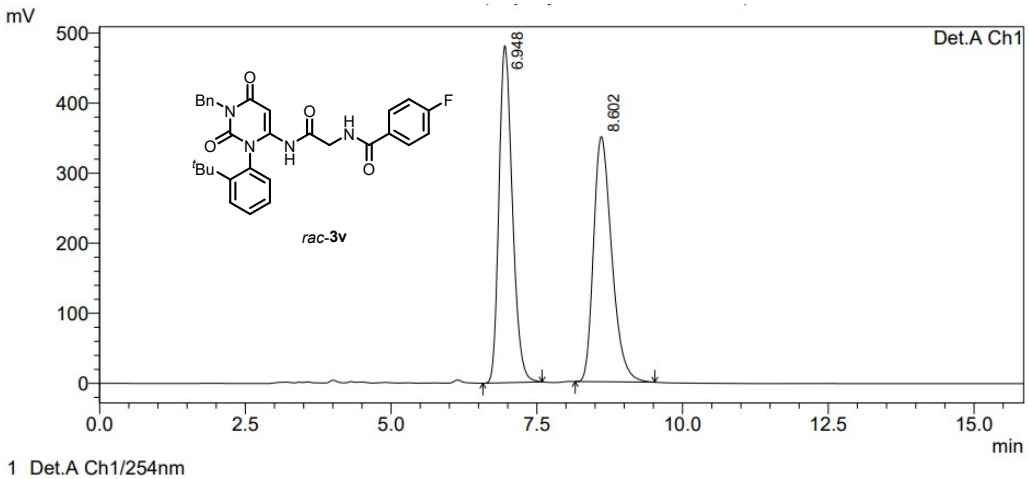


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

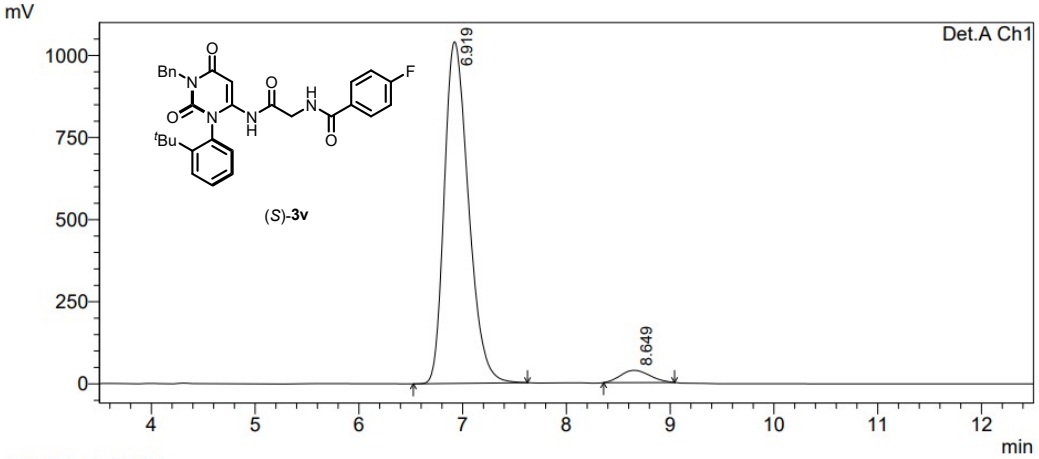
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.030	51406	6358	0.328	0.461
2	5.626	15612336	1372417	99.672	99.539
Total		15663742	1378776	100.000	100.000



PeakTable

Detector A Ch1 254nm

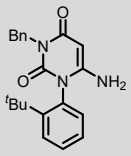
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.948	7700545	480720	50.305	57.884
2	8.602	7607126	349768	49.695	42.116
Total		15307671	830487	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.919	16857529	1040004	95.826	96.529
2	8.649	734266	37400	4.174	3.471
Total		17591796	1077404	100.000	100.000



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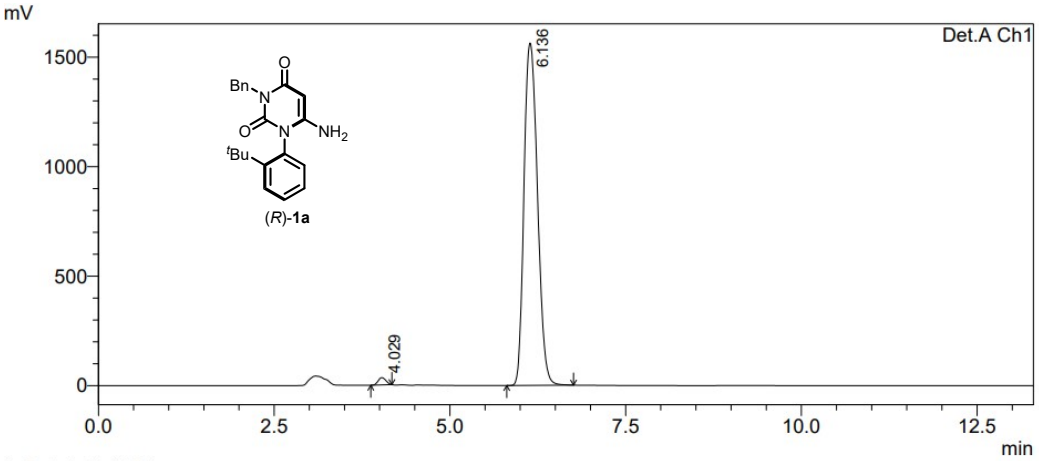
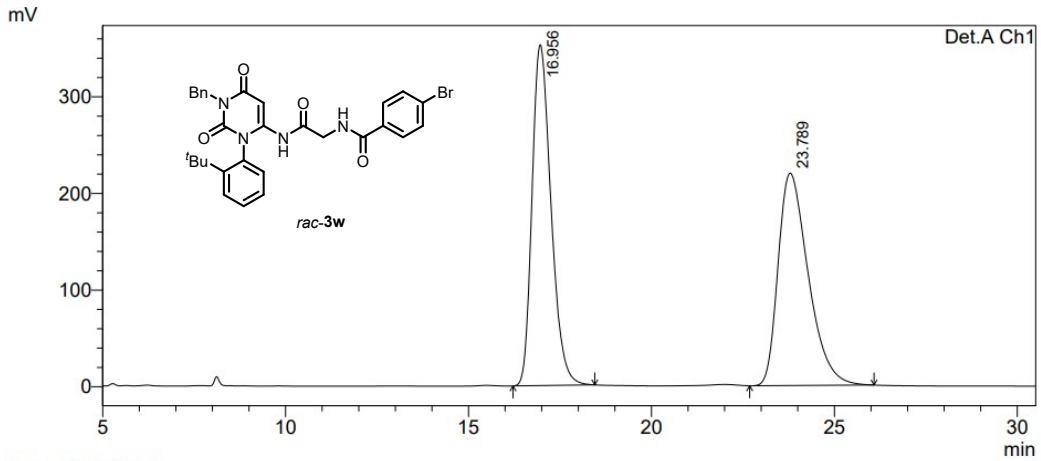


