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Supplementary information

Enantioselective catalytic desymmetric ester aminolysis

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Table of Contents

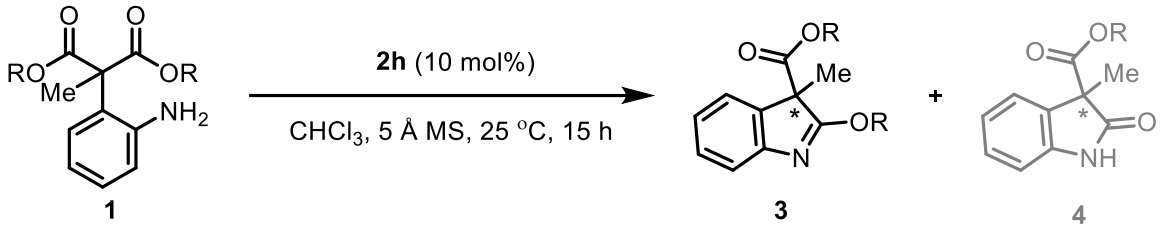
1. General information

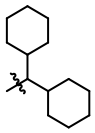
NMR spectra were recorded on Brucker AV 400 MHz spectrometer. Chemical shifts are given in ppm. The spectra are calibrated to the residual ^{1}H and ^{13}C signals of the solvents. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), doublet-doublet (dd), quintet (quint), multiplet (m), and broad (brs). The *ee* values were determined by HPLC (SHIMADZU, LC-20 AT) using a Daicel chiral column. Mass spectrometry analysis was carried out using an electrospray spectrometer Waters Micromass Q-TOF Premier Mass Spectrometer. Melting points were measured with SGW X-4 micro melting point apparatus. Optical rotations were measured on a Rudolph Research Analytical Autopol VI automatic polarimeter using a 50 mm path-length cell at 589 nm.

Materials and Methods: Unless otherwise stated, starting materials were purchased from commercial sources Adamas-Beta®, Leyan, Bide pharmatech Ltd., J&K®, Aladdin®, Energy chemical, and used without any purification. More sensitive compounds were stored in a desiccator or in a glove box if required. Solvents were purchased in HPLC quality, degassed by purging thoroughly with nitrogen and dried over activated molecular sieves of appropriate size. Alternatively, they were purged with argon and passed through alumina columns in a solvent purification system (Innovative Technology). Reactions were monitored by thin layer chromatography (TLC) using Xinnuo TLC silica gel 60 F254. Compounds were visualized by UV-light at 254 nm and by dipping the plates in an aqueous potassium permanganate solution followed by heating. Flash column chromatography was performed over silica gel (230-400 mesh). The $CDCl_3$ used in the NMR experiments was stored over anhydrous K_2CO_3 before use. Chiral phosphoric acid **2h** (CAS: 929294-27-9) was purchased from Leyan.

2. Optimization of the reaction conditions

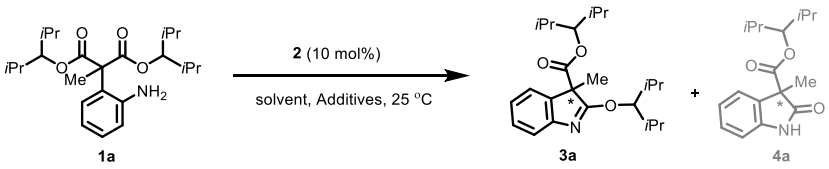
Table S1: Substituent effect[a]

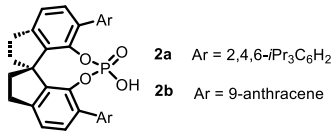


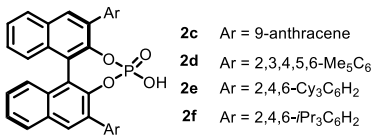
Entry	R	Yield (%)[b] 3	Ee (%)[c] 3	Yield (%)[b] 4	Ee (%)[c] 4	3:4
1	*t*Bu	trace	-	60	5	-
2		73	55	6	47	12:1
3		91	89	7	82	13:1

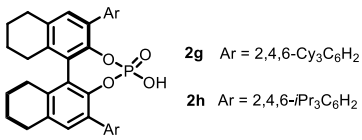
[a]Standard conditions: **1** (0.05 mmol), **2h** (10 mol%), M.S. (15 mg), solvent (*c* 0.1 M), sealed tube, argon, 15 h. [b]Isolated yields. [c]Determined by HPLC analysis.

Table S2: Survey of reaction conditions[a]







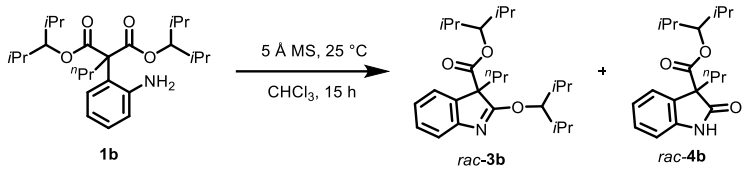


Entry	2	Solvent	Additives	Yield (%)[b] 3a	Ee (%)[c] 3a	Yield (%)[b] 4a	Ee (%)[c] 4a	3a:4a
1	**2a**	$CHCl_3$	5 Å	8	54	9	60	1:1
2	**2b**	$CHCl_3$	5 Å	76	83	7	61	11:1
3	**2c**	$CHCl_3$	5 Å	90	68	8	48	11:1
4	**2d**	$CHCl_3$	5 Å	91	62	8	70	11:1
5	**2e**	$CHCl_3$	5 Å	92	85	7	77	13:1
6	**2f**	$CHCl_3$	5 Å	86	86	8	84	11:1

7	**2g**	$CHCl_3$	5 Å	91	87	7	86	13:1
8	**2h**	$CHCl_3$	5 Å	91	89	7	82	13:1
9	**2h**	Tol	5 Å	81	80	17	22	4:1
10	**2h**	DCM	5 Å	66	86	8	70	8:1
11	**2h**	DCE	5 Å	64	86	7	61	9:1
12	**2h**	1,4-Dioxane	5 Å	76	86	16	90	5:1
13	**2f**	$CHCl_3$	3 Å	79	86	7	70	11:1
14	**2f**	$CHCl_3$	4 Å	84	86	5	71	17:1
15[d]	**2f**	$CHCl_3$	K_2SO_4	85	84	10	15	9:1
16[d]	**2f**	$CHCl_3$	Na_2SO_4	57	84	8	21	7:1

[a]Standard conditions: **1a** (0.05 mmol), **2** (10 mol%), M.S. (15 mg), solvent (*c* 0.1 M), sealed tube, argon, 15 h. Abbreviations: M.S. = molecular sieves. [b]Isolated yields. [c]Determined by HPLC analysis. [d]100 mg.

Table S3: Survey of background reactivity[a]

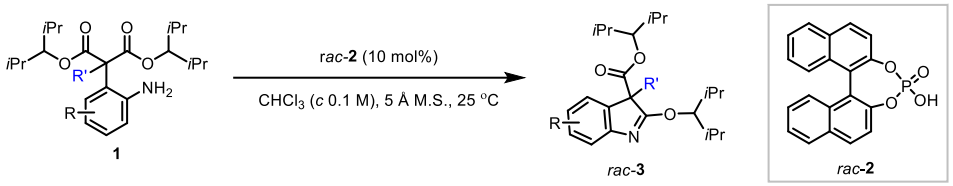


Entry	Yield (%)[b] *rac*-**3b**	Yield (%)[b] *rac*-**4b**	*rac*-**3b**:*rac*-**4b**
1	6	11	1:2

[a]Standard conditions: **1b** (0.05 mmol), M.S. (15 mg), solvent (*c* 0.1 M), sealed tube, argon, 15 h. [b]Isolated yields.

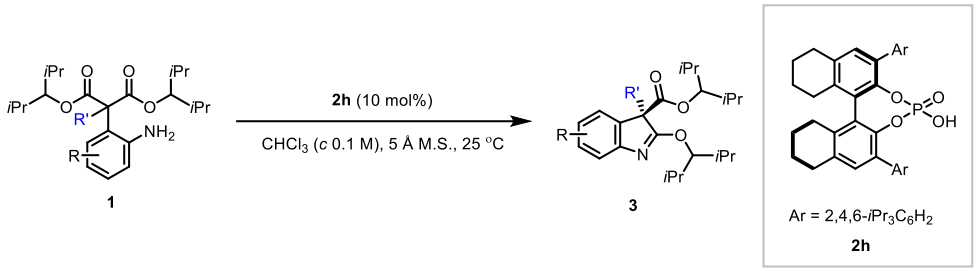
3. Synthesis and characterization data of compounds 3

General procedure for the synthesis of racemic 3



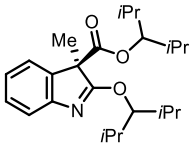
A suspension of **1** (0.05 mmol, 1.0 equiv.), *rac*-**2** (10 mol%), 5 Å molecular sieves (15.0 mg) in $CHCl_3$ (0.5 mL) was stirred in a dry sealed tube under argon. The reaction mixture was stirred at 25 °C for 18 h. After completion of the reaction (monitored by TLC), the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel eluting with petroleum ether/ethyl acetate (10:1, v/v) to afford the products *rac*-**3**.

General procedure for the enantioselective synthesis of 3



A suspension of **1** (0.05 mmol, 1.0 equiv.), **2h** (10 mol%), 5 Å molecular sieves (15.0 mg) in $CHCl_3$ (0.5 mL) was stirred in a dry sealed tube under argon. The reaction mixture was stirred at 25 ℃ for indicated time under argon. After completion of the reaction (monitored by TLC), the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel eluting with petroleum ether/ethyl acetate (10:1, v/v) to afford the products **3**.

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-methyl-*3H*-indole -3-carboxylate (3a)



15 h, 17.6 mg, 91% yield, 89% *ee,* white solid, m.p. = 60 – 62 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.32 (m, 1H), 7.30 – 7.26 (m, 2H), 7.07 – 7.03 (m, 1H), 5.14 – 4.93 (m, 1H), 4.59 (dd, *J* = 8.4, 4.0 Hz, 1H), 2.19 – 2.00 (m, 2H), 1.90 – 1.76 (m, 2H), 1.70 (s, 3H), 1.09 – 1.01 (m, 6H), 0.98 – 0.96 (m, 6H), 0.90 (d, *J* = 6.6 Hz, 3H), 0.86 (d, *J* = 6.8 Hz, 3H), 0.63 (d, *J* = 6.7 Hz, 3H), 0.54 (d, *J* = 6.8 Hz, 3H).

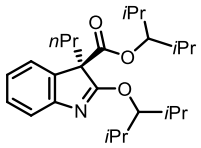
^{13}C NMR (101 MHz, Chloroform-*d*) δ 180.8, 170.3, 153.8, 137.9, 129.0, 123.3, 121.9, 118.4, 88.7, 84.6, 59.2, 30.4, 30.0, 29.6, 29.2, 20.4, 19.8, 19.5, 19.4, 19.2, 18.9, 18.2, 16.7, 15.5.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{24}H_{37}NNaO_3]^+$ 410.2666; Found 410.2669.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.3 min (minor), 9.6 min (major).

$[\alpha]^{23}_D$ -42.9 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-propyl-*3H*-indole -3-carboxylate (3b)



15 h, 20.1 mg, 97% yield, 91% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.15 (m, 3H), 7.00 – 6.96 (m, 1H), 4.95 (t, *J* = 5.8 Hz, 1H), 4.55 (dd, *J* = 8.2, 4.2 Hz, 1H), 2.30 – 2.07 (m, 2H), 2.05 – 1.98 (m, 2H), 1.82 – 1.74 (m, 2H), 1.08 – 1.01 (m, 2H), 1.00 – 0.98 (m, 6H), 0.93 (d, *J* = 6.8 Hz, 6H), 0.85 – 0.75 (m, 9H), 0.58 (d, *J* = 6.7 Hz, 3H), 0.49 (d, *J* = 6.8 Hz, 3H).

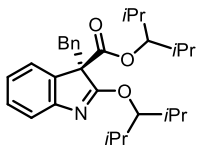
^{13}C NMR (101 MHz, Chloroform-*d*) δ 179.7, 170.1, 154.1, 136.1, 128.8, 123.2, 122.4, 118.24, 88.8, 84.5, 64.0, 35.9, 30.6, 29.0, 29.6, 29.3, 19.9, 19.6, 19.3, 18.8, 18.6, 17.2, 17.1, 15.8, 14.1.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{26}H_{41}NNaO_3]^+$ 438.2979; Found 438.2984.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.8 mL/min, 254 nm; t_R = 4.5 min (minor), 4.8 min (major).

$[\alpha]^{23}_D$ -30.2 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-3-benzyl-2-((2,4-dimethylpentan-3-yl)oxy)-*3H*-indole -3-carboxylate (3c)



15 h, 21.1 mg, 91% yield, 91% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.21 (m, 2H), 7.18 – 7.07 (m, 3H), 7.05 – 6.93 (m, 4H), 4.95 (t, *J* = 5.5 Hz, 1H), 4.62 – 4.59 (m, 1H), 3.82 (d, *J* = 14.1 Hz, 1H), 3.26 (d, *J* = 14.2 Hz, 1H), 2.17 – 2.03 (m, 1H), 2.01 – 1.92 (m, 1H), 1.92 – 1.74 (m, 2H), 1.01 (d, *J* = 6.8 Hz, 6H), 0.89 – 0.87 (m, 6H), 0.83 – 0.80 (m, 6H), 0.63 (d, *J* = 6.7 Hz, 3H), 0.55 (d, *J* = 6.8 Hz, 3H).

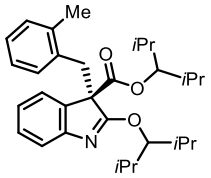
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.9, 169.7, 154.1, 135.9, 135.5, 130.3, 128.9, 127.9, 127.0, 123.9, 122.9, 118.3, 89.2, 85.0, 64.3, 39.4, 30.2, 30.1, 29.6, 29.2, 19.73, 19.67, 19.6, 19.3, 18.7, 18.2, 18.0, 15.9.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{41}NNaO_3]^+$ 486.2979; Found 486.2984.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.4 min (minor), 9.9 min (major).

$[\alpha]^{23}_D$ -64.7 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(2-methylbenzyl)-*3H*-indole-3-carboxylate (3d)



15 h, 23.1 mg, 97% yield, 93% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.28 (m, 1H), 7.25 – 7.21 (m, 1H), 7.12 – 7.10 (m, 1H), 7.06 – 7.02 (m, 2H), 7.01 – 6.96 (m, 1H), 6.88 – 6.84 (m, 1H), 6.71 – 6.64 (m, 1H), 4.97 (t, *J* = 5.7 Hz, 1H), 4.58 (dd, *J* = 8.0, 4.2 Hz, 1H), 3.79 (d, *J* = 14.9 Hz, 1H), 3.25 (d, *J* = 14.9 Hz, 1H), 2.10 – 2.03 (m, 1H), 2.01 – 1.92 (m, 1H), 1.91 (s, 3H), 1.85 – 1.73 (m, 2H), 1.02 (t, *J* = 6.6 Hz, 6H), 0.86 (d, *J* = 6.9 Hz, 3H), 0.81 – 0.78 (m, 9H), 0.60 (d, *J* = 6.7 Hz, 3H), 0.53 (d, *J* = 6.9 Hz, 3H).

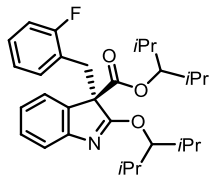
^{13}C NMR (101 MHz, Chloroform-*d*) δ 179.4, 170.0, 154.1, 137.6, 135.5, 135.0, 130.2, 129.6, 128.9, 126.9, 125.8, 123.8, 122.9, 118.2, 89.2, 85.0, 63.7, 35.0, 30.4, 30.1, 29.7, 29.2, 20.0, 19.8, 19.6, 19.4, 18.7, 18.2, 17.5, 15.9.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{43}NNaO_3]^+$ 500.3135; Found 500.3133.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.3 min (minor), 9.8 min (major).

$[\alpha]^{23}_D$ -63.9 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(2-fluorobenzyl)-*3H*-indole-3-carboxylate (3e)



15 h, 21.6 mg, 90% yield, 89% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26 – 7.20 (m, 2H), 7.13 – 7.08 (m, 1H), 7.04 – 6.97 (m, 2H), 6.97 – 6.91 (m, 1H), 6.89 – 6.85 (m, 2H), 4.95 (t, *J* = 5.5 Hz, 1H), 4.60 (dd, *J* = 8.1, 4.2 Hz, 1H), 3.75 (d, *J* = 14.7 Hz, 1H), 3.44 (d, *J* = 14.7 Hz, 1H), 2.14 – 1.91 (m, 2H), 1.85 – 1.76 (m, 2H), 1.00 (d, *J* = 6.8 Hz, 6H), 0.92 – 0.78 (m, 12H), 0.62 (d, *J* = 6.7 Hz, 3H), 0.51 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.0, 169.8, 161.3 (d, *J* = 247.1 Hz), 154.0, 135.5, 131.1 (d, *J* = 3.6 Hz), 129.1, 128.6 (d, *J* = 8.2 Hz), 123.6 (d, *J* = 3.7 Hz), 123.5 (d, *J* = 14.7 Hz), 123.3, 123.1, 118.3, 115.2 (d, *J* = 22.9 Hz), 89.3, 85.1, 63.5, 30.6, 30.5, 30.3, 30.0, 29.7, 29.2, 19.8, 19.6, 19.5, 19.3, 18.8, 18.2, 17.8, 15.8.

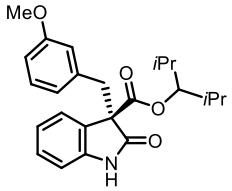
^{19}F NMR (377 MHz, Chloroform-*d*) δ -115.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{40}FNNaO_3]^+$ 504.2884; Found 504.2886.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.3 min (minor), 9.8 min (major).

$[\alpha]^{23}_D$ -21.7 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-3-(3-methoxybenzyl)-2-oxoindoline-3-carboxylate (4f)



15 h, 18.3 mg, 93% yield, 92% *ee,* white solid, m.p. = 105 – 107 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (s, 1H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.23 – 7.11 (m, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.93 (t, *J* = 7.9 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.61 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.54 (d, *J* = 7.5 Hz, 1H), 4.59 (t, *J* = 6.1 Hz, 1H), 3.56 (s, 2H), 3.53 (s, 3H), 1.82 (m, 1H), 1.76 – 1.68 (m, 1H), 0.88 (d, *J* = 6.8 Hz, 3H), 0.81 (d, *J* = 6.7 Hz, 3H), 0.67 (d, *J* = 6.8 Hz, 3H), 0.48 (d, *J* = 6.6 Hz, 3H).

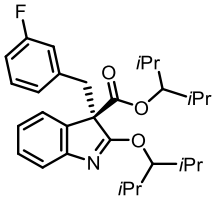
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.0, 169.2, 159.0, 141.7, 136.3, 129.1, 128.8, 128.6, 124.3, 122.7, 122.4, 114.9, 113.3, 110.0, 84.7, 61.7, 55.2, 39.1, 29.7, 29.5, 19.6, 19.5, 17.1, 16.6.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{24}H_{29}NNaO_4]^+$ 418.1989; Found 418.1991.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 90:10, 1.0 mL/min, 254 nm; t_R = 7.1 min (major), 9.2 min (minor).