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.029	254531	33060	1.205	2.073
2	6.136	20859699	1561931	98.795	97.927
Total		21114230	1594991	100.000	100.000

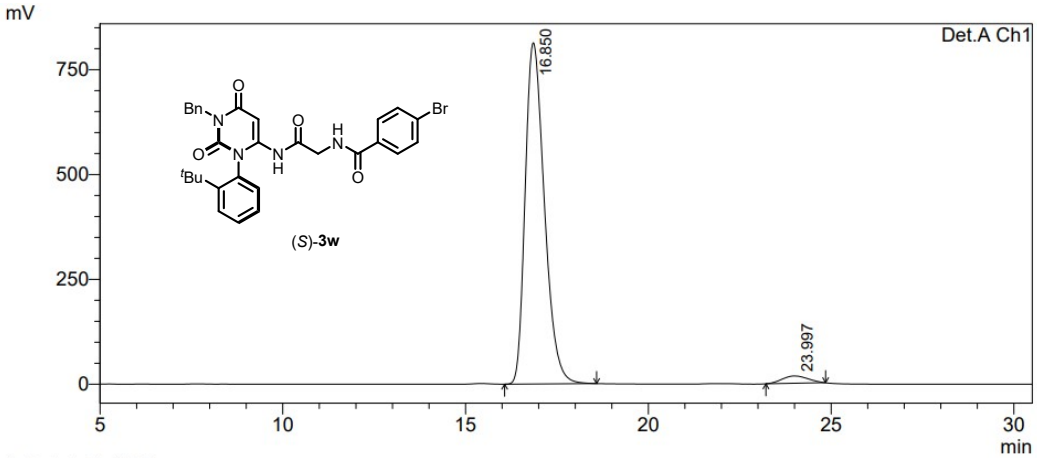


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.956	12677645	352158	50.202	61.604
2	23.789	12575556	219493	49.798	38.396
Total		25253201	571651	100.000	100.000

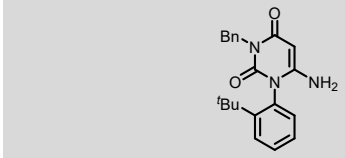


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.850	29665925	811044	97.208	97.898
2	23.997	852217	17417	2.792	2.102
Total		30518141	828461	100.000	100.000



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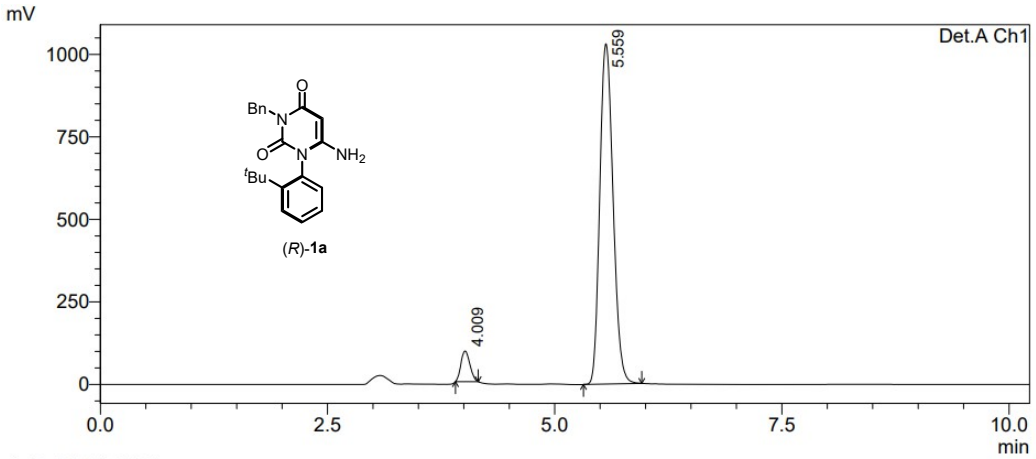
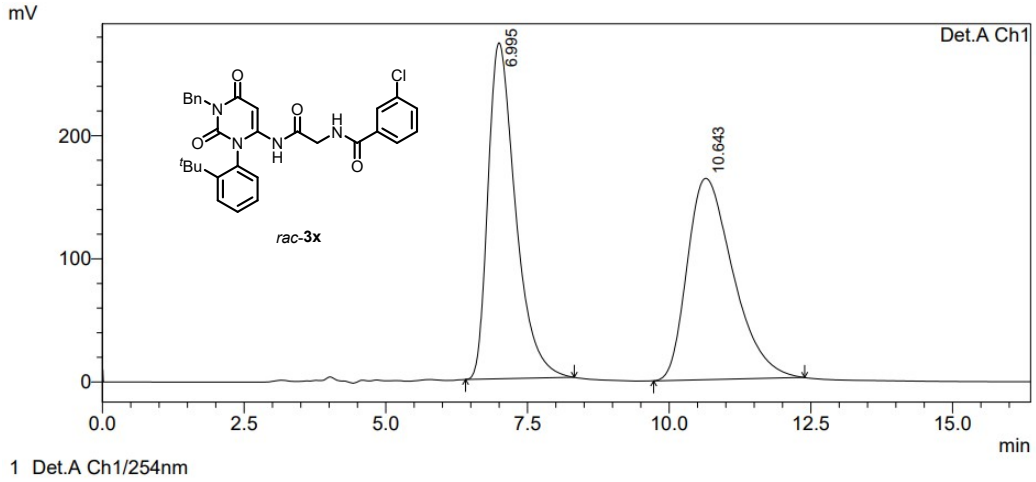


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.009	638896	93004	5.749	8.274
2	5.559	10474716	1031037	94.251	91.726
Total		11113612	1124042	100.000	100.000

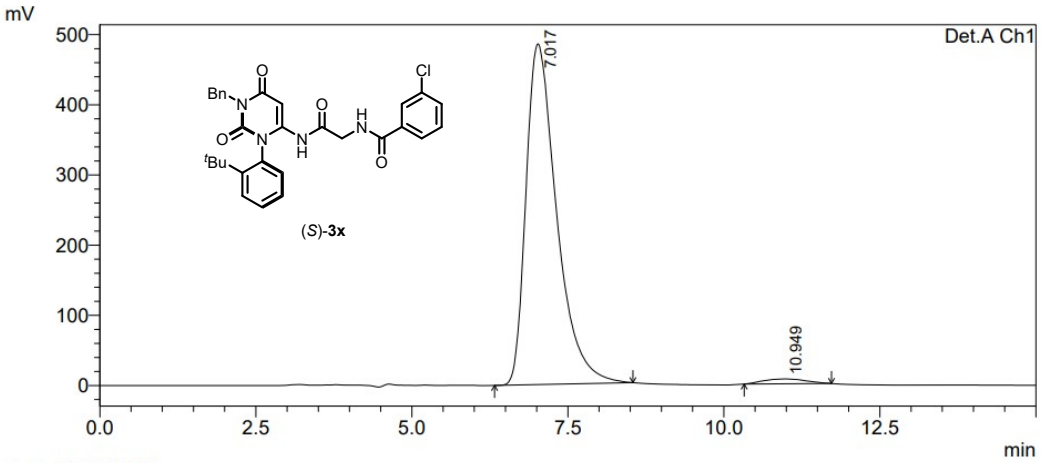


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.995	9219716	271993	50.050	62.452
2	10.643	9201286	163531	49.950	37.548
Total		18421001	435524	100.000	100.000

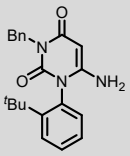


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.017	16577302	485424	98.036	98.543
2	10.949	332048	7178	1.964	1.457
Total		16909350	492602	100.000	100.000



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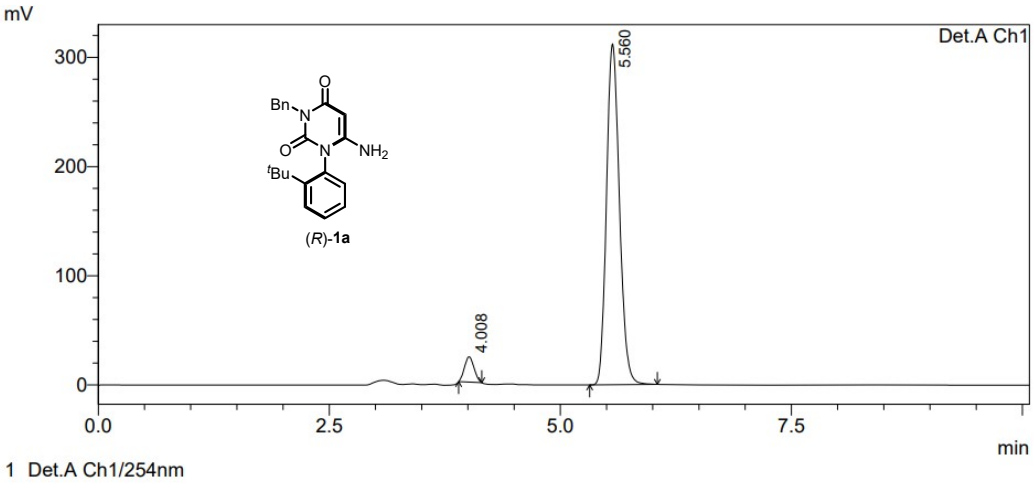
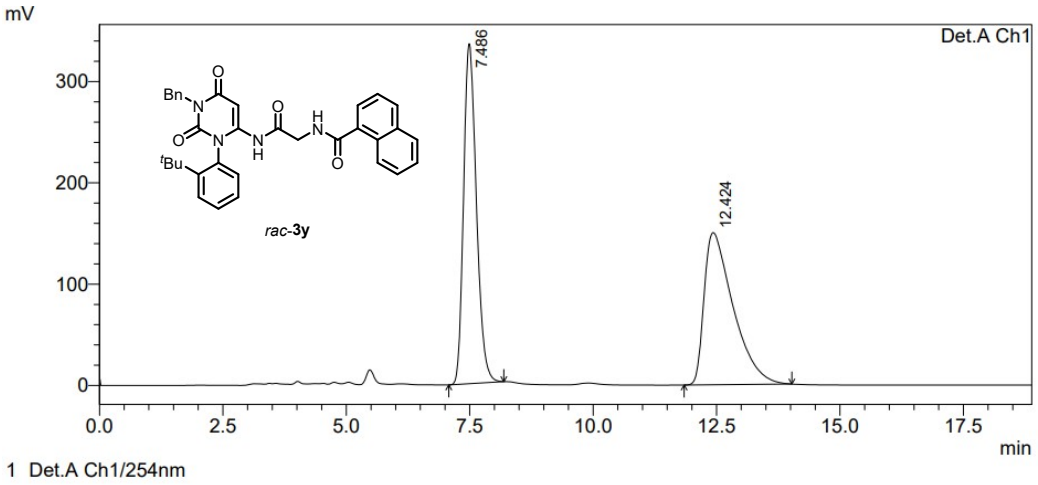


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.008	165195	23105	5.162	6.887
2	5.560	3035132	312363	94.838	93.113
Total		3200327	335468	100.000	100.000

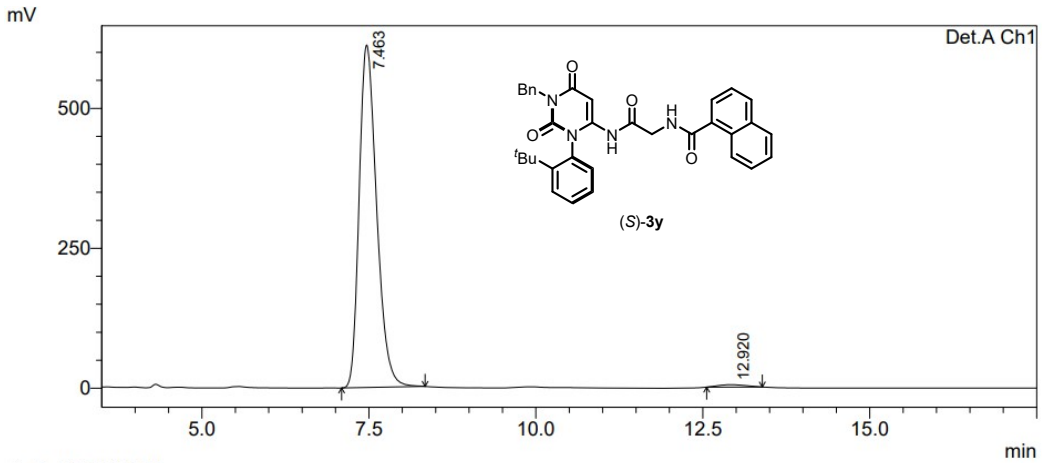


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.486	6059130	335464	49.700	69.100
2	12.424	6132180	150009	50.300	30.900
Total		12191310	485473	100.000	100.000