$[\alpha]^{23}_D$ -58.1 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(3-fluorobenzyl)-*3H*-indole-3-carboxylate (3g)



15 h, 21.1 mg, 88% yield, 91% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 1.9 Hz, 1H), 7.07 – 7.04 (m, 1H), 7.03 – 6.96 (m, 2H), 6.88 – 6.80 (m, 1H), 6.75 (d, *J* = 7.8 Hz, 2H), 4.93 (t, *J* = 5.5 Hz, 1H), 4.59 (dd, *J* = 8.1, 4.1 Hz, 1H), 3.74 (d, *J* = 14.3 Hz, 1H), 3.28 (d, *J* = 14.3 Hz, 1H),

2.21 – 2.01 (m, 1H), 2.01 – 1.91 (m, 1H), 1.87 – 1.70 (m, 2H), 0.98 (m, 6H), 0.86 (m, 6H), 0.80 (m, 6H), 0.61 (d, *J* = 6.8 Hz, 3H), 0.51 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.7, 169.6, 162.5 (d, *J* = 245.7 Hz), 154.0, 138.4 (d, *J* = 7.3 Hz), 135.3, 129.4, 129.3 (d, *J* = 8.2 Hz), 126.0 (d, *J* = 2.9 Hz), 123.3 (d, *J* = 53.2 Hz), 118.5, 117.2 (d, *J* = 21.8 Hz), 113.9 (d, *J* = 21.1 Hz), 89.4, 85.2, 64.0, 38.99, 38.97, 30.2, 30.1, 29.6, 29.2, 19.7, 19.5, 19.3, 18.7, 18.1, 18.0, 15.8.

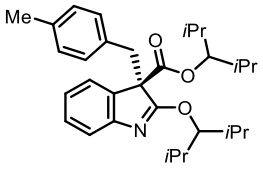
^{19}F NMR (377 MHz, Chloroform-*d*) δ -114.0.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{40}FNNaO_3]^+$ 504.2884; Found 504.2886.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 10.6 min (major), 13.0 min (minor).

$[\alpha]^{23}_D$ -54.4 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(4-methylbenzyl)-*3H*-indole-3-carboxylate (3h)



15 h, 20.3 mg, 85% yield, 87% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 6.7 Hz, 2H), 7.01 – 6.99 (m, 2H), 6.89 (dd, *J* = 7.8 Hz, 4H), 4.92 (t, *J* = 5.6 Hz, 1H), 4.59 (m, 1H), 3.77 (d, *J* = 14.0 Hz, 1H), 3.19 (d, *J* = 14.1 Hz, 1H), 2.24 (s, 3H), 2.11 – 2.04 (m, 1H), 1.97 – 1.95 (m, 1H), 1.85 – 1.73 (m, 2H), 0.99 (d, *J* = 6.8 Hz, 6H), 0.87 (t, *J* = 6.7 Hz, 6H), 0.79 (t, *J* = 5.9 Hz, 6H), 0.62 (d, *J* = 6.7 Hz, 3H), 0.54 (d, *J* = 6.8 Hz, 3H).

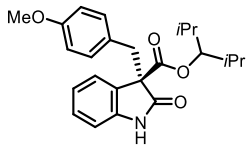
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.8, 169.6, 153.9, 136.3, 135.4, 132.5, 130.0, 128.7, 128.5, 123.8, 122.7, 89.0, 84.7, 64.2, 38.9, 30.1, 29.9, 29.5, 29.1, 21.0, 19.6, 19.5, 19.4, 19.2, 18.5, 18.1, 17.9, 15.8.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{43}NNaO_3]^+$ 500.3135; Found 500.3129.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.5 min (minor), 10.0 min (major).

$[\alpha]^{23}_{D}$ -32.4 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-3-(4-methoxybenzyl)-2-oxoindoline-3-carboxylate (4i)



15 h, 18.8 mg, 95% yield, 92% *ee,* white solid, m.p. = 108 – 110 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (s, 1H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.04 – 7.00 (m, 1H), 6.88 – 6.78 (m, 2H), 6.69 (d, *J* = 7.7 Hz, 1H), 6.62 – 6.48 (m, 2H), 4.59 (t, *J* = 6.0 Hz, 1H), 3.66 (s, 3H), 3.52 (d, *J* = 1.6 Hz, 2H), 1.86 – 1.78 (m, 1H), 1.76 – 1.66 (m, 1H), 0.88 (d, *J* = 6.8 Hz, 3H), 0.81 (d, *J* = 6.6 Hz, 3H), 0.67 (d, *J* = 6.8 Hz, 3H), 0.49 (d, *J* = 6.6 Hz, 3H).

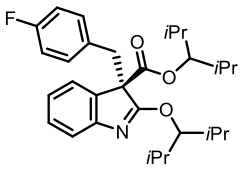
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.0, 169.3, 158.4, 141.6, 131.3, 129.0, 128.6, 126.9, 124.4, 122.4, 113.3, 109.9, 84.6, 61.8, 55.1, 38.3, 29.7, 29.5, 19.5, 17.2, 16.6.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{24}H_{29}NNaO_4]^+$ 418.1989; Found 418.1986.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 95:5, 1.0 mL/min, 254 nm; t_R = 18.5 min (major), 20.1 min (minor).

$[\alpha]^{23}_{D}$ -96.4 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(4-fluorobenzyl)-*3H*-indole-3-carboxylate (3j)



15 h, 21.2 mg, 88% yield, 94% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.24 (m, 2H), 7.00 – 6.95 (m, 4H), 6.80 (t, *J* = 8.6 Hz, 2H), 4.93 (t, *J* = 5.6 Hz, 1H), 4.60 – 4.57 (m, 1H), 3.75 (d, *J* = 14.2 Hz, 1H), 3.20 (d, *J* = 14.2 Hz, 1H), 2.10 – 2.03 (m, 1H), 2.02 – 1.94 (m, 1H), 1.84 – 1.75 (m,

2H), 0.99 (d, *J* = 7.0 Hz, 6H), 0.91 – 0.84 (m, 6H), 0.79 (t, *J* = 6.2 Hz, 6H), 0.60 (d, *J* = 6.7 Hz, 3H), 0.52 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.6, 169.5, 161.9 (d, *J* = 246.4 Hz), 153.9, 135.1, 131.7 (d, *J* = 8.1 Hz), 129.0, 123.7, 122.8, 118.3, 114.6 (d, *J* = 21.2 Hz), 89.2, 85.0, 64.1, 38.5, 30.1, 30.0, 29.5, 29.1, 19.6, 19.54, 19.45, 19.2, 18.6, 18.1, 17.9, 15.7.

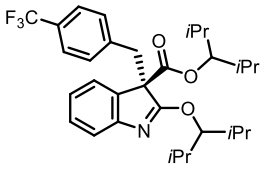
^{19}F NMR (377 MHz, Chloroform-*d*) δ -116.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{40}FNNaO_3]^+$ 504.2884; Found 504.2886.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 99:1, 0.5 mL/min, 254 nm; t_R = 8.1 min (major), 9.3 min (minor).

$[\alpha]^{23}_D$ -44.0 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(4-(trifluoromethyl)benzyl)-*3H*-indole-3-carboxylate (3k)



15 h, 24.1 mg, 91% yield, 91% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.20 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.00 – 6.97 (m, 2H), 4.90 (t, *J* = 5.5 Hz, 1H), 4.56 (dd, *J* = 8.2, 4.1 Hz, 1H), 3.76 (d, *J* = 14.3 Hz, 1H), 3.32 (d, *J* = 14.3 Hz, 1H), 2.08 – 1.96 (m, 1H), 1.92 –1.88 (m, 1H), 1.86 – 1.70 (m, 2H), 0.97 – 0.94 (m, 6H), 0.82 – 0.78 (m, 12H), 0.56 (d, *J* = 6.8 Hz, 3H), 0.45 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.6, 169.6, 154.0, 140.2, 135.2, 130.6, 129.3, 129.26 (q, *J* = 32.2 Hz), 125.6 (q, *J* = 273.3 Hz), 125.0 (q, *J* = 3.7 Hz), 123.5, 123.2, 118.6, 89.5, 85.3, 63.8, 39.0, 30.2, 30.0, 29.6, 29.2, 19.7, 19.6, 19.5, 19.3, 18.8, 18.1, 17.9, 15.7.

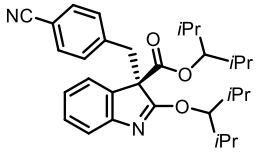
^{19}F NMR (377 MHz, Chloroform-*d*) δ -62.6.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{40}F_3NNaO_3]^+$ 554.2852; Found 554.2853.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.4 min (major), 12.0 min (minor).

$[\alpha]^{23}_D$ -60.7 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-3-(4-cyanobenzyl)-2-oxoindoline-3-carboxylate (3l)



15 h, 19.6 mg, 80% yield, 92% *ee,* white solid. m.p. = 115 – 118 ºC.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 (d, *J* = 7.8 Hz, 2H), 7.27 – 7.26 (m, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 7.01 – 6.95 (m, 2H), 4.93 (t, *J* = 5.6 Hz, 1H), 4.59 – 4.56 (m, 1H), 3.77 (d, *J* = 14.3 Hz, 1H), 3.34 (d, *J* = 14.3 Hz, 1H), 2.09 – 2.01 (m, 1H), 1.94 – 1.98 (m, 1H), 1.83 – 1.75 (m, 2H), 0.97 (t, *J* = 6.7 Hz, 6H), 0.88 – 0.78 (m, 12H), 0.58 (d, *J* = 6.7 Hz, 3H), 0.47 (d, *J* = 6.9 Hz, 3H).

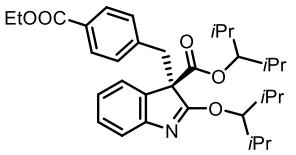
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.4, 169.4, 153.8, 141.5, 134.8, 131.6, 130.9, 129.3, 123.3, 123.1, 118.8, 118.5, 110.7, 89.5, 85.3, 63.5, 39.1, 30.1, 29.9, 29.4, 29.0, 19.6, 19.5, 19.4, 19.1, 18.7, 18.0, 17.8, 15.5.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{40}N_2NaO_3]^+$ 511.2931; Found 511.2933.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 95:5, 0.7 mL/min, 254 nm; t_R = 6.4 min (major), 8.8 min (minor).

$[\alpha]^{23}_D$ -50.4 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-3-((4-ethoxycarbonyl)benzyl)-2-oxoindoline-3-carboxylate (3m)



15 h, 22.0 mg, 82% yield, 92% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 – 7.77 (m, 2H), 7.26 – 7.23 (m, 2H), 7.07 (d, *J* = 8.3 Hz, 2H), 6.99 – 6.95 (m, 2H), 4.93 (t, *J* = 5.4 Hz, 1H), 4.59 (q, *J* = 8.0, 4.2 Hz, 1H), 4.32 (dd, *J* = 7.1 Hz, 2H), 3.82 (d, *J* = 14.2 Hz, 1H), 3.31 (d, *J* = 14.2 Hz, 1H), 2.12 –2.02 (m, 1H), 2.01 – 1.92 (m, 1H), 1.85 – 1.75 (m, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.00 – 0.97 (m, 6H), 0.88 – 0.84 (m, 6H), 0.82 – 0.80 (m, 6H), 0.60 (d, *J* = 6.7 Hz, 3H), 0.51 (d, *J* = 6.9 Hz, 3H).

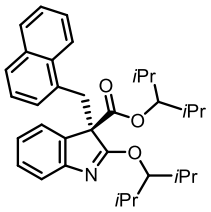
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.5, 169.5, 166.5, 153.9, 141.1, 135.0, 130.2, 129.1, 123.6, 122.9, 118.4, 89.3, 85.1, 63.8, 60.8, 39.1, 30.1, 29.9, 29.5, 29.1, 19.6, 19.5, 19.4, 19.2, 18.6, 18.1, 17.9, 15.7, 14.3.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{33}H_{45}NNaO_5]^+$ 558.3190; Found 558.3185.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 95:5, 0.7 mL/min, 254 nm; t_R = 5.9 min (major), 9.1 min (minor).

$[\alpha]^{23}_D$ -44.0 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(naphthalen-1-ylmethyl)-*3H*-indole-3-carboxylate (3n)



15 h, 24.6 mg, 96% yield, 95% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.25 – 7.17 (m, 2H), 7.14 (t, *J* = 8.1 Hz, 1H), 7.08 (d, *J* = 4.8 Hz, 2H), 7.05 – 7.01 (m, 1H), 6.62 – 6.54 (m, 2H), 4.82 (t, *J* = 5.7 Hz, 1H), 4.46 (dd, *J* = 8.0, 4.2 Hz, 1H), 4.10 (d, *J* = 15.3 Hz, 1H), 3.70 (d, *J* = 15.3 Hz, 1H), 1.96 – 1.86 (m, 1H), 1.73 – 1.57 (m, 3H), 0.88 (t, *J* = 7.0 Hz, 6H), 0.69 – 0.66 (m, 6H), 0.61 (d, *J* = 6.9 Hz, 3H), 0.49 (d, *J* = 6.7 Hz, 3H), 0.43 (d, *J* = 6.7 Hz, 3H), 0.33 (d, *J* = 6.8 Hz, 3H).

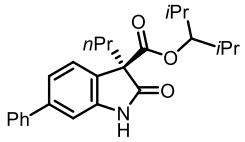
^{13}C NMR (101 MHz, Chloroform-*d*) δ 179.3, 170.0, 154.0, 135.4, 133.7, 132.9, 132.3, 128.9, 128.6, 127.6, 127.2, 125.7, 125.3, 125.1, 124.11, 124.08, 122.9, 118.3, 89.3, 85.1, 63.9, 34.4, 30.3, 29.9, 29.6, 29.2, 19.67, 19.65, 19.5, 19.4, 18.7, 18.1, 17.5, 15.8.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{34}H_{43}NNaO_3]^+$ 536.3135; Found 536.3142.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.8 min (minor), 10.2 min (major).

$[\alpha]^{23}_D$ -91.5 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl (*R*)-2-oxo-6-phenyl-3-propylindoline-3-carboxylate (4o)



40 ºC, 48 h, 18.2 mg, 93% yield, 61% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-d) δ 9.13 (s, 1H), 7.58 (d, J = 8.9 Hz, 2H), 7.49 – 7.42 (m, 2H), 7.38 – 7.35 (m, 1H), 7.28 (s, 2H), 7.17 (s, 1H), 4.57 (t, J = 6.1 Hz, 1H), 2.34 – 2.23 (m, 2H), 1.85 – 1.80 (m, 1H), 1.75 – 1.70 (m, 1H), 1.22 – 1.21 (m, 1H), 1.11 – 1.05 (m, 1H), 0.90 – 0.84 (m, 6H), 0.81 (d, J = 6.7 Hz, 3H), 0.67 (d, J = 6.8 Hz, 3H), 0.52 (d, J = 6.7 Hz, 3H).

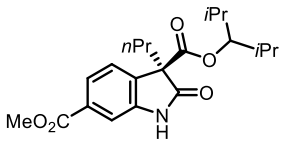
^{13}C NMR (101 MHz, Chloroform-d) δ 177.5, 169.3, 142.3, 140.6, 128.8, 128.2, 127.7, 127.1, 123.9, 121.5, 108.8, 84.3, 60.5, 35.6, 29.6, 29.4, 19.5, 19.4, 17.1, 17.0, 16.6, 14.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{25}H_{31}NNaO_3]^+$ 416.2196; Found 416.2198.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 95:5, 1.0 mL/min, 254 nm; t_R = 12.4 min (minor), 13.7 min (major).

$[\alpha]^{23}_D$ +9.5 (*c* 1.0, $CHCl_3$).

3-(2,4-dimethylpentan-3-yl)6-methyl(*R*)-2-oxo-3-propylindoline-3,6-dicarboxylate (4p)



40 ºC, 48 h, 15.3 mg, 82% yield, 82% *ee,* yellow solid, m.p. = 112 – 114 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (s, 1H), 7.77 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.59 (d, *J* = 1.5 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 4.55 (t, *J* = 6.0 Hz, 1H), 3.92 (s, 3H), 2.35 – 2.20 (m, 2H), 1.85 – 1.78 (m, 1H), 1.74 – 1.68 (m, 1H), 1.20 – 1.14 (m, 1H), 1.01 – 0.96 (m, 1H), 0.86 (t, *J* = 6.6 Hz, 6H), 0.78 (d, *J* = 6.7 Hz, 3H), 0.65 (d, *J* = 6.9 Hz, 3H), 0.48 (d, *J* = 6.7 Hz, 3H).

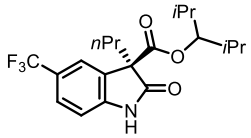
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.5, 168.6, 166.5, 141.8, 134.3, 130.9, 124.4, 123.6, 110.6, 84.6, 60.6, 52.4, 35.6, 29.5, 29.4, 19.4, 17.1, 16.9, 16.6, 14.1.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{21}H_{29}NNaO_5]^+$ 398.1938; Found 398.1935.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 90:10, 1.0 mL/min, 254 nm; t_R = 6.9 min (major), 8.9 min (minor).

$[\alpha]^{23}_D$ +40.0 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-oxo-3-propyl-5-(trifluoromethyl)indoline-3-carboxylate (4q)



24 h, 17.7 mg, 92% yield, 80% *ee,* white solid, m.p. = 125 – 127 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.33 (s, 1H), 7.55 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.48 (d, *J* = 1.8 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 4.56 (t, *J* = 6.1 Hz, 1H), 2.40 – 2.22 (m, 2H), 1.85 – 1.69 (m, 2H), 1.23 – 1.11 (m, 1H), 1.09 – 0.94 (m, 1H), 0.89 (d, *J* = 7.2 Hz, 3H), 0.84 (d, *J* = 6.8 Hz, 3H), 0.76 (d, *J* = 6.7 Hz, 3H), 0.67 (d, *J* = 6.8 Hz, 3H), 0.48 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 177.3, 168.5, 144.8, 130.0, 126.4 (q, *J* = 3.8 Hz), 125.2 (q, *J* = 33.3 Hz), 125.0 (q, *J* = 272.7 Hz), 121.1 (q, *J* = 3.9 Hz), 110.0, 84.9, 84.8, 60.7, 35.7, 29.6, 29.5, 19.5, 19.4, 17.2, 17.0, 16.6, 14.2.

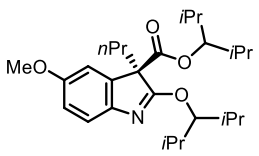
^{19}F NMR (377 MHz, Chloroform-*d*) δ -61.7.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{20}H_{26}F_3NNaO_3]^+$ 408.1757; Found 408.1759.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 98:2, 1.0 mL/min, 254 nm; t_R = 13.1 min (major), 15.1 min (minor).

$[\alpha]^{23}_D$ -33.8 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-5-methoxy-3-propyl-*3H*-indole-3-carboxylate (3r)



15 h, 21.9 mg, 98% yield, 95% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 8.4 Hz, 1H), 6.83 (d, *J* = 2.6 Hz, 1H), 6.78 (dd, *J* = 8.4, 2.6 Hz, 1H), 4.95 – 4.92 (m, 1H), 4.61 – 4.58 (m, 1H), 3.76 (s, 3H), 2.27 – 2.17 (m, 1H), 2.15 – 1.96 (m, 3H), 1.87 – 1.79 (m, 2H), 1.04 – 0.93 (m, 12H), 0.88 – 0.83 (m, 9H), 0.64 (d, *J* = 6.7 Hz, 3H), 0.58 (d, *J* = 6.8 Hz, 3H).