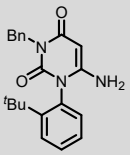


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.463	11127021	611270	98.924	99.315
2	12.920	121037	4213	1.076	0.685
Total		11248058	615483	100.000	100.000



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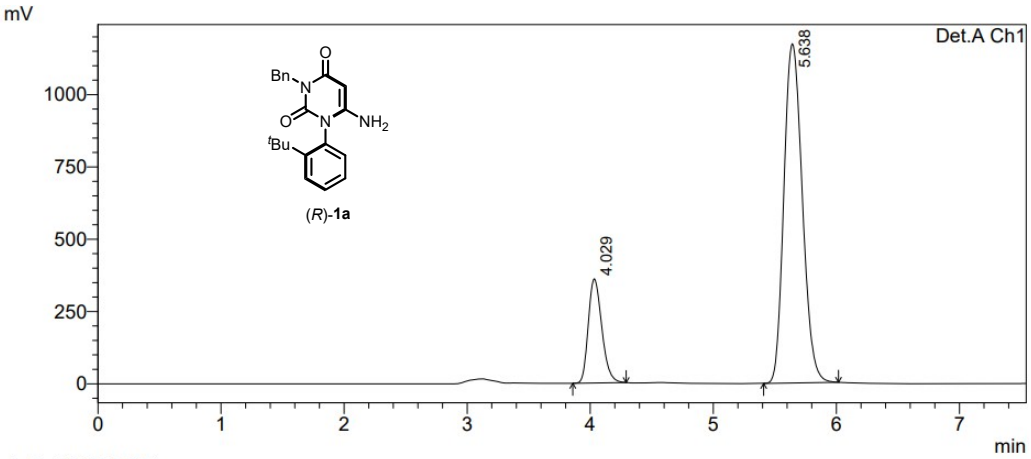

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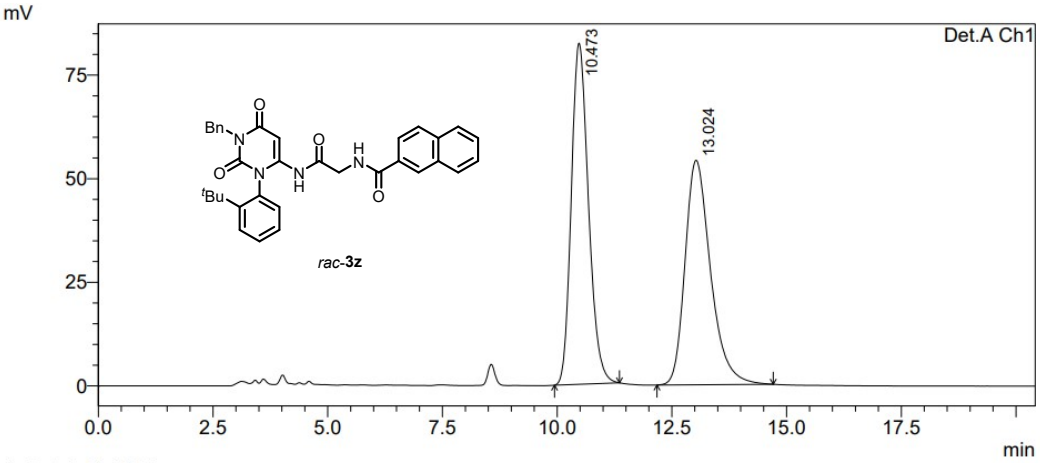
1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.029	2748065	360550	18.387	23.550
2	5.638	12197989	1170444	81.613	76.450
Total		14946054	1530994	100.000	100.000

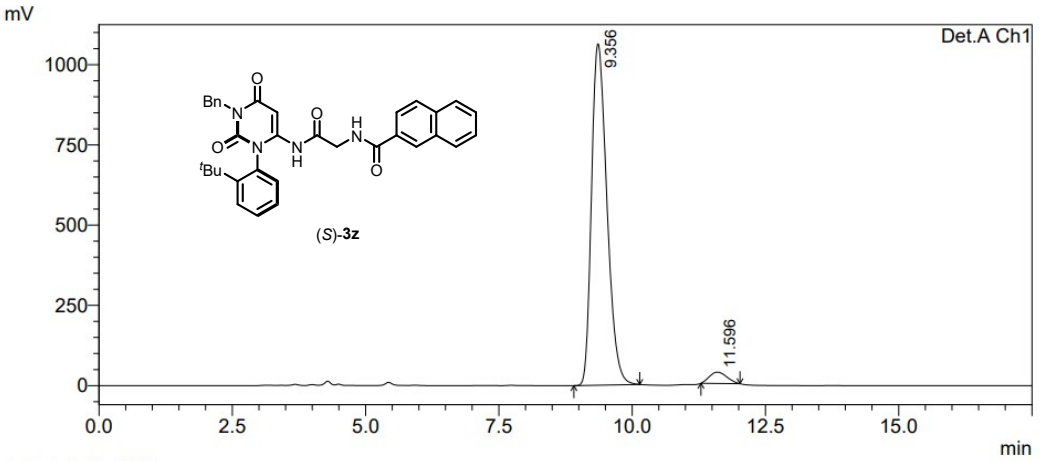


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.473	2145019	82278	50.603	60.308
2	13.024	2093861	54152	49.397	39.692
Total		4238880	136430	100.000	100.000

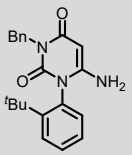


1 Det.A Ch1/254nm

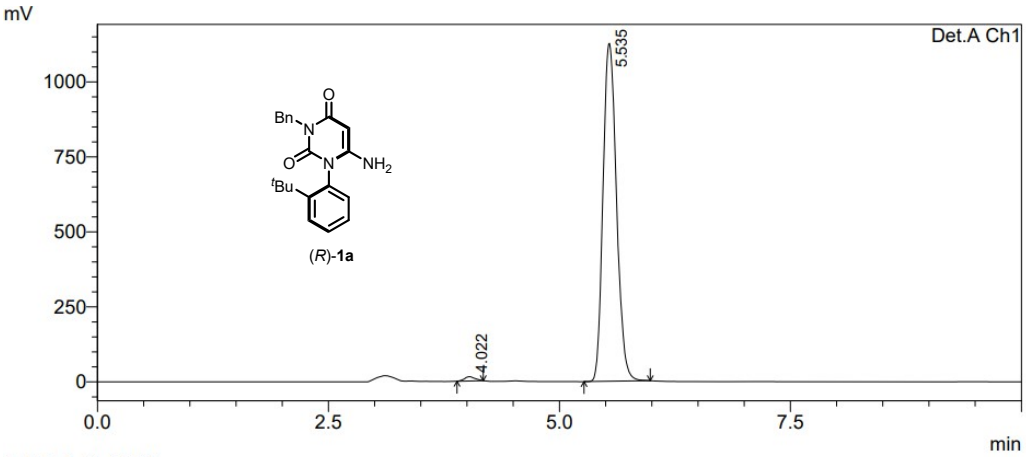
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.356	21395605	1062352	96.364	96.762
2	11.596	807347	35545	3.636	3.238
Total		22202951	1097898	100.000	100.000



rac-**1a**



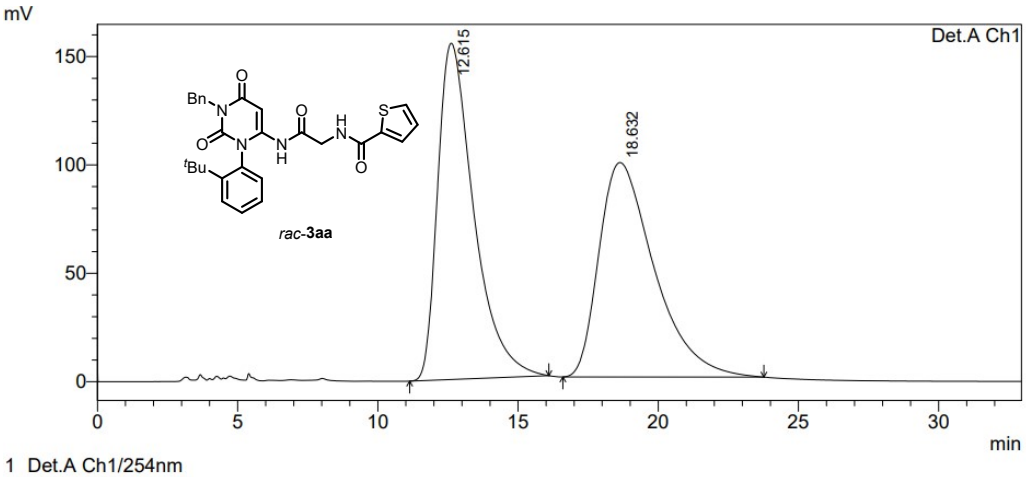
(*R*)-**1a**

1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

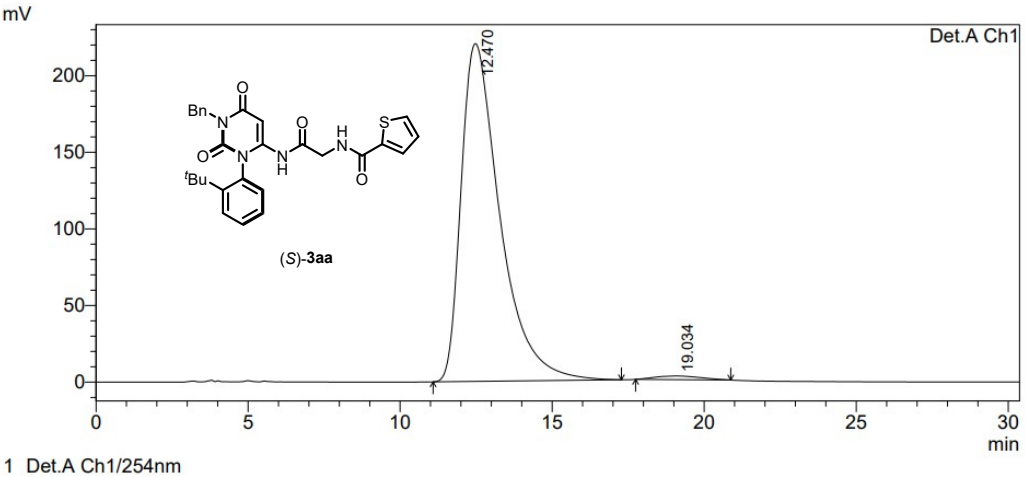
Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.022	113183	14147	0.980	1.240
2	5.535	11431523	1126759	99.020	98.760
Total		11544706	1140907	100.000	100.000



PeakTable

Detector A Ch1 254nm

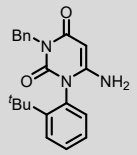
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.615	13871593	155129	50.545	61.080
2	18.632	13572237	98847	49.455	38.920
Total		27443830	253976	100.000	100.000



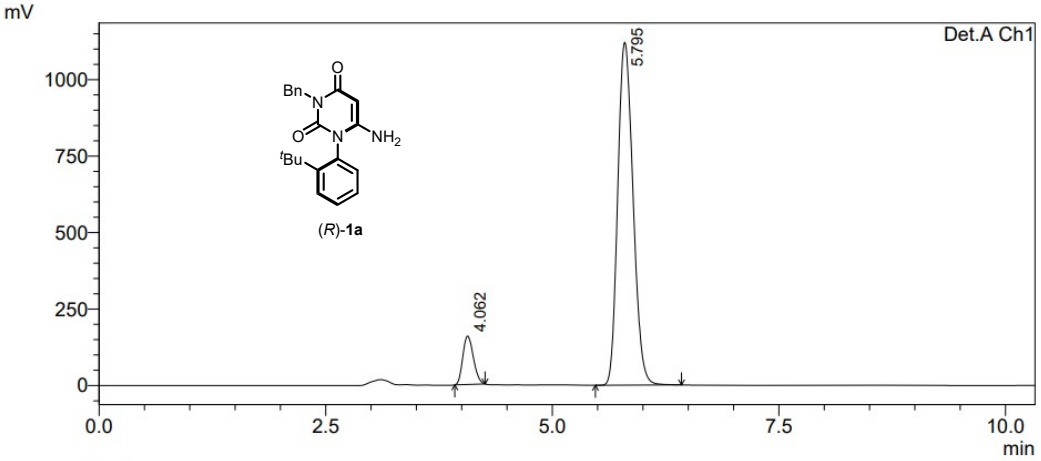
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.470	19583032	220515	98.748	98.936
2	19.034	248280	2371	1.252	1.064
Total		19831312	222886	100.000	100.000