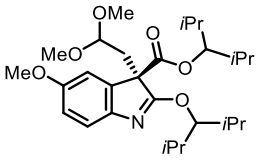
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.3, 170.1, 156.4, 147.4, 137.3, 118.4, 113.7, 109.26, 88.5, 84.5, 64.4, 56.0, 36.0, 30.6, 29.8, 29.6, 29.3, 20.0, 19.60, 19.55, 19.3, 18.7, 18.6, 17.12, 17.06, 15.9, 14.1.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{27}H_{43}NNaO_4]^+$ 468.3084; Found 468.3084.

Chiral HPLC: Chiralpak IC, hexane:*i*PrOH = 99:1, 0.2 mL/min, 254 nm; t_R = 21.4 min (minor), 22.1 min (major).

$[\alpha]^{23}_D$ -7.5 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-5-methoxy-3-propyl-*3H*-indole-3-carboxylate (3s)



15 h, 21.6 mg, 88% yield, 69% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.20 (d, *J* = 8.4 Hz, 1H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.81 – 6.78 (m, 1H), 4.93 (t, *J* = 5.6 Hz, 1H), 4.59 – 4.53 (m, 1H), 4.14 – 4.12 (m, 1H), 3.76 (s, 3H), 3.09 (s, 3H), 3.06 (s, 3H), 2.72 – 2.67 (m, 1H), 2.55 – 2.49 (m, 1H), 2.13 – 2.01 (m, 2H), 1.94 – 1.78 (m, 2H), 1.06 – 0.97 (m, 12H), 0.84 (dd, *J* = 10.4, 6.7 Hz, 6H), 0.66 (d, *J* = 6.7 Hz, 3H), 0.57 (d, *J* = 6.9 Hz, 3H).

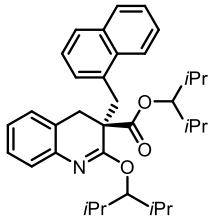
^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.1, 169.6, 156.2, 147.5, 136.3, 118.5, 114.2, 109.9, 102.0, 88.8, 84.9, 61.9, 56.0, 54.4, 52.7, 36.5, 30.6, 29.9, 29.7, 29.3, 19.8, 19.6, 19.5, 19.3, 18.7, 18.6, 17.5, 15.9.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{28}H_{45}NNaO_6]^+$ 514.3139; Found 514.3140.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 99:1, 1.0 mL/min, 254 nm; t_R = 7.8 min (major), 10.5 min (minor).

$[\alpha]^{23}_D$ -17.2 (*c* 1.0, $CHCl_3$).

2,4-dimethylpentan-3-yl(*R*)-2-((2,4-dimethylpentan-3-yl)oxy)-3-(naphthalen-1-ylmet-hyl)-3,4-dihydroquinoline-3-carboxylate (3t)



6 d, 23.5 mg, 89% yield, 64% *ee,* colorless oil. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 – 8.01 (m, 1H), 7.88 – 7.81 (m, 1H), 7.74 (d, *J* = 8.2 Hz, 1H), 7.53 (d, *J* = 7.1 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.12 – 7.04 (m, 2H), 6.87 – 6.83 (m, 1H), 6.78 (d, *J* = 7.4 Hz, 1H), 5.33 (t, *J* = 5.9 Hz, 1H), 4.52 (dd, *J* = 7.2, 4.9 Hz, 1H), 4.12 (d, *J* = 14.5 Hz, 1H), 3.74 (d, *J* = 14.6 Hz,

1H), 3.04 (d, *J* = 15.8 Hz, 1H), 2.88 (d, *J* = 15.8 Hz, 1H), 2.15 – 2.08 (m, 2H), 1.78 – 1.60 (m, 2H), 1.09 – 1.01 (m, 12H), 0.74 (d, *J* = 6.8 Hz, 3H), 0.64 (d, *J* = 6.6 Hz, 3H), 0.52 (d, *J* = 6.7 Hz, 3H), 0.39 (d, *J* = 6.9 Hz, 3H).

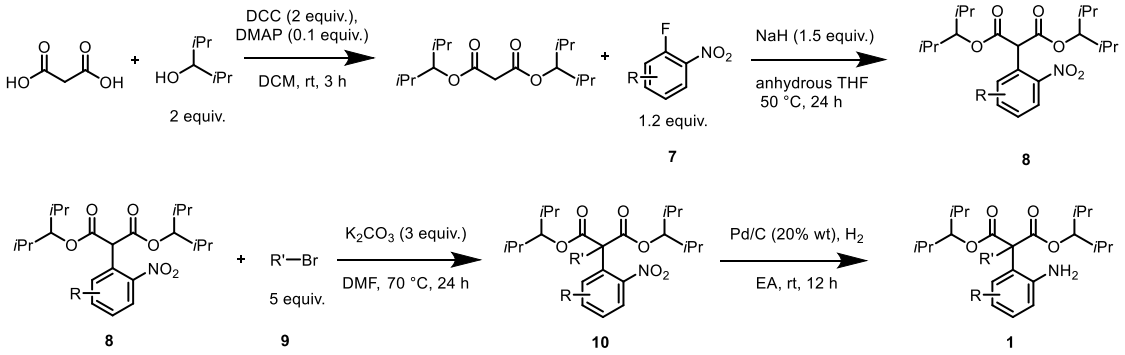
^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.7, 164.1, 143.3, 134.0, 133.4, 133.1, 129.1, 128.9, 127.8, 127.4, 127.3, 126.2, 125.9, 125.4, 125.3, 124.6, 124.4, 124.3, 84.7, 83.8, 52.0, 35.2, 34.7, 30.3, 30.2, 29.7, 29.1, 20.1, 19.9, 19.5, 19.3, 18.2, 18.1, 18.0, 16.5.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{35}H_{45}NNaO_3]^+$ 550.3292; Found 550.3299.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 99:1, 0.4 mL/min, 254 nm; t_R = 9.4 min (major), 10.0 min (minor).

$[\alpha]^{23}_D$ +23.4 (*c* 1.0, $CHCl_3$).

4. Synthesis and characterization data of compound 1



DMAP (3.0 mmol, 0.1 equiv.), 2,4-dimethyl-3-pentanol (60.0 mmol, 2.0 equiv.) were added to a solution of Malonic acid (30.0 mmol) in DCM (100 mL) at room temperature. Then DCC (60.0 mmol, 2.0 equiv.) was added to the reaction mixture at 0 °C. The reaction mixture was stirred at room temperature for 3 h. After completion of the reaction (monitored by TLC), vacuum filtration was carried out, and the filter cake was washed with DCM. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by column chromatography on silica gel, eluting with petroleum ether to afford bis(1-isopropyl-2-methylpropyl) malonate as colorless oil with 98% yield.

To a solution of sodium hydride (60% dispersion in mineral oil, 45.0 mmol, 1.5 equiv.) in anhydrous THF (50 mL) in a flame-dried flask was added bis(1-isopropyl-2-

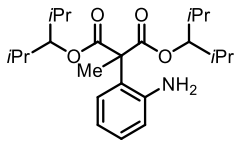
methylpropyl) malonate (30.0 mmol, 1.0 equiv.) at 0 °C under argon. The reaction mixture was stirred at room temperature for 1 h and a solution of **7** (36.0 mmol, 1.2 equiv.) in anhydrous THF (20 mL) was slowly added. The reaction mixture was stirred at 50 ℃ under N_2 for 24 h. After completion of the reaction (monitored by TLC), the reaction was quenched by saturated aqueous NH_4Cl, extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/ethyl acetate (200:1, v/v) to afford **8** as yellow oil with 38-54% yields.

9 (15.0 mmol, 5.0 equiv.) was added to a solution of **8** and K_2CO_3 (9.0 mmol, 3.0 equiv.) in DMF (10 mL) at 70 °C. The reaction mixture was stirred for 24 h. After completion of the reaction (monitored by TLC), the reaction was quenched by saturated aqueous NaCl, extracted with ethyl acetate. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated under vacuum. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/ethyl acetate (30:1, v/v) to afford **10** as colorless oil with 29-95% yields.

Pd/C (20% wt) was added to the solution of **10** in EA (10 mL) under H_2 at room temperature for 12 h. After completion of the reaction (monitored by TLC), the reaction was filtered and concentrated under vacuum. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/ethyl acetate (80:1, v/v) to afford **1** as colorless oil with 28-48% yields.

Note: All compounds were stored at −20 °C.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-methylmalonate (1a)



Colorless oil.

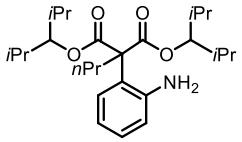
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.26 (m, 1H), 7.11 – 7.07 (m, 1H), 6.78 – 6.76 (m, 1H), 6.66 (dd, *J* = 7.9, 1.3 Hz, 1H), 4.65 (t, *J* = 5.9 Hz, 2H), 4.46 (s, 2H), 2.01

(s, 3H), 1.97 – 1.82 (m, 4H), 0.92 – 0.88 (m, 12H), 0.82 (d, *J* = 6.9 Hz, 6H), 0.76 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.8, 146.4, 128.9, 127.0, 123.8, 118.5, 118.2, 84.5, 58.2, 29.80, 29.77, 23.0, 19.8, 19.7, 17.44, 17.36.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{24}H_{39}NNaO_4]^+$ 428.2771; Found 428.2780.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-propylmalonate (1b)



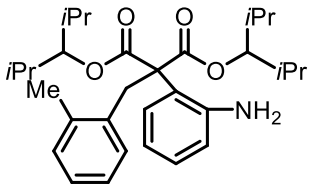
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 (d, *J* = 1.5 Hz, 1H), 7.08 – 7.04 (m, 1H), 6.77 – 6.73 (m, 1H), 6.62 (dd, *J* = 7.9, 1.4 Hz, 1H), 4.62 (t, *J* = 5.6 Hz, 2H), 4.40 (s, 2H), 2.51 – 2.36 (m, 2H), 2.01 – 1.77 (m, 4H), 1.45 – 1.39 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H), 0.90 – 0.86 (m, 12H), 0.77 (d, *J* = 6.9 Hz, 6H), 0.70 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.5, 146.4, 128.6, 127.5, 123.0, 118.4, 118.2, 84.3, 61.7, 36.7, 29.8, 29.7, 19.8, 19.6, 18.7, 17.9, 17.3, 14.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{26}H_{43}NNaO_4]^+$ 456.3084; Found 456.3087.

Bis(2,4-dimethylpentan-3-yl) 2-(2-aminophenyl)-2-(2-methylbenzyl)malonate (1d)



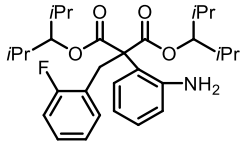
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 7.10 – 7.00 (m, 2H), 6.96 (t, *J* = 8.0 Hz, 1H), 6.71 – 6.61 (m, 2H), 4.59 (t, *J* = 5.5 Hz, 2H), 4.37 (s, 2H), 3.90 (s, 2H), 2.35 (s, 3H), 1.98 – 1.80 (m, 2H), 1.78 – 1.65 (m, 2H), 0.86 – 0.82 (m, 12H), 0.56 (d, *J* = 6.9 Hz, 6H), 0.48 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.7, 147.0, 136.5, 135.1, 129.8, 129.3, 129.0, 128.7, 126.2, 125.8, 120.8, 118.4, 118.1, 84.7, 61.5, 37.0, 29.9, 29.7, 20.2, 19.9, 19.3, 17.5, 17.0.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{45}NNaO_4]^+$ 518.3241; Found 518.3246.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(2-fluorobenzyl)malonate (1e)



Colorless oil.

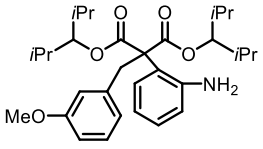
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.20 (m, 1H), 7.12 – 7.05 (m, 3H), 6.97 – 6.92 (m, 1H), 6.87 – 6.83 (m, 1H), 6.71 – 6.60 (m, 2H), 4.58 (t, *J* = 5.7 Hz, 2H), 4.29 (s, 2H), 3.98 (s, 2H), 1.85 – 1.78 (m, 2H), 1.77 – 1.72 (m, 2H), 0.81 – 0.76 (m, 12H), 0.61 (d, *J* = 6.9 Hz, 6H), 0.54 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.7, 161.4 (d, *J* = 244.9 Hz), 146.6, 130.8 (d, *J* = 3.5 Hz), 129.1, 128.9, 127.9 (d, *J* = 8.6 Hz), 124.3 (d, *J* = 13.8 Hz), 123.6 (d, *J* = 3.6 Hz), 121.4, 118.6 (d, *J* = 18.5 Hz), 114.7 (d, *J* = 22.6 Hz), 85.1, 61.4, 31.2 (d, *J* = 5.3 Hz), 29.8, 29.6, 19.7, 19.4, 17.7, 17.1.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -115.9.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{42}FNNaO_4]^+$ 522.2990; Found 522.2994.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(3-methoxybenzyl)malonate (1f)



Colorless oil.

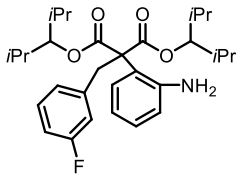
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 7.3 Hz, 1H), 7.12 – 7.04 (m, 2H), 6.82 (d, *J* = 7.6 Hz, 1H), 6.76 – 6.71 (m, 2H), 6.70 – 6.63 (m, 2H), 4.62 (t, *J* = 5.6 Hz,

2H), 4.27 (s, 2H), 3.95 (s, 2H), 3.65 (s, 3H), 1.93 – 1.84 (m, 2H), 1.83 – 1.73 (m, 2H), 0.81 – 0.81 (m, 12H), 0.68 (d, *J* = 6.9 Hz, 6H), 0.64 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.1, 159.2, 146.2, 138.3, 129.0, 128.9, 128.8, 122.9, 122.8, 118.69, 118.66, 115.4, 112.6, 85.2, 62.7, 55.2, 39.3, 29.8, 29.6, 19.6, 19.5, 18.0, 17.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{45}NNaO_5]^+$ 534.3190; Found 534.3193.

Bis(2,4-dimethylpentan-3-yl) 2-(2-aminophenyl)-2-(3-fluorobenzyl)malonate (1g)



Colorless oil.

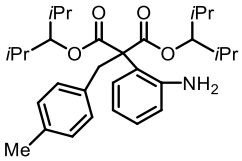
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.22 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.14 – 7.07 (m, 2H), 7.00 – 6.90 (m, 2H), 6.86 – 6.77 (m, 1H), 6.76 – 6.66 (m, 2H), 4.63 (t, *J* = 5.6 Hz, 2H), 4.23 (s, 2H), 3.94 (s, 2H), 1.94 – 1.87 (m, 2H), 1.83 – 1.76 (m, 2H), 0.84 – 0.81 (m, 12H), 0.71 (d, *J* = 6.9 Hz, 6H), 0.66 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.9, 162.40 (d, *J* = 244.3 Hz), 146.0, 139.3 (d, *J* = 7.8 Hz), 129.1 (d, *J* = 8.2 Hz), 128.9, 128.7, 126.0 (d, *J* = 2.7 Hz), 122.9, 118.8 (d, *J* = 8.7 Hz), 117.3 (d, *J* = 21.9 Hz), 113.3 (d, *J* = 21.1 Hz), 85.3, 62.8, 38.9, 29.7, 29.5, 19.5, 19.4, 17.9, 17.3.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -114.3.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{42}FNNaO_4]^+$ 522.2990; Found 522.3001.

Bis(2,4-dimethylpentan-3-yl) 2-(2-aminophenyl)-2-(4-methylbenzyl)malonate (1h)



Colorless oil.

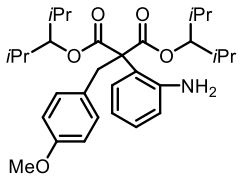
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (d, *J* = 8.0 Hz, 1H), 7.09 (d, *J* = 7.9 Hz, 3H), 6.96 (d, *J* = 7.4 Hz, 2H), 6.70 (dd, *J* = 24.5, 7.8 Hz, 2H), 4.60 (d, *J* = 5.3 Hz, 2H), 4.28

(s, 2H), 3.92 (s, 2H), 2.25 (s, 3H), 1.93 – 1.88 (m, 2H), 1.81 – 1.73 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 12H), 0.64 (t, *J* = 8.2 Hz, 12H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.9, 146.0, 135.8, 133.4, 130.0, 128.7, 128.5, 122.9, 118.5, 84.9, 62.5, 39.1, 29.7, 29.5, 21.0, 19.5, 19.3, 18.0, 17.3.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{45}NNaO_4]^+$ 518.3241; Found 518.3242.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(4-methoxybenzyl)malonate (1i)



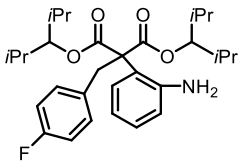
White solid, m.p. = 92 – 94 ºC.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.16 – 7.11 (m, 2H), 7.09 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.75 – 6.68 (m, 3H), 6.65 (dd, *J* = 7.9, 1.3 Hz, 1H), 4.61 (t, *J* = 5.6 Hz, 2H), 4.26 (s, 2H), 3.89 (s, 2H), 3.73 (s, 3H), 1.93 – 1.87 (m, 2H), 1.81 – 1.73 (m, 2H), 0.84 – 0.81 (m, 12H), 0.69 – 0.64 (m, 12H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.1, 158.3, 146.2, 131.4, 128.82, 128.80, 128.76, 123.1, 118.64, 118.62, 113.3, 85.1, 62.8, 55.3, 38.8, 29.8, 29.7, 19.7, 19.5, 18.1, 17.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{34}H_{45}NNaO_5]^+$ 534.3190; Found 534.3200.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(4-(fluorobenzyl)malonate (1j)



Colorless oil.

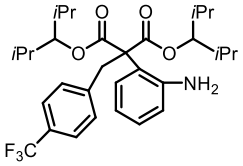
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.23 (d, *J* = 8.0 Hz, 1H), 7.15 (dd, *J* = 8.3, 5.2 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.83 (t, *J* = 8.5 Hz, 2H), 6.71 (q, *J* = 8.0 Hz, 2H), 4.62 (t, *J* = 5.6 Hz, 2H), 4.26 (s, 2H), 3.91 (s, 2H), 1.93 – 1.84 (m, 2H), 1.82 – 1.74 (m, 2H), 0.82 (t, *J* = 6.9 Hz, 12H), 0.70 (d, *J* = 6.7 Hz, 6H), 0.66 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.9, 161.6 (d, *J* = 245.4 Hz), 145.8, 132.3 (d, *J* = 3.0 Hz), 131.8 (d, *J* = 8.1 Hz), 128.8, 128.7, 122.9, 118.8, 118.7, 114.5 (d, *J* = 21.0 Hz), 114.4, 85.2, 38.4, 29.7, 29.5, 19.5, 19.4, 17.9, 17.3.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -116.1

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{30}H_{42}FNNaO_4]^+$ 522.2990; Found 522.2981.

Bis(2,4-dimethylpentan-3-yl) 2-(2-aminophenyl)-2-(4-(trifluoromethyl)benzyl)malonate (1k)



White solid, m.p. = 58 – 59 ºC.

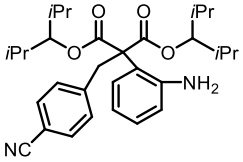
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.23 – 7.17 (m, 1H), 7.11 (m, 1H), 6.76 – 6.64 (m, 2H), 4.63 (t, *J* = 5.7 Hz, 2H), 4.23 (s, 2H), 4.00 (s, 2H), 1.93 – 1.84 (m, 2H), 1.82 – 1.74 (m, 2H), 0.83 – 0.80 (m, 12H), 0.70 (d, *J* = 6.8 Hz, 6H), 0.65 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.0, 146.1, 141.2, 130.8, 129.1, 128.82, 128.77 (q, *J* = 32.4 Hz), 127.0 (q, *J* = 272.8 Hz), 124.7 (q, *J* = 3.7 Hz), 122.9, 119.1, 119.0, 85.6, 63.0, 39.2, 29.8, 29.5, 19.6, 19.5, 18.0, 17.5.

^{19}F NMR (377 MHz, Chloroform-*d*) δ -62.5.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{42}F_3NNaO_4]^+$ 572.2958; Found 572.2957.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(4-cyanobenzyl)malonate (1l)



Colorless oil.

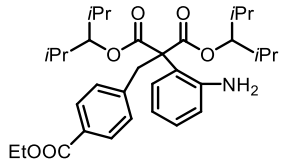
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 5.7 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.71 (d, *J* = 8.2 Hz, 2H), 4.64 (t, *J* = 5.8 Hz, 2H), 4.20 (s, 2H),

3.99 (s, 2H), 1.92 – 1.78 (m, 4H), 0.81 (t, *J* = 6.2 Hz, 12H), 0.73 (d, *J* = 6.9 Hz, 6H), 0.67 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.8, 145.7, 142.7, 131.4, 131.1, 129.1, 128.8, 122.8, 119.2, 119.0, 110.1, 85.6, 63.1, 38.9, 29.7, 29.5, 19.48, 19.46, 17.8, 17.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{31}H_{42}N_2NaO_4]^+$ 529.3037; Found 529.3034.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(4-ethoxycarbonylbenzyl)malonate (1m)



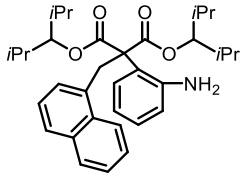
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.26 (s, 1H), 7.24 (s, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.11 –7.07 (m, 1H), 6.69 (t, *J* = 7.7 Hz, 2H), 4.63 (t, *J* = 5.7 Hz, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 4.01 (s, 2H), 1.92 –1.84 (m, 2H), 1.82 –1.75 (m, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 0.85 – 0.79 (m, 12H), 0.69 (d, *J* = 6.9 Hz, 6H), 0.64 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.8, 166.6, 145.9, 142.2, 130.2, 129.0, 128.9, 128.8, 128.4, 122.5, 118.9, 118.7, 85.3, 62.7, 60.8, 39.1, 29.7, 29.5, 19.5, 19.4, 17.9, 17.3, 14.3.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{33}H_{47}NNaO_6]^+$ 576.3296; Found 576.3299.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminophenyl)-2-(naphthalen-1-ylmethyl)malonate (1n)



Colorless oil.

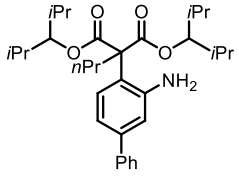
^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.5 Hz, 1H), 7.80 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.48 – 7.43 (m, 1H), 7.39 – 7.32

(m, 2H), 7.25 – 7.14 (m, 1H), 7.07 – 7.02 (m, 1H), 6.70 – 6.56 (m, 2H), 4.56 (t, *J* = 5.6 Hz, 2H), 4.43 (s, 2H), 4.38 (s, 2H), 1.88 – 1.76 (m, 2H), 1.66 – 1.56 (m, 2H), 0.78 – 0.73 (m, 12H), 0.45 (d, *J* = 6.9 Hz, 6H), 0.34 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.7, 147.0, 133.6, 132.5, 131.9, 129.3, 129.10, 129.05, 127.0, 126.7, 126.2, 125.5, 125.3, 122.7, 120.5, 118.5, 118.1, 84.8, 61.4, 36.3, 29.8, 29.6, 19.8, 19.2, 17.5, 16.9.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{34}H_{45}NNaO_4]^+$ 554.3241; Found 554.3235.

Bis(2,4-dimethylpentan-3-yl)-2-(3-amino-[1,1'-biphenyl]-4-yl)-2-propylmalonate (1o)



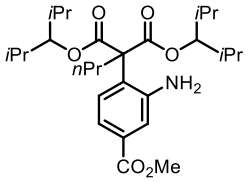
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.40 (dd, *J* = 8.3, 6.8 Hz, 2H), 7.36 – 7.27 (m, 2H), 7.00 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.87 (d, *J* = 1.9 Hz, 1H), 4.66 (t, *J* = 5.6 Hz, 2H), 4.49 (s, 2H), 2.70 – 2.31 (m, 2H), 1.96 – 1.87 (m, 4H), 1.56 – 1.40 (m, 2H), 1.02 (t, *J* = 7.3 Hz, 3H), 0.91 (m, 12H), 0.92 – 0.89 (d, *J* = 6.9 Hz, 6H), 0.74 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.5, 146.7, 141.3, 140.9, 128.7, 128.1, 127.3, 127.1, 122.2, 117.3, 116.8, 84.4, 61.7, 36.7, 29.80, 29.79, 19.8, 19.7, 18.7, 17.9, 17.4, 14.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{32}H_{47}NNaO_4]^+$ 532.3397; Found 532.3400.

Bis(2,4-dimethylpentan-3-yl)-2-(2-amino-4-(methoxycarbonyl)phenyl)-2-propylmalonate (1p)



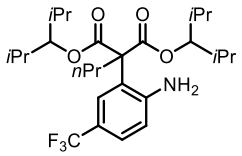
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.24 (d, *J* = 1.7 Hz, 1H), 7.06 – 7.02 (m, 1H), 6.75 – 6.71 (m, 1H), 6.60 (dd, *J* = 7.9, 1.4 Hz, 1H), 4.61 (t, *J* = 5.6 Hz, 2H), 4.38 (s, 2H), 2.54 – 2.36 (m, 2H), 2.02 – 1.80 (m, 4H), 1.46 – 1.37 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H), 0.88 – 0.84 (m, 12H), 0.76 (d, *J* = 6.9 Hz, 6H), 0.69 (d, *J* = 6.8 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.5, 146.5, 128.6, 127.5, 123.1, 118.4, 118.2, 84.3, 61.7, 36.7, 29.8, 19.8, 19.6, 18.8, 17.9, 17.3, 14.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{28}H_{45}NNaO_6]^+$ 514.3139; Found 514.3149.

Bis(2,4-dimethylpentan-3-yl)-2-(2-amino-5-(trifluoromethyl)phenyl)-2-propylmalonate (1q)



White solid, m.p. = 52 – 55 ºC.

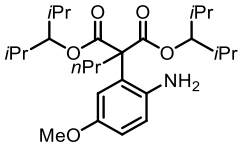
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 2.1 Hz, 1H), 7.30 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.65 (d, *J* = 8.3 Hz, 1H), 4.78 (s, 2H), 4.62 (t, *J* = 5.6 Hz, 2H), 2.52 – 2.38 (m, 2H), 1.96 – 1.83 (m, 4H), 1.50 – 1.37 (m, 2H), 1.01 (t, *J* = 7.3 Hz, 3H), 0.91 – 0.86 (m, 12H), 0.76 (d, *J* = 6.9 Hz, 6H), 0.68 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.8, 149.4, 125.7 (q, *J* = 3.7 Hz), 125.0 (q, *J* = 4.1 Hz), 124.9 (q, *J* = 271.7 Hz), 122.1, 119.8 (q, *J* = 32.6 Hz), 117.3, 84.7, 61.5, 36.4, 29.6, 19.7, 19.5, 18.6, 17.7, 17.1, 14.1.

^{19}F NMR (376 MHz, Chloroform-*d*) δ -61.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{27}H_{42}F_3NNaO_4]^+$ 524.2958; Found 524.2960.

Bis(2,4-dimethylpentan-3-yl)-2-(2-amino-5-methoxyphenyl)-2-propylmalonate (1r)



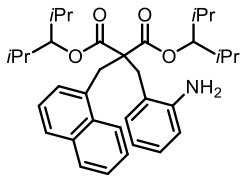
Yellow solid, m.p. = 51 – 53 ºC.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.89 (d, *J* = 2.8 Hz, 1H), 6.68 (dd, *J* = 8.6, 2.8 Hz, 1H), 6.58 (d, *J* = 8.6 Hz, 1H), 4.62 (t, *J* = 5.6 Hz, 2H), 4.08 (s, 2H), 3.74 (s, 3H), 2.50 – 2.31 (m, 2H), 1.97 – 1.84 (m, 4H), 1.48 – 1.39 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H), 0.90 – 0.86 (m, 12H), 0.79 (d, *J* = 6.9 Hz, 6H), 0.73 (d, *J* = 6.7 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.3, 152.7, 140.2, 125.0, 119.3, 114.4, 113.8, 84.4, 61.9, 56.1, 36.8, 29.8, 19.8, 19.6, 18.8, 17.9, 17.4, 14.4.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{27}H_{45}NNaO_5]^+$ 486.3190; Found 486.3184.

Bis(2,4-dimethylpentan-3-yl)-2-(2-aminobenzyl)-2-(naphthalen-1-ylmethyl)malonate (1t)



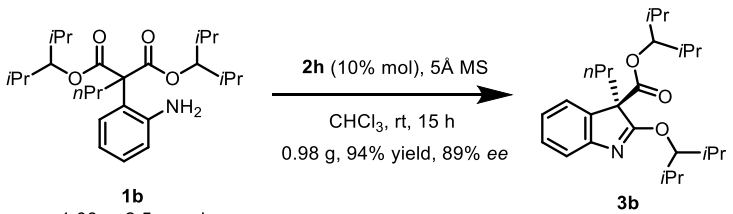
Colorless oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 8.2 Hz, 1H), 7.85 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.59 (d, *J* = 7.2 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.37 (t, *J* = 7.7 Hz, 1H), 6.95 – 6.85 (m, 1H), 6.86 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.59 – 6.45 (m, 2H), 4.65 (t, *J* = 5.8 Hz, 2H), 4.06 (s, 2H), 3.86 (s, 2H), 3.57 (s, 2H), 1.90 – 1.74 (m, 4H), 0.81 – 0.78 (m, 12H), 0.68 (d, *J* = 6.7 Hz, 6H), 0.63 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.5, 146.0, 134.1, 132.9, 132.8, 131.9, 129.0, 127.9, 127.5, 126.3, 126.2, 125.6, 125.3, 123.5, 121.2, 118.5, 116.9, 85.6, 59.9, 33.3, 33.0, 29.9, 29.5, 19.7, 19.6, 17.9, 17.1.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{35}H_{47}NNaO_4]^+$ 568.3397; Found 568.3405.

5. Gram-scale reaction

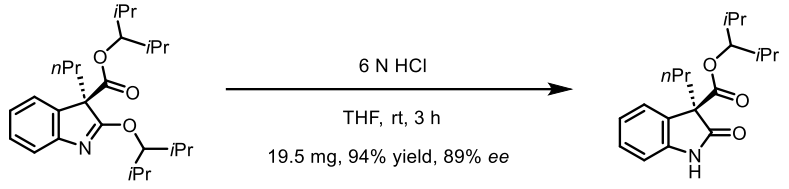


1b
1.08 g, 2.5 mmol

3b

A suspension of **1b** (2.5 mmol, 1.08 g), **2h** (0.25 mmol, 10 mol%) and 5Å MS (750 mg) in $CHCl_3$ (25 mL) was stirred in a 100 mL round-bottom flask at room temperature for 15 h under argon. After completion of the reaction (monitored by TLC), the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/ethyl acetate (10:1, v/v) to afford the product **3b** in 94% yield (980 mg) with 89% *ee* as a colorless oil.

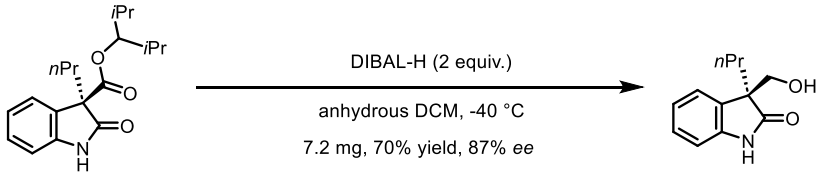
6. Synthetic transformations



3b

4b

6 N HCl (0.075 mmol, 1.5 equiv.) was added to the solution of **3b** (0.05 mmol, 1.0 equiv.) in THF (0.5 mL) at room temperature. Then the mixture was stirred for 3 h at room temperature. After completion of the reaction (monitored by TLC), the solvent was removed in vacuo. The residue was purified by column chromatography on silica gel, eluting with petroleum ether/ethyl acetate (10:1, v/v) to give the compound **4b** in 94% yield (19.5 mg) with 89% *ee* as a white solid.



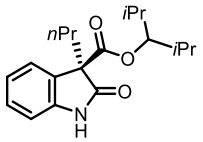
4b

5

DIBAL-H (1.0 M in Tol, 0.1 mmol, 2.0 equiv.) was added to a solution of **4b** (0.05 mmol, 1.0 equiv.) in anhydrous DCM (0.5 mL) at -40 ℃. And the mixture was stirred for 2 h. After completion of the reaction (monitored by TLC), the solvent was removed

in vacuo. The residue was purified by column chromatography on silica gel, eluting with ethyl acetate to give the compound **5** in 70% yield (7.2 mg) with 87% *ee* as a colorless oil.

2,4-dimethylpentan-3-yl (*R*)-2-oxo-3-propylindoline-3-carboxylate (4b)



19.5 mg, 94% yield, 89% *ee,* white solid, m.p. = 89 – 91 ºC. The product was isolated by flash chromatography with petroleum ether/ethyl acetate (10:1, v/v).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.02 (s, 1H), 7.26 – 7.19 (m, 2H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 4.54 (t, *J* = 6.1 Hz, 1H), 2.33 – 2.17 (m, 2H), 1.84 – 1.75 (m, 1H), 1.72 – 1.65 (m, 1H), 1.22 – 1.11 (m, 1H), 1.05 – 0.94 (m, 1H), 0.88 – 0.84 (m, 6H), 0.78 (d, *J* = 6.7 Hz, 3H), 0.65 (d, *J* = 6.8 Hz, 3H), 0.46 (d, *J* = 6.7 Hz, 3H).

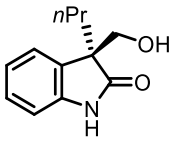
^{13}C NMR (101 MHz, Chloroform-*d*) δ 177.3, 169.3, 141.7, 129.3, 128.8, 123.6, 122.5, 109.9, 84.1, 60.5, 35.5, 29.5, 29.4, 19.4, 19.4, 17.0, 17.0, 16.5, 14.1.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{19}H_{27}NNaO_3]^+$ 340.1883; Found 340.1882.

Chiral HPLC: Chiralpak IG, hexane:*i*PrOH = 95:5, 0.7 mL/min, 254 nm; t_R = 12.1 min (major), 13.4 min (minor).

$[\alpha]^{23}_D$ -61.6 (*c* 1.0, $CHCl_3$).

(*S*)-3-(hydroxymethyl)-3-propylindolin-2-one (5)



7.2 mg, 70% yield, 87% *ee,* colorless oil. The product was isolated by flash chromatography with ethyl acetate.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 (s, 1H), 7.25 – 7.16 (m, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.7 Hz, 1H), 3.91 (d, *J* = 10.9 Hz, 1H), 3.78 (d, *J* = 10.8 Hz, 1H),

2.02 – 1.94 (m, 2H), 1.78 – 1.70 (m, 1H), 1.17 – 1.06 (m, 1H), 1.03 – 0.91 (m, 1H), 0.81 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.8, 141.4, 130.7, 128.3, 123.3, 122.7, 110.0, 67.3, 55.5, 35.2, 17.4, 14.2.

HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $[C_{12}H_{15}NNaO_2]^+$ 228.0995; Found 228.0993.

Chiral HPLC: Chiralpak AD-H, hexane:*i*PrOH = 70:30, 1.0 mL/min, 254 nm; t_R = 5.0 min (major), 9.3 min (minor).

$[\alpha]^{23}_D$ +16.4 (*c* 1.0, $CHCl_3$)

7. References

[1] C. Xie, J. Kim, B. Mai, S. Cao, R. Ye, X. Wang, P. Liu, O. Kwon. Enantioselective Synthesis of Quaternary Oxindoles: Desymmetrizing Staudinger–Aza–Wittig Reaction Enabled by a Bespoke HypPhos Oxide Catalyst. *J. Am. Chem. Soc.* **2022**, *144*, 21318-21327.

[2] A. H. Horchar, J. E. Dean, A. R. Lake, J. E. Carsley, T. R. Lillevig, S. Liu and K. S. Petersen. Synthesis of Lactams via a Chiral Phosphoric Acid-Catalyzed Aniline Cyclization. *J. Org. Chem.* **2024**, *89*, 12725-12738.

[3] Zheng, W.-Y.; Wang, Z.-Q.; Li, X.-Z.; Li, Z.-C.; Wu, H.; Rexit, A. A.; He, Y.-P. Enantioselective Catalytic Urech Hydantoin Synthesis. *Org. Chem. Front.* **2025**, *12*, 4417-4423.

8. Crystallographic data for 4f (CCDC 2430733)

Bond precision:	C-C =0.0019 A	Wavelength=1.54184	
Cell:	a=11.74413(4)	b=11.74413(4)	c=32.511796(15)
	alpha=90	beta=90	gamma=90
Temperature:	108 K		
	Calculated		Reported
Volume	4429.86(4)		4429.85(4)
Space group	P 43 21 2		P 43 21 2
Hall group	P 4nw 2abw		P 4nw 2abw
Moiety formula	C24 H29 N O4		C24 H29 N O4
Sum formula	C24 H29 N O4		C24 H29 N O4
Mr	395.4		395.48
Dx,g cm-3	1.186		1.186
Z	8		8
Mu (mm-1)	0.644		0.644
F000	1696.0		1696.0
F000’	1701.07		
h,k,lmax	141440		141439
Nref	4624[2737]		4585
Tmin,Tmax	0.902,0.914		0.868,1.000
Tmin’	0.902		
Correction method= # Reported T Limits: Tmin=0.868Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness= 1.68/0.99		Theta(max)= 76.024	
R(reflections)= 0.0261(4485)		wR2(reflections)= 0.0658(4585)	
S = 1.054	Npar= 267		

Table 1. Crystal data and structure refinement for a.