rac-**1a**

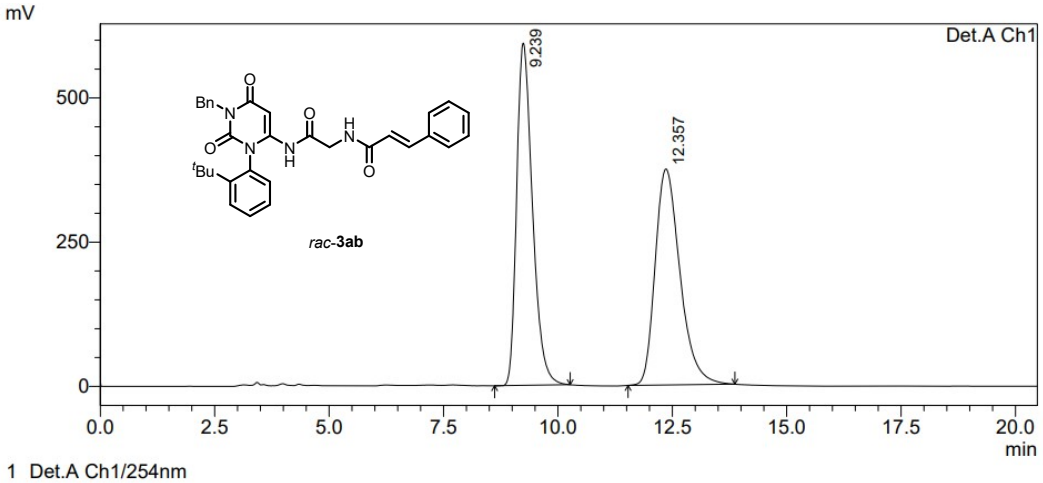


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.062	1286136	158578	8.895	12.391
2	5.795	13172933	1121245	91.105	87.609
Total		14459069	1279823	100.000	100.000

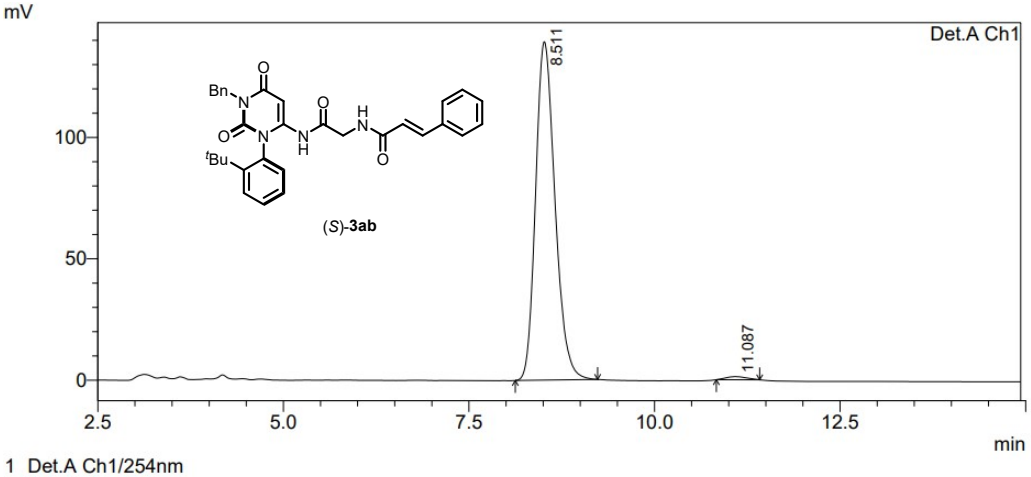


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.239	14264201	593104	50.281	61.331
2	12.357	14104818	373958	49.719	38.669
Total		28369019	967062	100.000	100.000

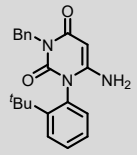


1 Det.A Ch1/254nm

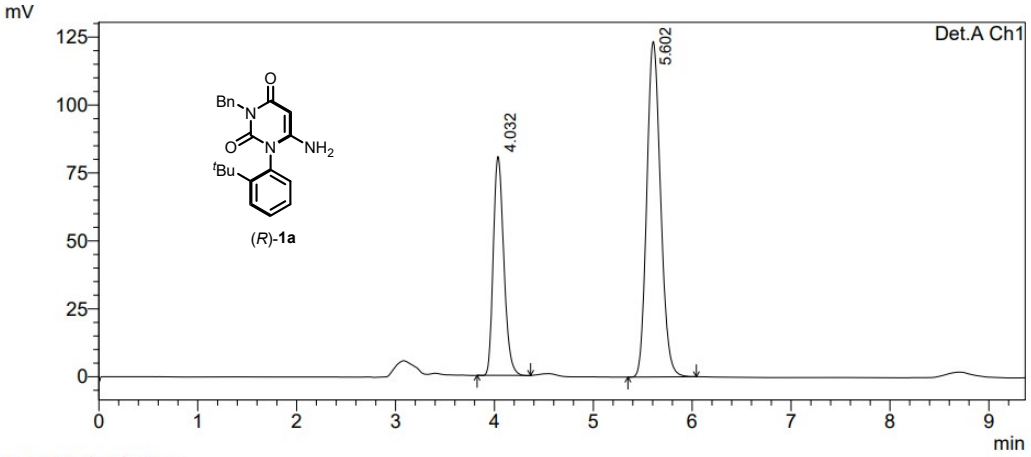
PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.511	2531688	139295	99.000	99.086
2	11.087	25585	1284	1.000	0.914
Total		2557274	140579	100.000	100.000



rac-**1a**

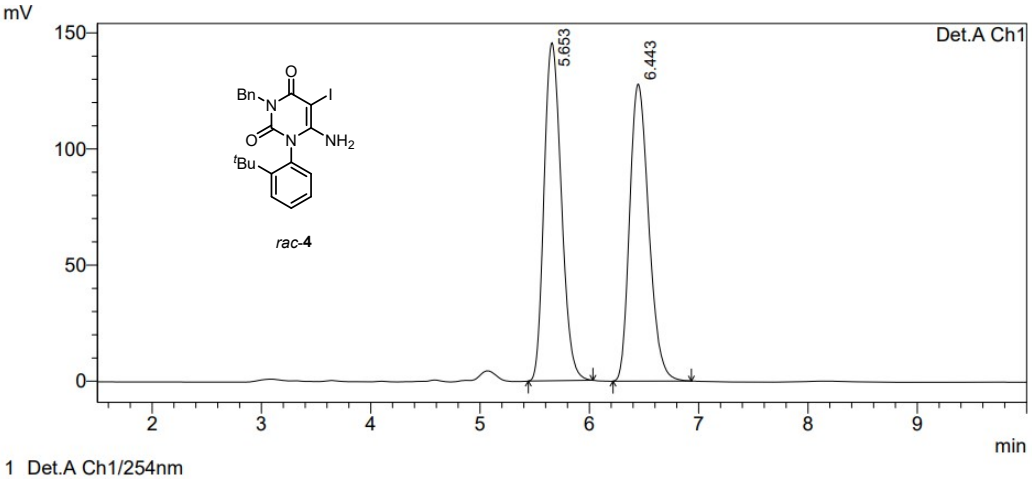


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.032	594334	80543	33.193	39.463
2	5.602	1196231	123557	66.807	60.537
Total		1790564	204100	100.000	100.000