Identification code	a
Empirical formula	C24 H29 N O4
Formula weight	395.48
Temperature	108(2) K
Wavelength	1.54184Å

Crystal system	Tetragonal	
Space group	$P4_32_12$	
Unit cell dimensions	a = 11.74413(4) Å	a= 90 °
	b = 11.74413(4) Å	b= 90 °
	c = 32.11796(15) Å	g = 90 °
Volume	4429.85(4) $?^3$	
Z	8	
Density (calculated)	1.186 Mg/m^3	
Absorption coefficient	0.644 mm^{-1}	
F(000)	1696	
Crystal size	0.160 x 0.150 x 0.140 mm^3	
Theta range for data collection	4.008 to 76.024?	
Index ranges	-14<=h<=14, -14<=k<=14, -29<=l<=39	
Reflections collected	68000	
Independent reflections	4585 [R(int) = 0.0236]	
Completeness to theta = 67.684?	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86791	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4585 / 1 / 267	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0654	
R indices (all data)	R1 = 0.0266, wR2 = 0.0657	
Absolute structure parameter	0.01(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.150 and -0.166 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^x 10^3)for a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2650(1)	6825(1)	3008(1)	30(1)
C(1)	3039(1)	3970(1)	3478(1)	22(1)
O(2)	5830(1)	4103(1)	3066(1)	24(1)
N(2)	4743(1)	3068(1)	2601(1)	21(1)
C(9)	5146(1)	3346(1)	2982(1)	20(1)
C(11)	5552(1)	1823(1)	3495(1)	21(1)
C(12)	3315(1)	5057(1)	3324(1)	22(1)
C(7)	3842(1)	1804(1)	3032(1)	19(1)
C(2)	3974(1)	2150(1)	2620(1)	20(1)
O(3)	6225(1)	1416(1)	3193(1)	22(1)
C(8)	4597(1)	2539(1)	3305(1)	20(1)
C(6)	3129(1)	912(1)	3132(1)	23(1)
C(10)	3964(1)	3205(1)	3648(1)	22(1)
C(13)	7167(1)	661(1)	3307(1)	23(1)
C(4)	2679(1)	721(1)	2400(1)	27(1)
C(14)	7107(1)	-365(1)	3013(1)	27(1)
C(5)	2540(1)	366(1)	2810(1)	26(1)
C(3)	3401(1)	1621(1)	2298(1)	25(1)
O(4)	5670(1)	1656(1)	3861(1)	30(1)
C(16)	8265(1)	1357(1)	3287(1)	29(1)
C(19)	7437(1)	-85(1)	2564(1)	33(1)
C(20)	2468(1)	5751(1)	3162(1)	24(1)
C(21)	1340(1)	5384(1)	3154(1)	28(1)
C(22)	1069(1)	4321(1)	3308(1)	31(1)
C(23)	1911(1)	3611(1)	3469(1)	27(1)
C(24)	3795(1)	7211(1)	2982(1)	31(1)
C(15)	5921(1)	-907(1)	3024(1)	35(1)
C(18)	8241(2)	2362(2)	3588(1)	42(1)
C(17)	9296(1)	598(2)	3378(1)	41(1)

Table 3. Bond lengths [Å] and angles [ ] for t.

O(1)-C(20)	1.3721(17)
O(1)-C(24)	1.4219(18)
C(1)-C(23)	1.3907(19)
C(1)-C(12)	1.4062(19)
C(1)-C(10)	1.5105(19)
O(2)-C(9)	1.2281(16)
N(2)-C(9)	1.3538(16)
N(2)-C(2)	1.4082(17)
N(2)-H(2)	0.8800
C(9)-C(8)	1.5449(17)
C(11)-O(4)	1.2005(15)
C(11)-O(3)	1.3392(16)
C(11)-C(8)	1.5293(18)
C(12)-C(20)	1.3869(19)
C(12)-H(12)	0.9500
C(7)-C(6)	1.3785(18)
C(7)-C(2)	1.3954(17)
C(7)-C(8)	1.5165(17)
C(2)-C(3)	1.3809(18)
O(3)-C(13)	1.4647(15)
C(8)-C(10)	1.5404(17)
C(6)-C(5)	1.3999(19)
C(6)-H(6)	0.9500
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(13)-C(16)	1.5282(19)
C(13)-C(14)	1.533(2)
C(13)-H(13)	1.0000
C(4)-C(5)	1.392(2)
C(4)-C(3)	1.395(2)
C(4)-H(4)	0.9500
C(14)-C(19)	1.529(2)
C(14)-C(15)	1.531(2)
C(14)-H(14)	1.0000
C(5)-H(5)	0.9500
C(3)-H(3)	0.9500

C(16)-C(18)	1.527(2)
C(16)-C(17)	1.532(2)
C(16)-H(16)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.394(2)
C(21)-C(22)	1.381(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.393(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

C(20)-O(1)-C(24)	117.48(11)
C(23)-C(1)-C(12)	119.14(13)
C(23)-C(1)-C(10)	120.80(12)
C(12)-C(1)-C(10)	120.06(12)
C(9)-N(2)-C(2)	111.69(10)
C(9)-N(2)-H(2)	124.2
C(2)-N(2)-H(2)	124.2
O(2)-C(9)-N(2)	126.86(12)
O(2)-C(9)-C(8)	124.82(11)
N(2)-C(9)-C(8)	108.32(11)
O(4)-C(11)-O(3)	125.68(13)
O(4)-C(11)-C(8)	124.40(12)
O(3)-C(11)-C(8)	109.92(10)

C(20)-C(12)-C(1)	120.03(12)
C(20)-C(12)-H(12)	120.0
C(1)-C(12)-H(12)	120.0
C(6)-C(7)-C(2)	120.63(12)
C(6)-C(7)-C(8)	130.80(11)
C(2)-C(7)-C(8)	108.56(11)
C(3)-C(2)-C(7)	121.78(12)
C(3)-C(2)-N(2)	128.65(12)
C(7)-C(2)-N(2)	109.57(11)
C(11)-O(3)-C(13)	118.72(10)
C(7)-C(8)-C(11)	110.23(10)
C(7)-C(8)-C(10)	114.82(11)
C(11)-C(8)-C(10)	110.39(10)
C(7)-C(8)-C(9)	101.85(10)
C(11)-C(8)-C(9)	107.37(10)
C(10)-C(8)-C(9)	111.68(10)
C(7)-C(6)-C(5)	118.46(12)
C(7)-C(6)-H(6)	120.8
C(5)-C(6)-H(6)	120.8
C(1)-C(10)-C(8)	113.08(10)
C(1)-C(10)-H(10A)	109.0
C(8)-C(10)-H(10A)	109.0
C(1)-C(10)-H(10B)	109.0
C(8)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
O(3)-C(13)-C(16)	107.63(11)
O(3)-C(13)-C(14)	106.61(10)
C(16)-C(13)-C(14)	115.63(12)
O(3)-C(13)-H(13)	108.9
C(16)-C(13)-H(13)	108.9
C(14)-C(13)-H(13)	108.9
C(5)-C(4)-C(3)	121.45(12)
C(5)-C(4)-H(4)	119.3
C(3)-C(4)-H(4)	119.3
C(19)-C(14)-C(15)	109.95(13)
C(19)-C(14)-C(13)	113.65(12)
C(15)-C(14)-C(13)	110.80(12)
C(19)-C(14)-H(14)	107.4

C(15)-C(14)-H(14)	107.4
C(13)-C(14)-H(14)	107.4
C(4)-C(5)-C(6)	120.27(13)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(2)-C(3)-C(4)	117.40(12)
C(2)-C(3)-H(3)	121.3
C(4)-C(3)-H(3)	121.3
C(18)-C(16)-C(13)	111.74(12)
C(18)-C(16)-C(17)	110.08(14)
C(13)-C(16)-C(17)	110.32(13)
C(18)-C(16)-H(16)	108.2
C(13)-C(16)-H(16)	108.2
C(17)-C(16)-H(16)	108.2
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(1)-C(20)-C(12)	124.40(13)
O(1)-C(20)-C(21)	115.10(12)
C(12)-C(20)-C(21)	120.49(13)
C(22)-C(21)-C(20)	119.42(14)
C(22)-C(21)-H(21)	120.3
C(20)-C(21)-H(21)	120.3
C(21)-C(22)-C(23)	120.73(13)
C(21)-C(22)-H(22)	119.6
C(23)-C(22)-H(22)	119.6
C(1)-C(23)-C(22)	120.18(13)
C(1)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
O(1)-C(24)-H(24A)	109.5
O(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	30(1)	27(1)	32(1)	4(1)	2(1)	2(1)
C(1)	26(1)	25(1)	14(1)	-4(1)	4(1)	-2(1)
O(2)	28(1)	24(1)	19(1)	1(1)	2(1)	-5(1)
N(2)	27(1)	23(1)	14(1)	3(1)	1(1)	-1(1)
C(9)	22(1)	21(1)	17(1)	2(1)	2(1)	2(1)
C(11)	22(1)	23(1)	18(1)	3(1)	-1(1)	-6(1)
C(12)	22(1)	25(1)	18(1)	-3(1)	2(1)	-2(1)
C(7)	21(1)	21(1)	16(1)	0(1)	-1(1)	2(1)
C(2)	22(1)	22(1)	18(1)	1(1)	1(1)	3(1)
O(3)	24(1)	25(1)	17(1)	3(1)	-1(1)	2(1)
C(8)	22(1)	21(1)	15(1)	2(1)	1(1)	-2(1)
C(6)	23(1)	24(1)	21(1)	1(1)	1(1)	0(1)
C(10)	28(1)	24(1)	14(1)	0(1)	3(1)	-2(1)
C(13)	23(1)	26(1)	21(1)	6(1)	-3(1)	1(1)
C(4)	25(1)	31(1)	26(1)	-8(1)	-5(1)	2(1)
C(14)	29(1)	25(1)	29(1)	3(1)	-2(1)	2(1)
C(5)	24(1)	25(1)	31(1)	-3(1)	-1(1)	-3(1)
C(3)	29(1)	30(1)	17(1)	-2(1)	-2(1)	4(1)
O(4)	28(1)	45(1)	17(1)	7(1)	-1(1)	1(1)
C(16)	24(1)	37(1)	25(1)	4(1)	-1(1)	-3(1)
C(19)	39(1)	35(1)	26(1)	-2(1)	0(1)	4(1)
C(20)	28(1)	24(1)	19(1)	-3(1)	4(1)	1(1)
C(21)	24(1)	36(1)	24(1)	-4(1)	0(1)	4(1)
C(22)	22(1)	39(1)	31(1)	-7(1)	4(1)	-5(1)
C(23)	28(1)	28(1)	26(1)	-2(1)	7(1)	-6(1)
C(24)	34(1)	28(1)	31(1)	3(1)	2(1)	-4(1)
C(15)	38(1)	27(1)	41(1)	1(1)	-3(1)	-6(1)
C(18)	35(1)	48(1)	41(1)	-9(1)	2(1)	-18(1)
C(17)	25(1)	58(1)	40(1)	7(1)	-6(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for a.

	x	y	z	U(eq)
H(2)	4938	3419	2369	26
H(12)	4081	5316	3332	26
H(6)	3040	673	3413	27
H(10A)	3621	2657	3845	27
H(10B)	4520	3674	3803	27
H(13)	7052	392	3600	28
H(4)	2274	341	2185	33
H(14)	7659	-946	3118	33
H(5)	2043	-250	2872	32
H(3)	3495	1861	2017	30
H(16)	8346	1663	2998	34
H(19A)	6945	524	2458	50
H(19B)	7346	-765	2391	50
H(19C)	8233	166	2555	50
H(21)	762	5862	3042	34
H(22)	300	4072	3305	37
H(23)	1714	2880	3573	33
H(24A)	4236	6689	2807	46
H(24B)	4128	7236	3262	46
H(24C)	3810	7975	2859	46
H(15A)	5678	-1001	3313	53
H(15B)	5947	-1652	2887	53
H(15C)	5380	-413	2877	53
H(18A)	7616	2875	3513	62
H(18B)	8965	2775	3572	62
H(18C)	8127	2082	3872	62
H(17A)	9204	243	3652	62
H(17B)	9990	1060	3376	62
H(17C)	9352	4	3165	62

_ Table 6. Torsion angles [deg]for t.

C(2)-N(2)-C(9)-O(2)	179.65(12)
C(2)-N(2)-C(9)-C(8)	-0.31(14)
C(23)-C(1)-C(12)-C(20)	-0.67(18)
C(10)-C(1)-C(12)-C(20)	178.83(11)
C(6)-C(7)-C(2)-C(3)	0.08(19)
C(8)-C(7)-C(2)-C(3)	179.06(12)
C(6)-C(7)-C(2)-N(2)	-179.90(12)
C(8)-C(7)-C(2)-N(2)	-0.92(14)
C(9)-N(2)-C(2)-C(3)	-179.19(13)
C(9)-N(2)-C(2)-C(7)	0.79(15)
O(4)-C(11)-O(3)-C(13)	2.65(19)
C(8)-C(11)-O(3)-C(13)	-177.22(10)
C(6)-C(7)-C(8)-C(11)	65.81(17)
C(2)-C(7)-C(8)-C(11)	-113.03(11)
C(6)-C(7)-C(8)-C(10)	-59.61(18)
C(2)-C(7)-C(8)-C(10)	121.55(12)
C(6)-C(7)-C(8)-C(9)	179.53(13)
C(2)-C(7)-C(8)-C(9)	0.69(13)
O(4)-C(11)-C(8)-C(7)	-116.45(14)
O(3)-C(11)-C(8)-C(7)	63.42(13)
O(4)-C(11)-C(8)-C(10)	11.45(18)
O(3)-C(11)-C(8)-C(10)	-168.68(10)
O(4)-C(11)-C(8)-C(9)	133.40(14)
O(3)-C(11)-C(8)-C(9)	-46.73(13)
O(2)-C(9)-C(8)-C(7)	179.80(12)
N(2)-C(9)-C(8)-C(7)	-0.23(13)
O(2)-C(9)-C(8)-C(11)	-64.36(16)
N(2)-C(9)-C(8)-C(11)	115.61(11)
O(2)-C(9)-C(8)-C(10)	56.78(17)
N(2)-C(9)-C(8)-C(10)	-123.26(12)
C(2)-C(7)-C(6)-C(5)	-0.17(19)
C(8)-C(7)-C(6)-C(5)	-178.89(13)
C(23)-C(1)-C(10)-C(8)	96.55(14)
C(12)-C(1)-C(10)-C(8)	-82.95(14)
C(7)-C(8)-C(10)-C(1)	-57.11(14)
C(11)-C(8)-C(10)-C(1)	177.56(11)

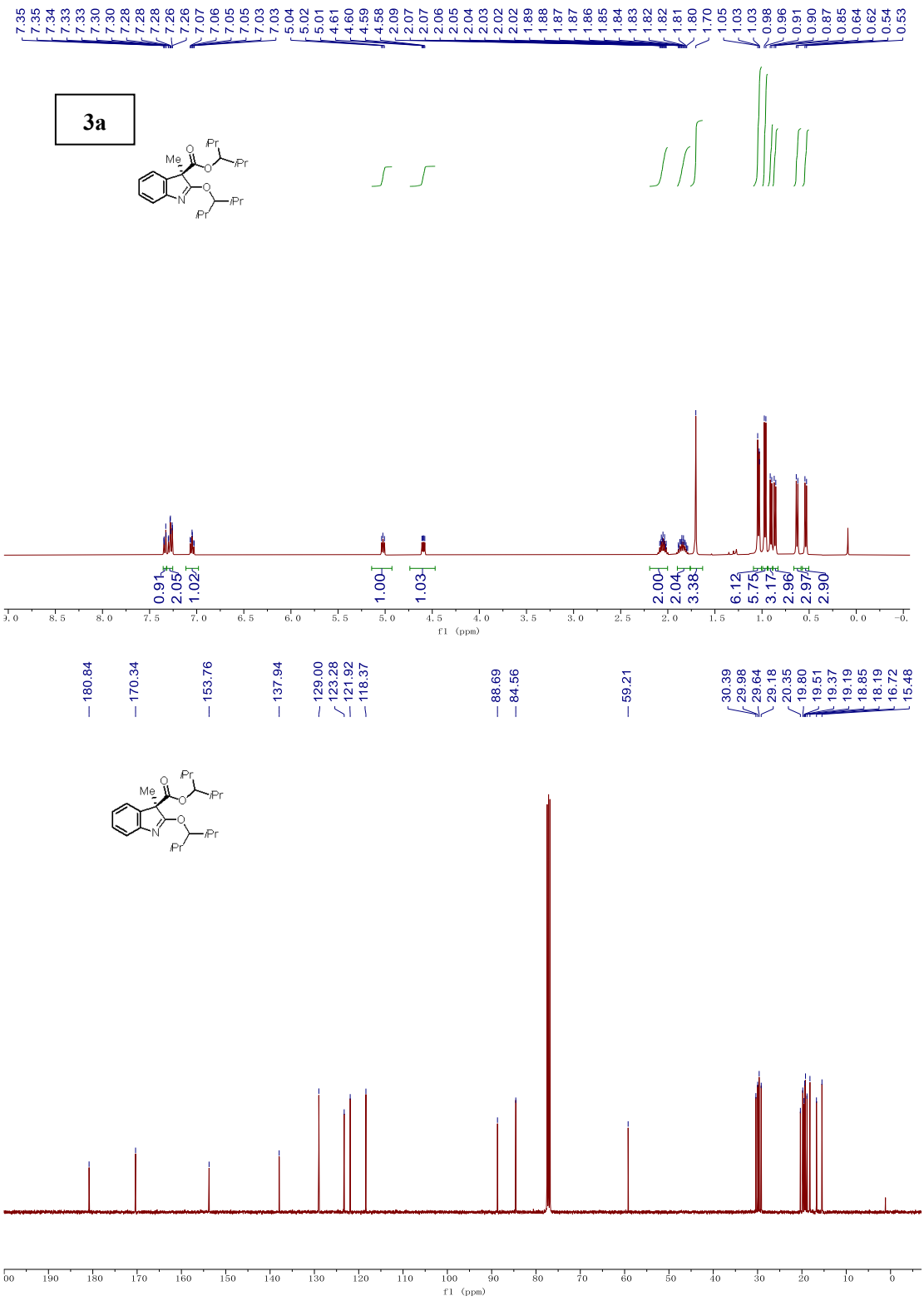
C(9)-C(8)-C(10)-C(1)	58.19(14)
C(11)-O(3)-C(13)-C(16)	-103.35(13)
C(11)-O(3)-C(13)-C(14)	132.01(12)
O(3)-C(13)-C(14)-C(19)	70.75(14)
C(16)-C(13)-C(14)-C(19)	-48.83(16)
O(3)-C(13)-C(14)-C(15)	-53.63(14)
C(16)-C(13)-C(14)-C(15)	-173.21(12)
C(3)-C(4)-C(5)-C(6)	0.0(2)
C(7)-C(6)-C(5)-C(4)	0.2(2)
C(7)-C(2)-C(3)-C(4)	0.0(2)
N(2)-C(2)-C(3)-C(4)	-179.99(13)
C(5)-C(4)-C(3)-C(2)	-0.1(2)
O(3)-C(13)-C(16)-C(18)	60.52(15)
C(14)-C(13)-C(16)-C(18)	179.55(12)
O(3)-C(13)-C(16)-C(17)	-176.67(11)
C(14)-C(13)-C(16)-C(17)	-57.64(16)
C(24)-O(1)-C(20)-C(12)	5.23(18)
C(24)-O(1)-C(20)-C(21)	-175.71(12)
C(1)-C(12)-C(20)-O(1)	179.58(11)
C(1)-C(12)-C(20)-C(21)	0.57(19)
O(1)-C(20)-C(21)-C(22)	-179.06(12)
C(12)-C(20)-C(21)-C(22)	0.0(2)
C(20)-C(21)-C(22)-C(23)	-0.5(2)
C(12)-C(1)-C(23)-C(22)	0.18(19)
C(10)-C(1)-C(23)-C(22)	-179.33(12)
C(21)-C(22)-C(23)-C(1)	0.4(2)

Symmetry transformations used to generate equivalent atoms:

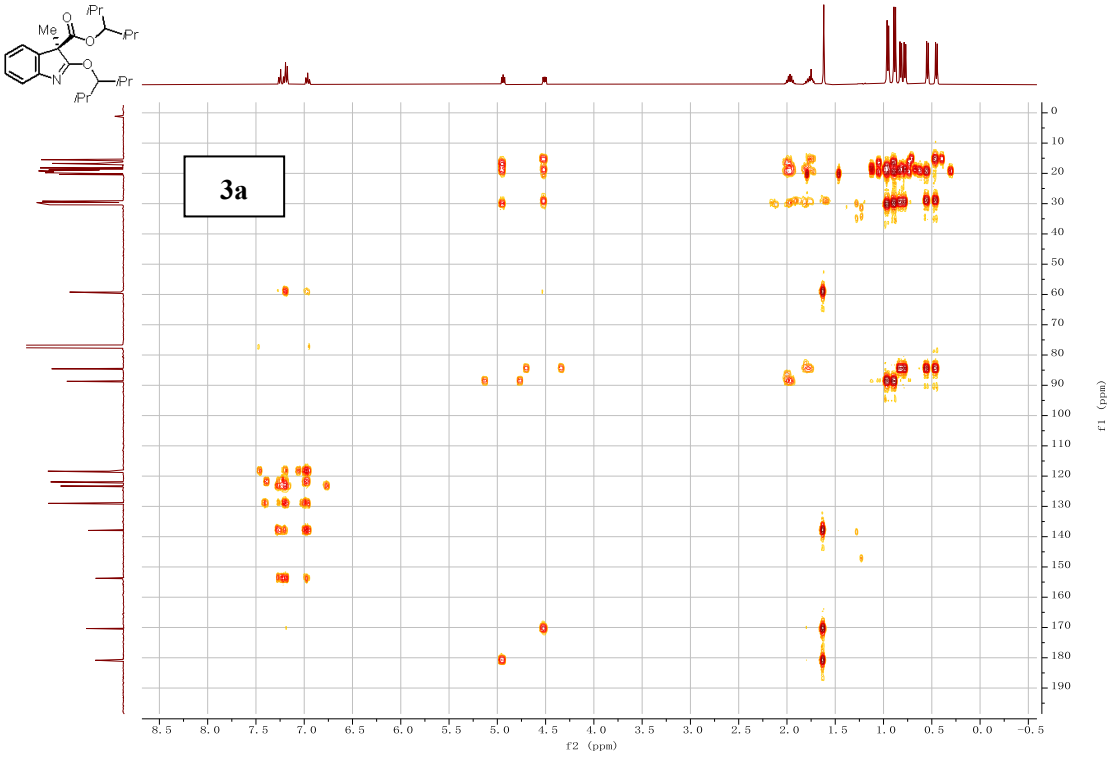
Table 7. Hydrogen bonds for t [Å and °].

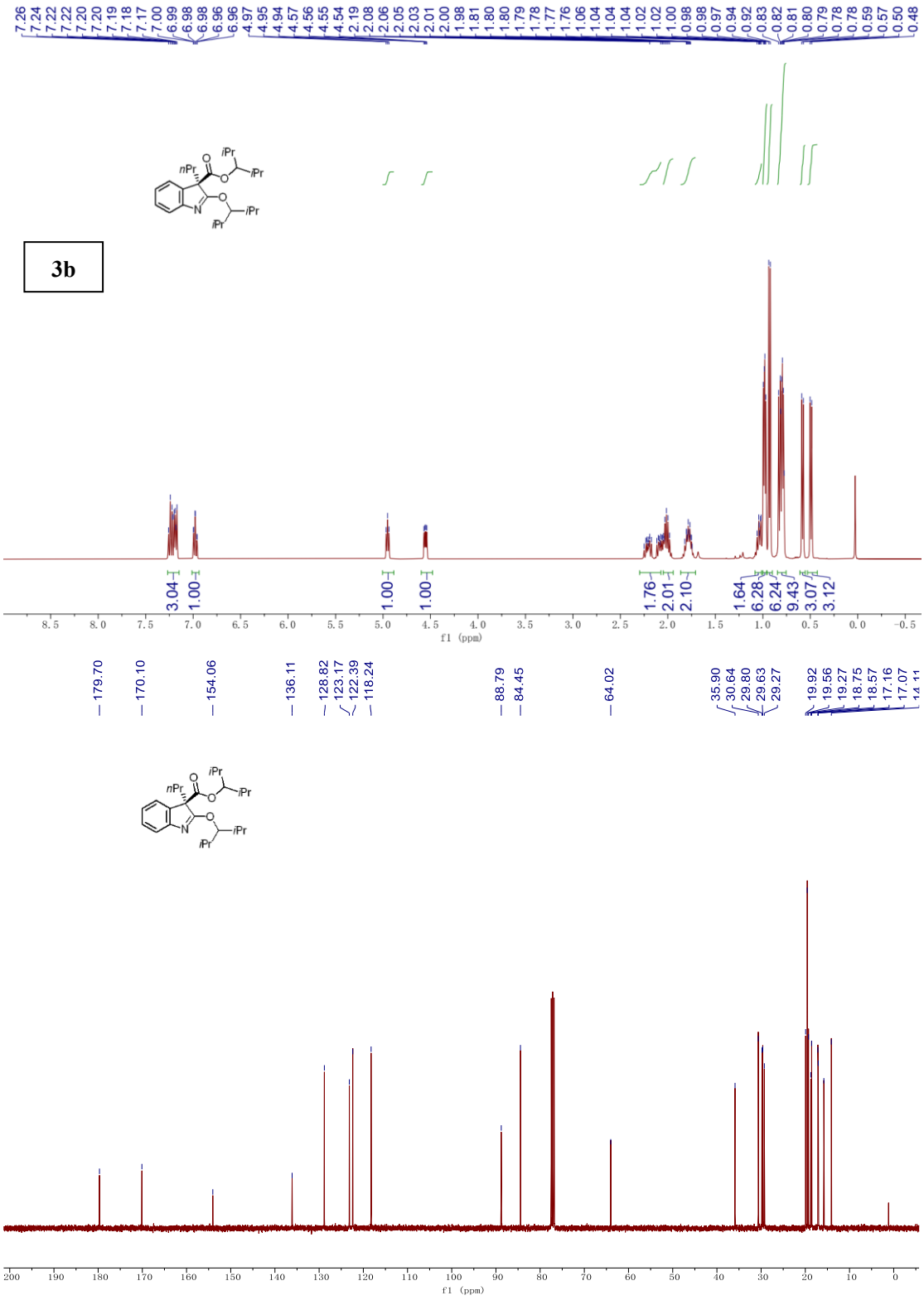
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

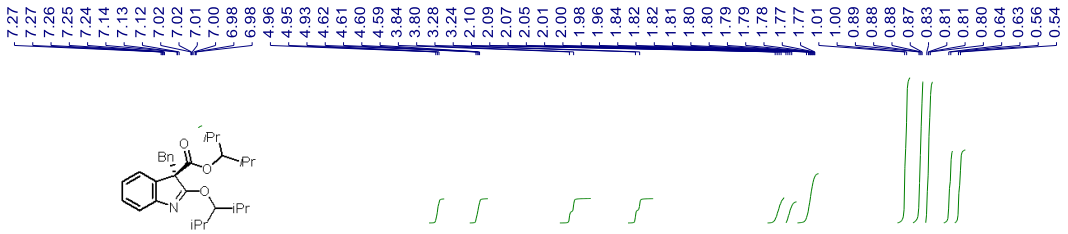
9. Copies of NMR spectra



HMBC spectrums of **3a**




3b
f1 (ppm)
f1 (ppm)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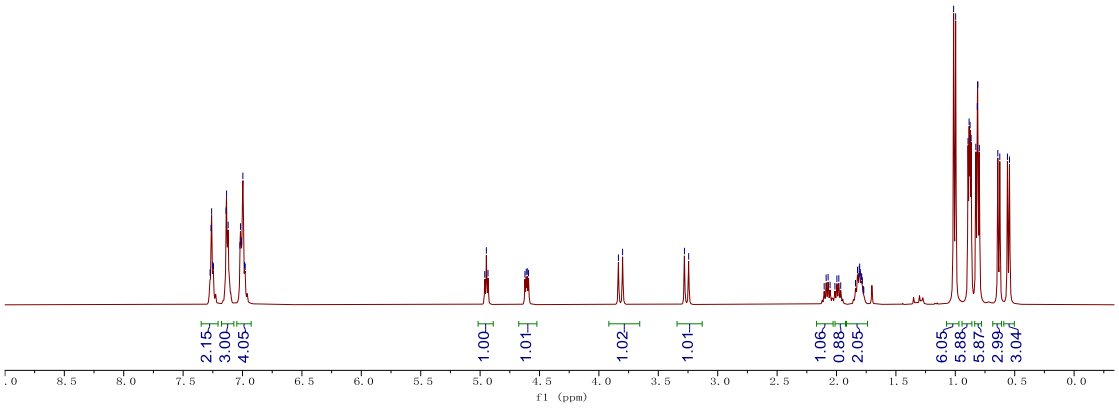
7.26
7.25
7.24
7.14
7.13
7.12
7.02
7.02
7.01
7.00
6.98
6.98
4.96
4.95
4.93
4.62
4.61
4.60
4.59
3.84
3.80
3.28
3.24
2.10
2.09
2.07
2.05
2.01
2.00
1.98
1.96
1.84
1.82
1.82
1.81
1.80
1.80
1.79
1.79
1.78
1.77
1.77
1.01
1.00
0.89
0.88
0.88
0.87
0.83
0.81
0.81
0.80
0.64
0.63
0.56
0.54
Bn
iPr
iPr
iPr
iPr
iPr

3c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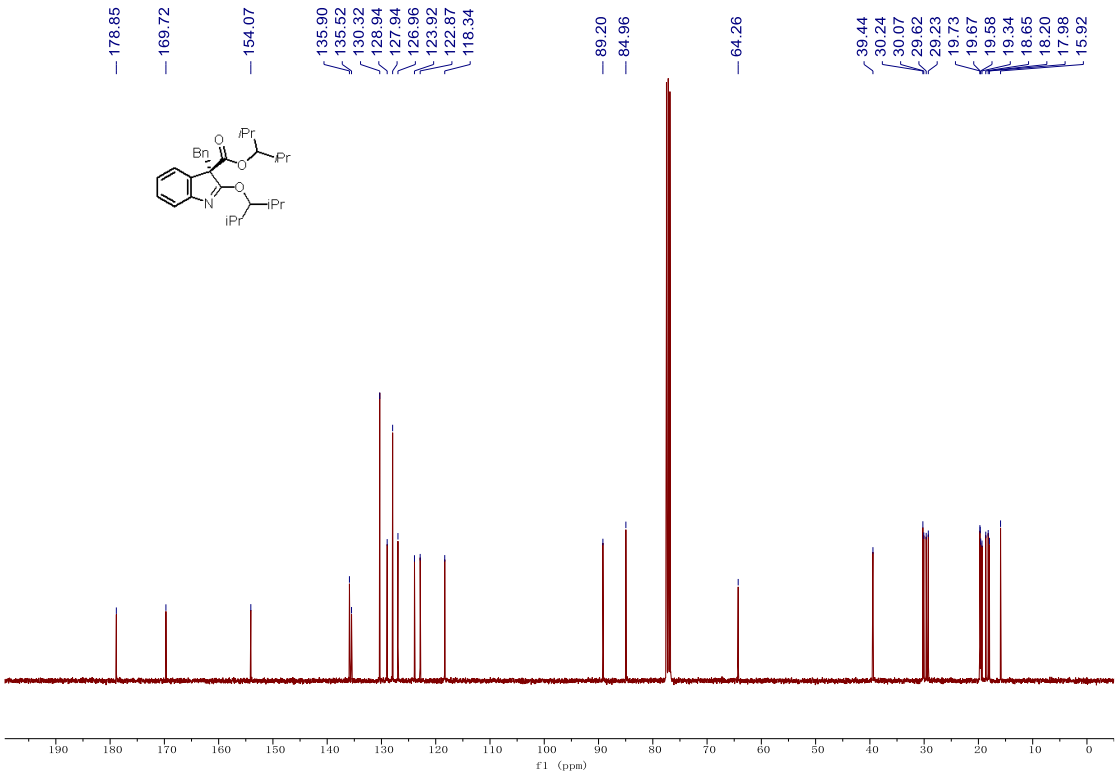
4.05
1.00
1.01
1.02
1.01
1.06
0.88
2.05
6.05
5.88
5.87
2.99
3.04
f1 (ppm)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127.94
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123.92
122.87
118.34
89.20
84.96
64.26
39.44
30.24
30.07
29.62
29.23
19.73
19.67
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18.65
18.20
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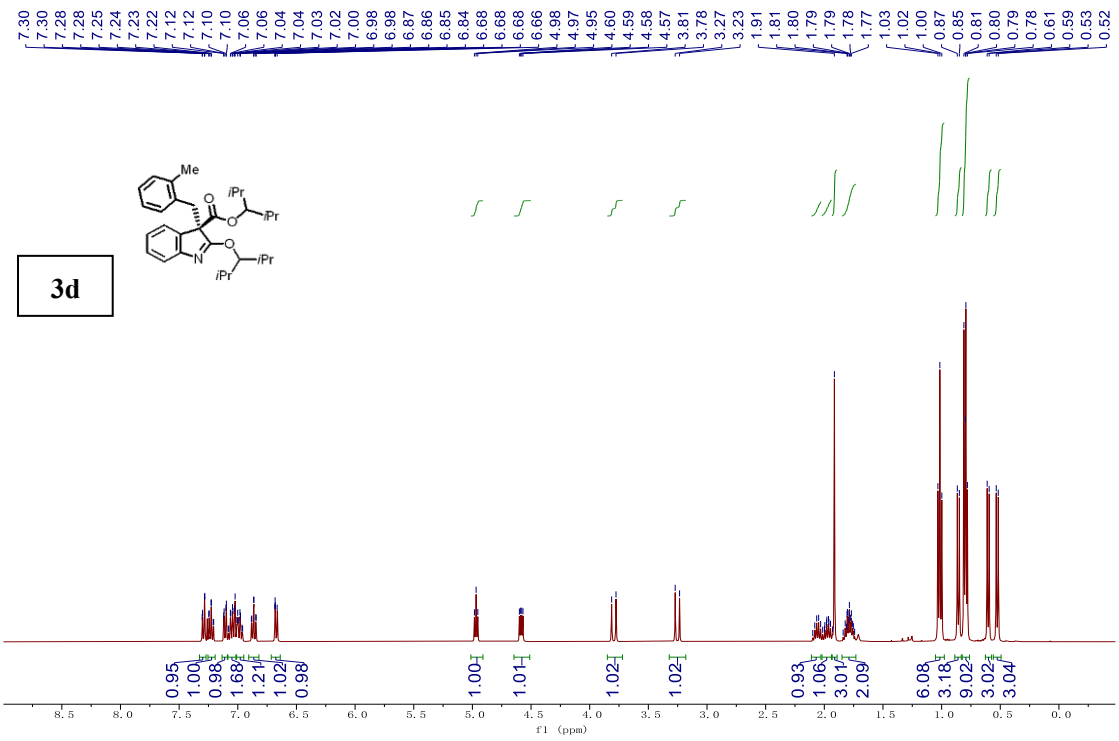
Bn
iPr
iPr
iPr
iPr
f1 (ppm)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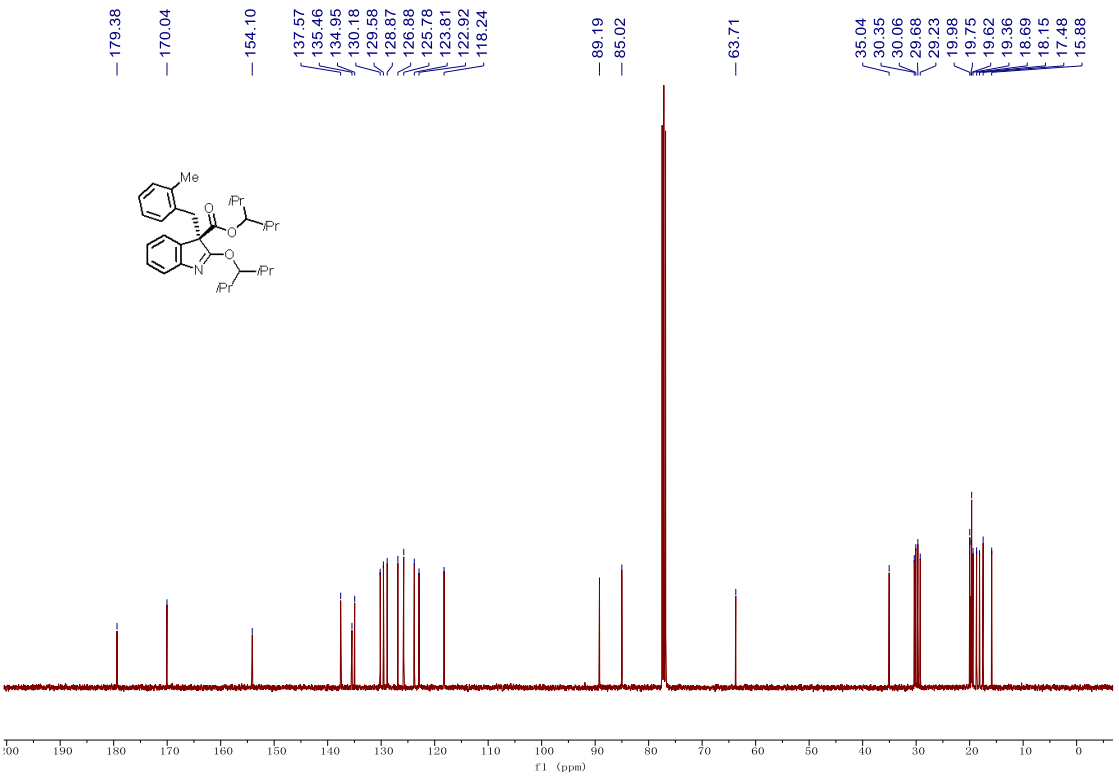
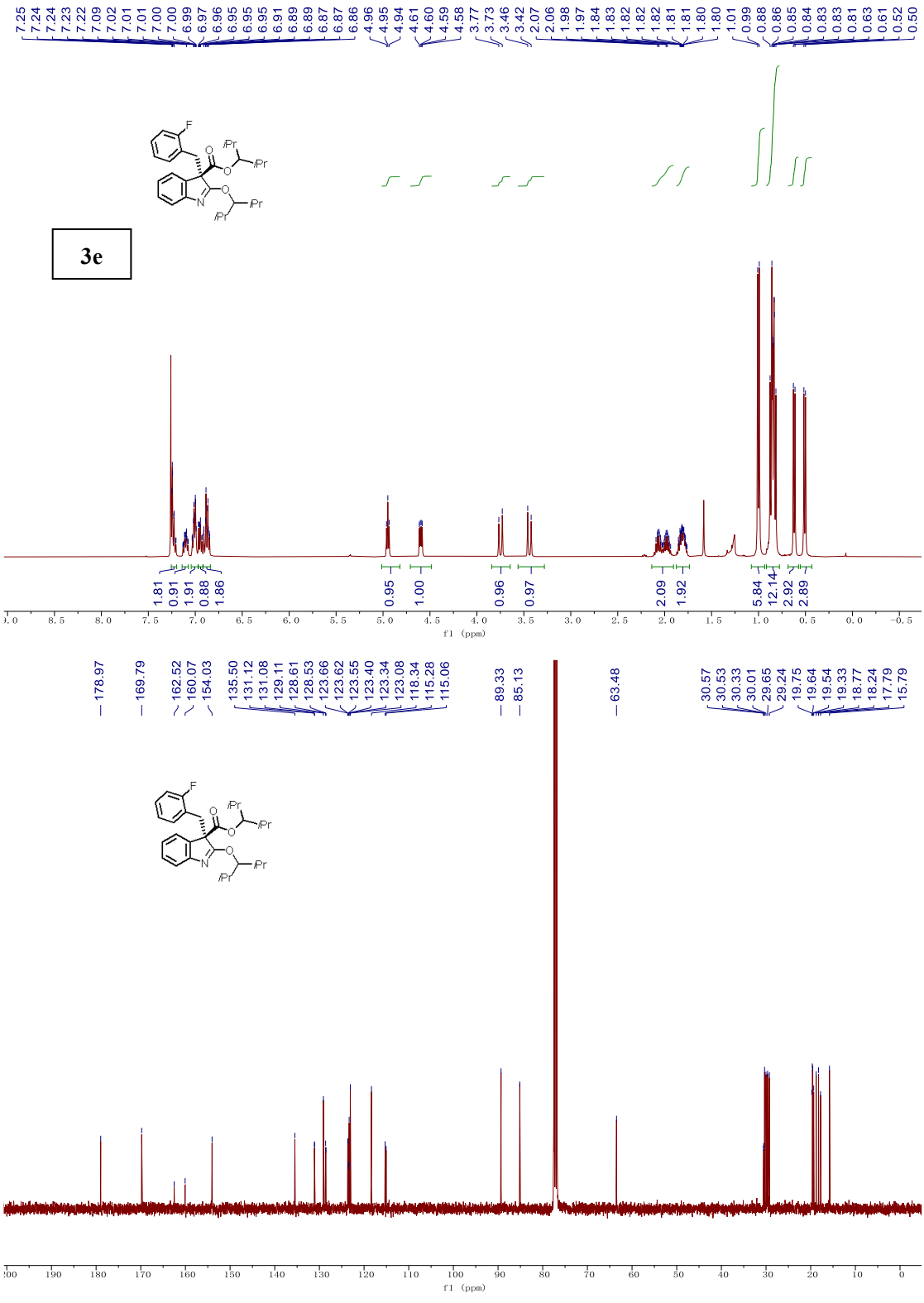
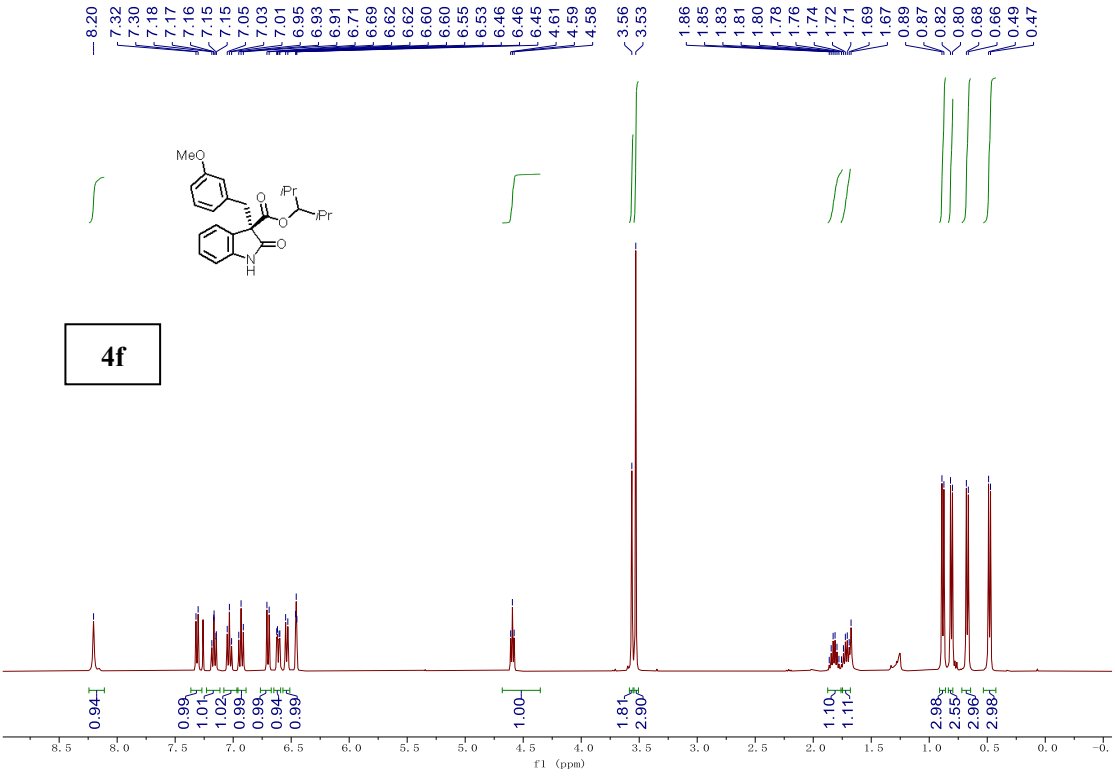
Me
iPr
iPr
iPr
iPr
3d
0.95 1.00 0.98 1.68 1.21 1.02 0.98 1.00 1.01 1.02 1.02 0.93 1.06 3.01 2.09 6.08 3.18 9.02 3.02 3.04
f1 (ppm)