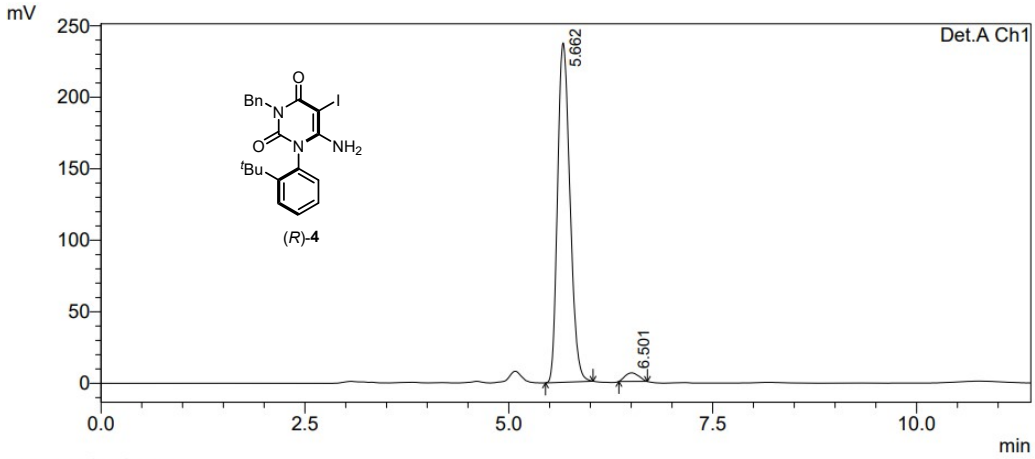


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.653	1596542	145669	50.678	53.255
2	6.443	1553819	127865	49.322	46.745
Total		3150362	273534	100.000	100.000

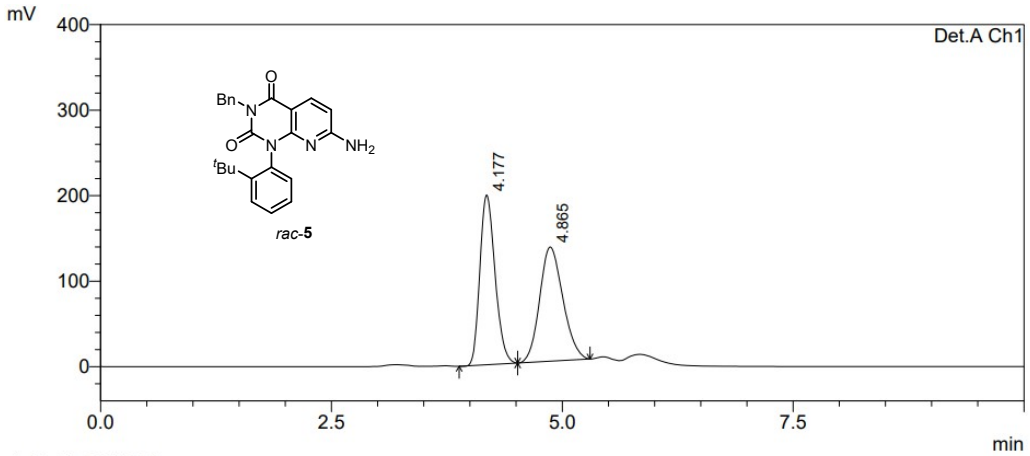


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.662	2508072	236709	97.252	97.526
2	6.501	70874	6004	2.748	2.474
Total		2578946	242713	100.000	100.000

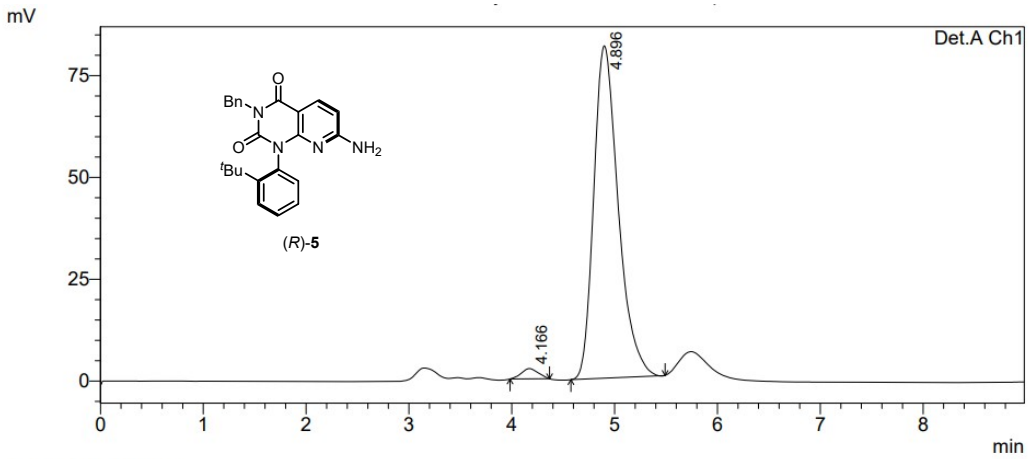


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.177	2269828	198378	49.312	59.813
2	4.865	2333141	133284	50.688	40.187
Total		4602969	331662	100.000	100.000