179.38 170.04 154.10 137.57 135.46 134.95 130.18 129.58 128.87 126.88 125.78 123.81 122.92 118.24 89.19 85.02 63.71 35.04 30.35 30.06 29.68 29.23 19.98 19.75 19.62 19.36 18.69 18.15 17.48 15.88
Me
iPr
iPr
iPr
iPr
f1 (ppm)


3e
f1 (ppm)
f1 (ppm)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7.32
7.30
7.18
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7.16
7.15
7.15
7.05
7.03
7.01
6.95
6.93
6.91
6.71
6.69
6.62
6.62
6.60
6.60
6.55
6.53
6.46
6.46
6.45
4.61
4.59
4.58
3.56
3.53
1.86
1.85
1.83
1.81
1.80
1.78
1.76
1.74
1.72
1.71
1.69
1.67
0.89
0.87
0.82
0.80
0.68
0.66
0.49
0.47
MeO
iPr
iPr
O
O
O
N
H
0.94
0.99
1.01
1.02
0.99
0.99
0.94
0.99
1.00
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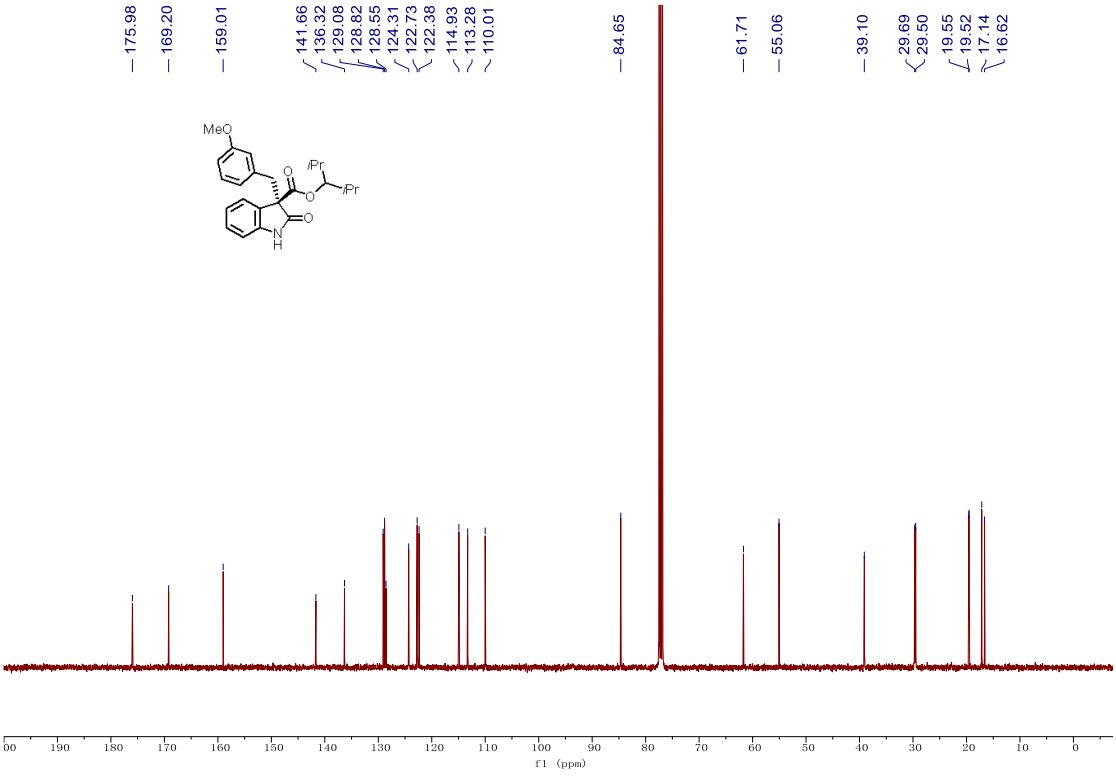
2.90
1.10
1.11
2.98
2.55
2.96
2.98
f1 (ppm)

4f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122.73
122.38
114.93
113.28
110.01
84.65
61.71
55.06
39.10
29.69
29.50
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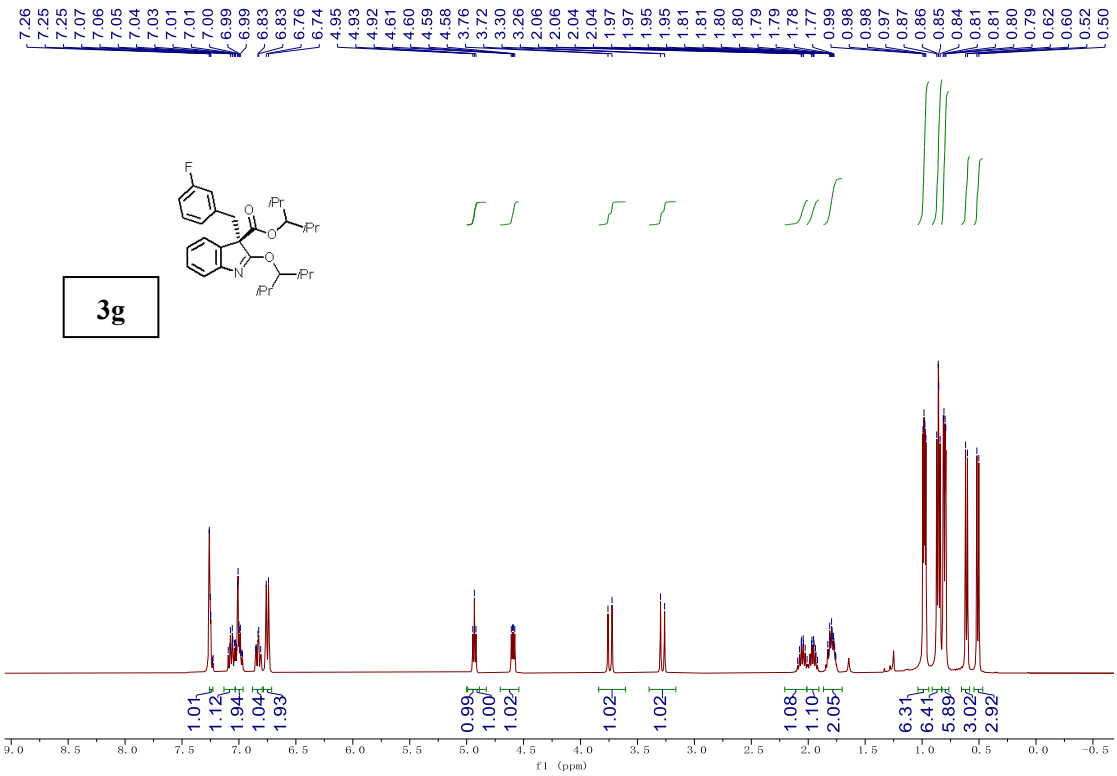
19.52
17.14
16.62
MeO
iPr
iPr
O
O
O
N
H
f1 (ppm)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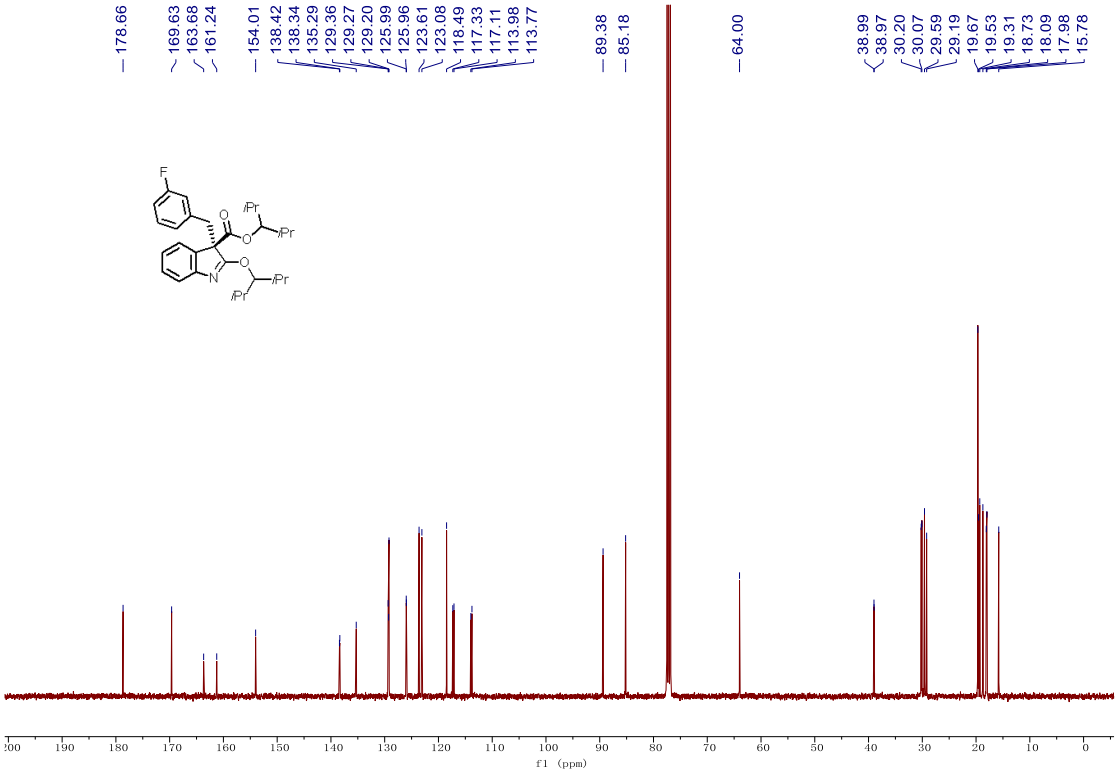
4.95 4.93 4.92 4.61 4.60 4.59 4.58 3.76 3.72 3.30 3.26 2.06 2.04 2.04 1.97 1.97 1.95 1.95 1.81 1.81 1.80 1.80 1.79 1.79 1.78 1.77 0.99 0.98 0.98 0.97 0.87 0.86 0.85 0.84 0.81 0.81 0.80 0.79 0.62 0.60 0.52 0.50
F
O
iPr
iPr
O
N
O
iPr
iPr
1.01 1.12 1.94 1.04 1.93 0.99 1.00 1.02 1.02 1.02 1.08 1.10 2.05 6.31 6.41 5.89 3.02 2.92
f1 (ppm)

3g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89.38 85.18 64.00
38.99 38.97 30.20 30.07 29.59 29.19 19.67 19.53 19.31 18.73 18.09 17.98 15.78
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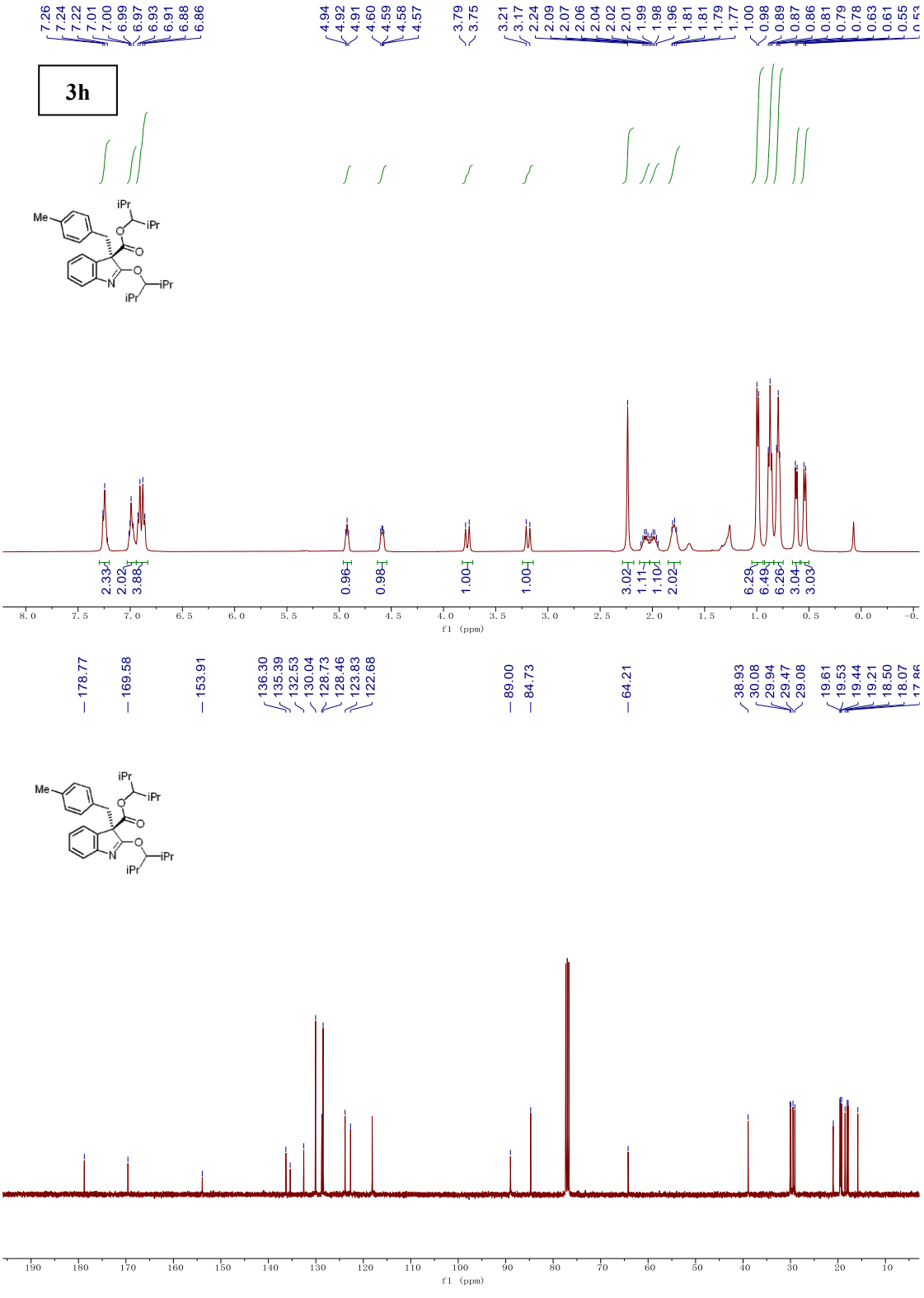
iPr
O
N
O
iPr
iPr
f1 (ppm)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O
N
O
iPr
iPr
7.26
7.24
7.22
7.01
7.00
6.99
6.97
6.93
6.91
6.88
6.86
4.94
4.92
4.91
4.60
4.59
4.58
4.57
3.79
3.75
3.21
3.17
2.24
2.09
2.07
2.06
2.04
2.02
2.01
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1.98
1.96
1.81
1.81
1.79
1.77
1.00
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0.89
0.87
0.86
0.81
0.79
0.78
0.63
0.61
0.55
2.33
2.02
3.88
0.96
0.98
1.00
1.00
3.02
1.11
1.10
2.02
6.29
6.49
6.26
3.04
3.03
f1 (ppm)
178.77
169.58
153.91
136.30
135.39
132.53
130.04
128.73
128.46
123.83
122.68
89.00
84.73
64.21
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29.47
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19.53
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19.21
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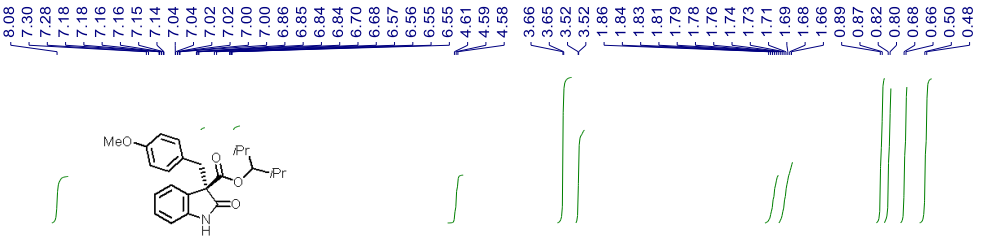
18.07
f1 (ppm)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7.16
7.15
7.14
7.04
7.04
7.02
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3.52
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1.81
1.79
1.78
1.76
1.74
1.73
1.71
1.69
1.68
1.66
0.89
0.87
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0.66
0.50
0.48
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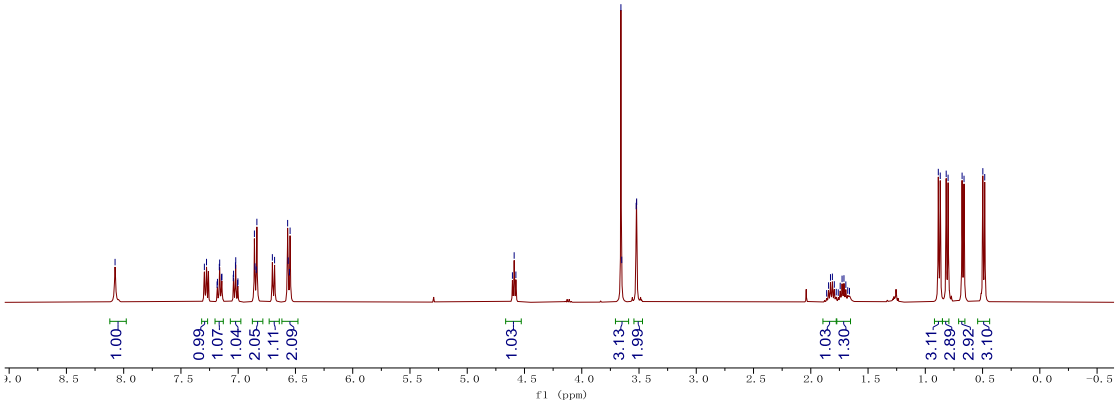
iPr
iPr
O
O
N
H
O