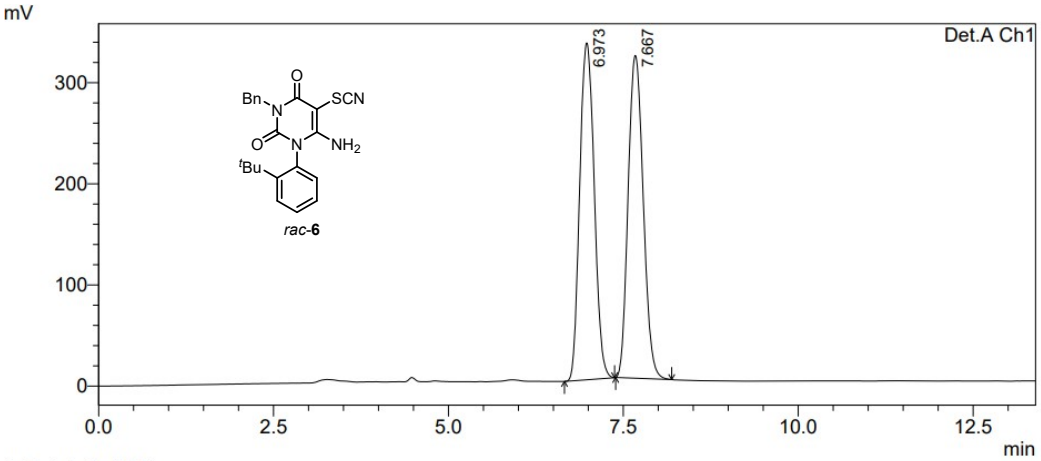


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	4.166	28800	2528	2.083	3.007
2	4.896	1353479	81547	97.917	96.993
Total		1382279	84076	100.000	100.000

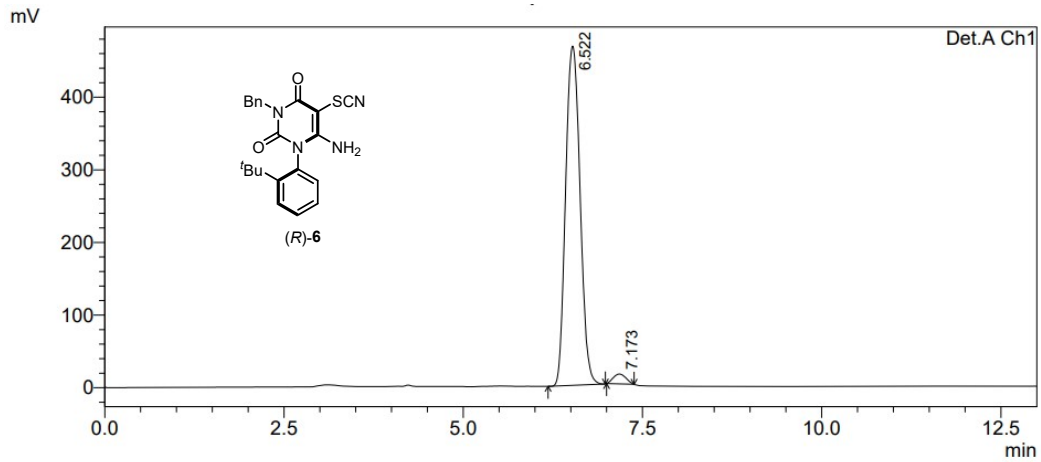


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.973	4808036	332355	50.074	51.016
2	7.667	4793764	319116	49.926	48.984
Total		9601800	651471	100.000	100.000

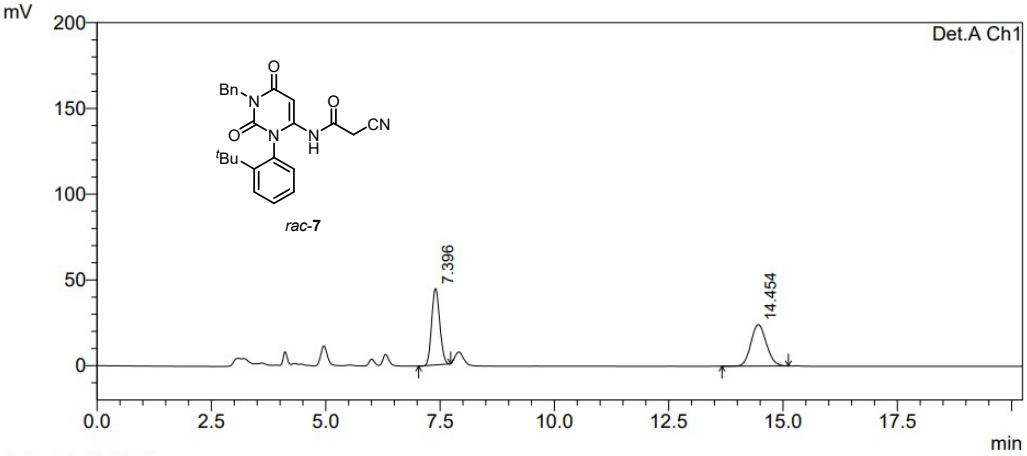


1 Det.A Ch1/254nm

PeakTable

Detector A Ch1 254nm

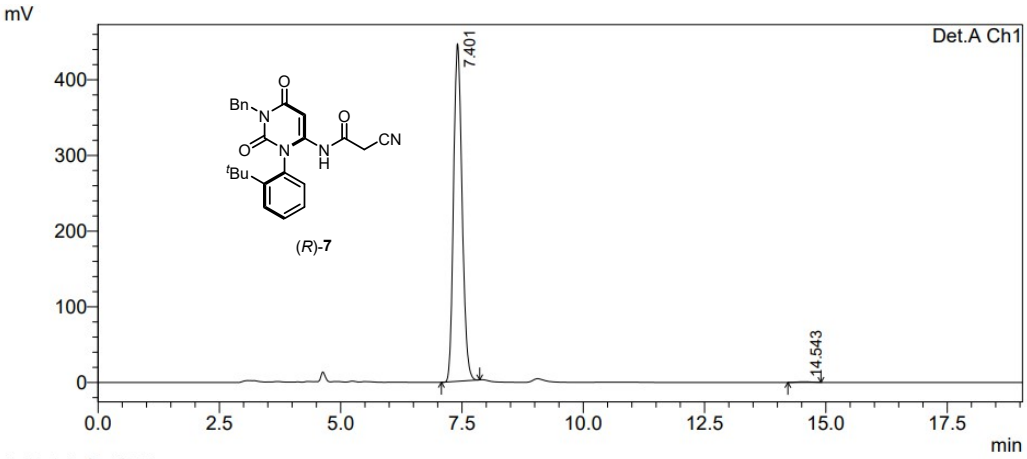
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.522	6541658	466605	97.501	97.179
2	7.173	167677	13545	2.499	2.821
Total		6709335	480149	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.396	547193	44541	49.065	64.772
2	14.454	568051	24225	50.935	35.228
Total		1115244	68765	100.000	100.000



PeakTable

Detector A Ch1 254nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.401	5452011	444931	99.668	99.805
2	14.543	18134	869	0.332	0.195
Total		5470145	445800	100.000	100.000