4i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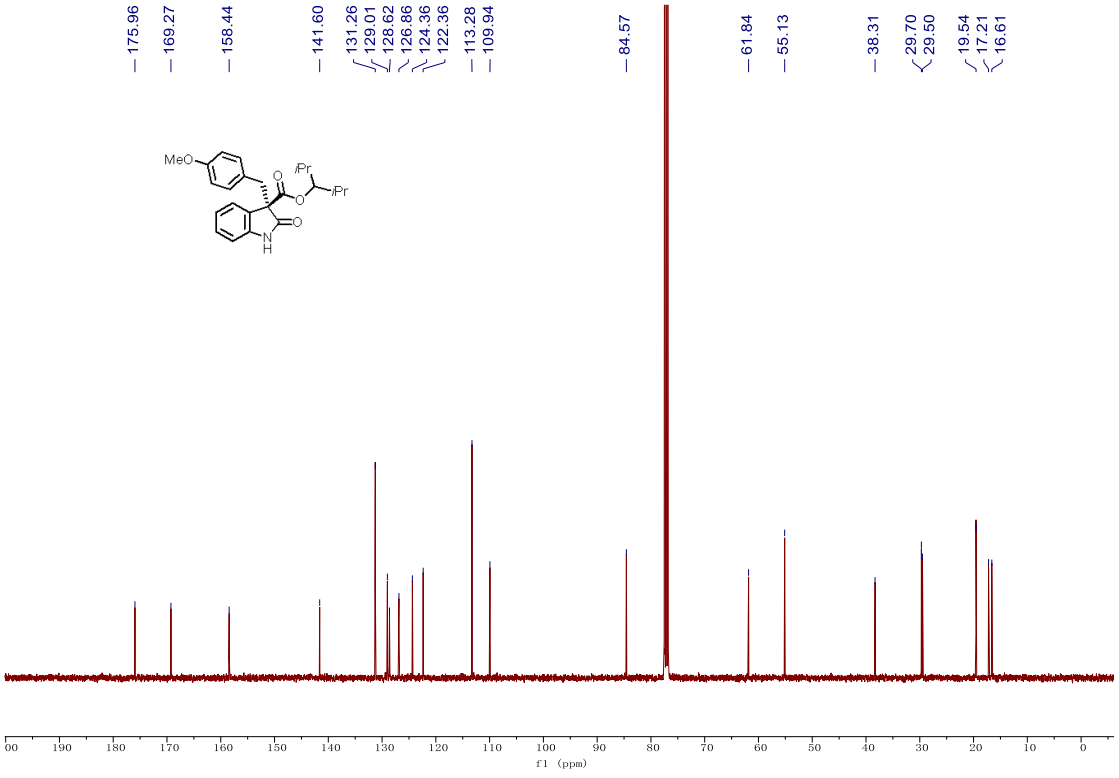
1.07
1.04
2.05
1.11
2.09
1.03
3.13
1.99
1.03
1.30
3.11
2.89
2.92
3.10
f1 (ppm)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158.44
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131.26
129.01
128.62
126.86
124.36
122.36
113.28
109.94
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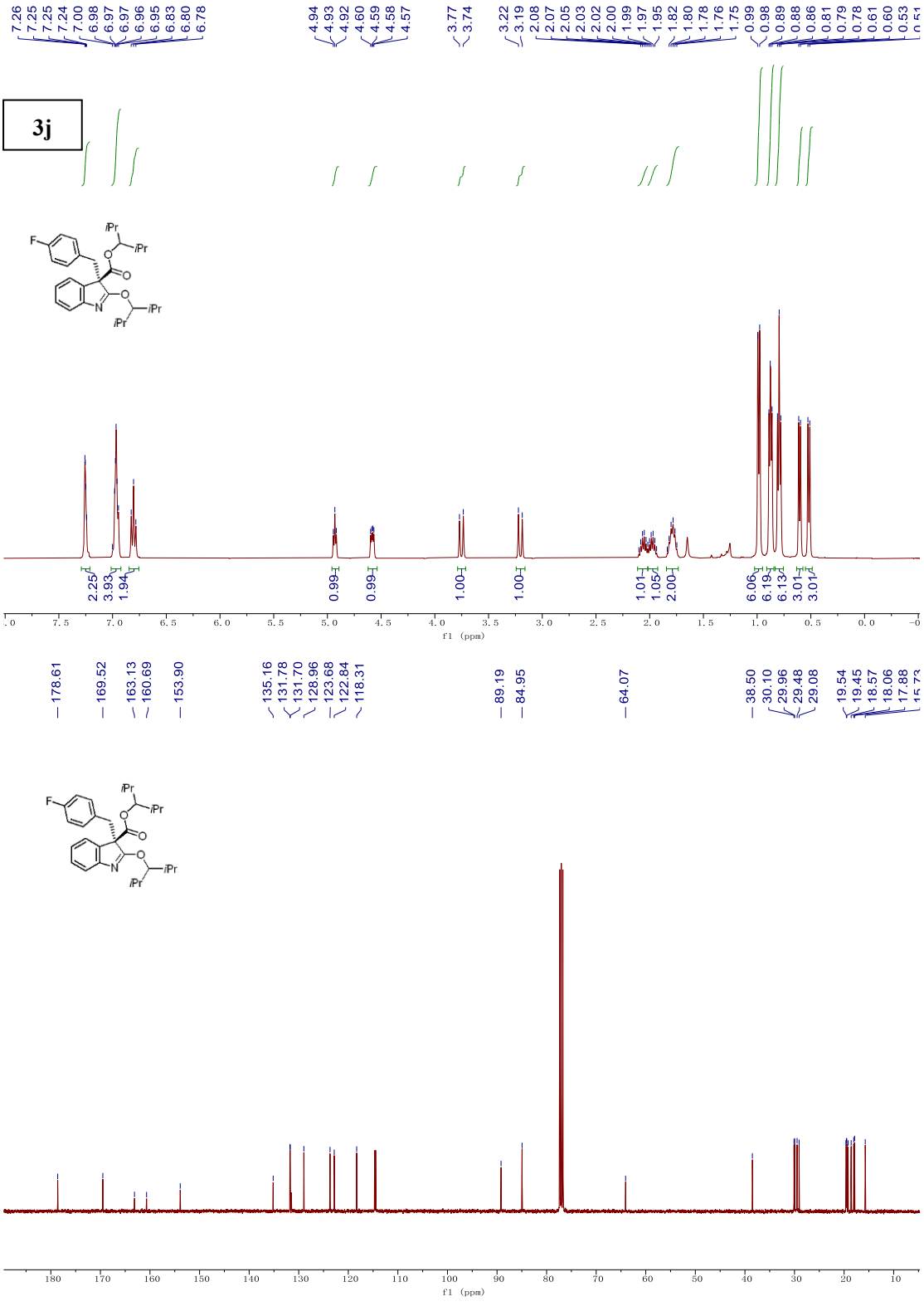
61.84
55.13
38.31
29.70
29.50
19.54
17.21
16.61
MeO
iPr
iPr
O
O
N
H
O
f1 (ppm)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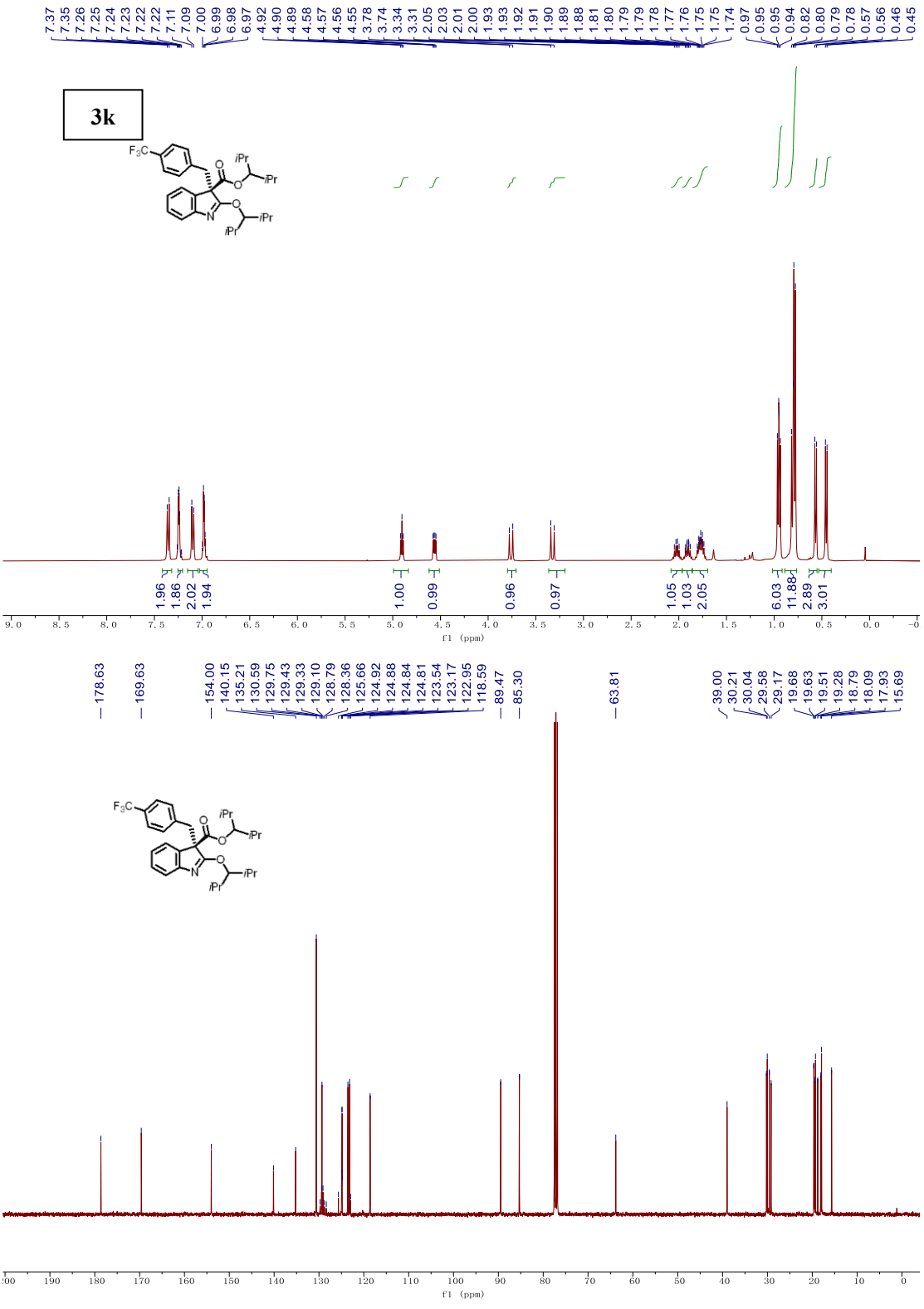
4.94 4.93 4.92 4.60 4.59 4.58 4.57
3.77 3.74
3.22 3.19
2.08 2.07 2.05 2.03 2.02 2.00 1.99 1.97 1.95 1.82 1.80 1.78 1.76 1.75
0.99 0.98 0.89 0.88 0.86 0.81 0.79 0.78 0.61 0.60 0.53
iPr
iPr
F
O
O
N
iPr
iPr
2.25 3.93 1.94 0.99 0.99 1.00 1.00 1.01 1.05 2.00 6.06 6.19 6.13 3.01 3.01
f1 (ppm)
178.61 169.52 163.13 160.69 153.90
135.16 131.78 131.70 128.96 123.68 122.84 118.31
89.19 84.95 64.07
38.50 30.10 29.96 29.48 29.08
19.54 19.45 18.57 18.06 17.88
f1 (ppm)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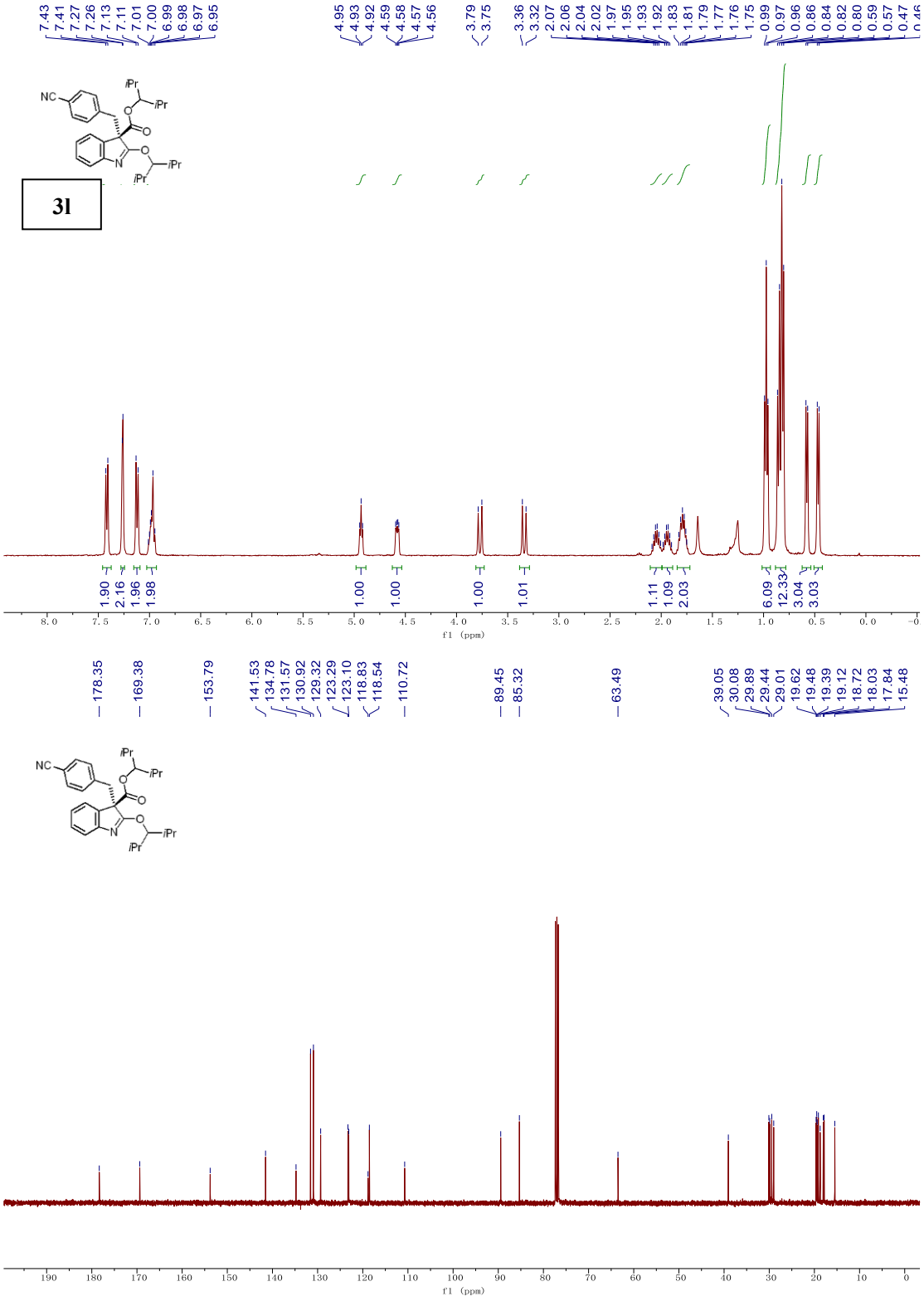
0.97 0.95 0.95 0.94 0.82 0.80 0.79 0.78 0.57 0.56 0.46 0.45
1.96 1.86 2.02 1.94 1.00 0.99 0.96 0.97 1.05 1.03 2.05 6.03 11.88 2.89 3.01
f1 (ppm)
178.63 169.63 154.00 140.15 135.21 130.59 129.75 129.43 129.33 129.10 128.79 128.36 125.66 124.92 124.88 124.84 124.81 123.54 123.17 122.95 118.59 89.47 85.30 63.81 39.00 30.21 30.04 29.58 29.17 19.68 19.63 19.51 19.28 18.79 18.09 17.93 15.69
f1 (ppm)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6.98
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6.95
4.95
4.93
4.92
4.59
4.58
4.57
4.56
3.79
3.75
3.36
3.32
2.07
2.06
2.04
2.02
1.97
1.95
1.93
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1.77
1.76
1.75
0.99
0.97
0.96
0.86
0.84
0.82
0.80
0.59
0.57
0.47
1.90
2.16
1.96
1.98
1.00
1.00
1.00
1.01
1.11
1.09
2.03
6.09
12.33
3.04
3.03
f1 (ppm)
178.35
169.38
153.79
141.53
134.78
131.57
130.92
129.32
123.29
123.10
118.83
118.54
110.72
89.45
85.32
63.49
39.05
30.08
29.89
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19.48
19.39
19.12
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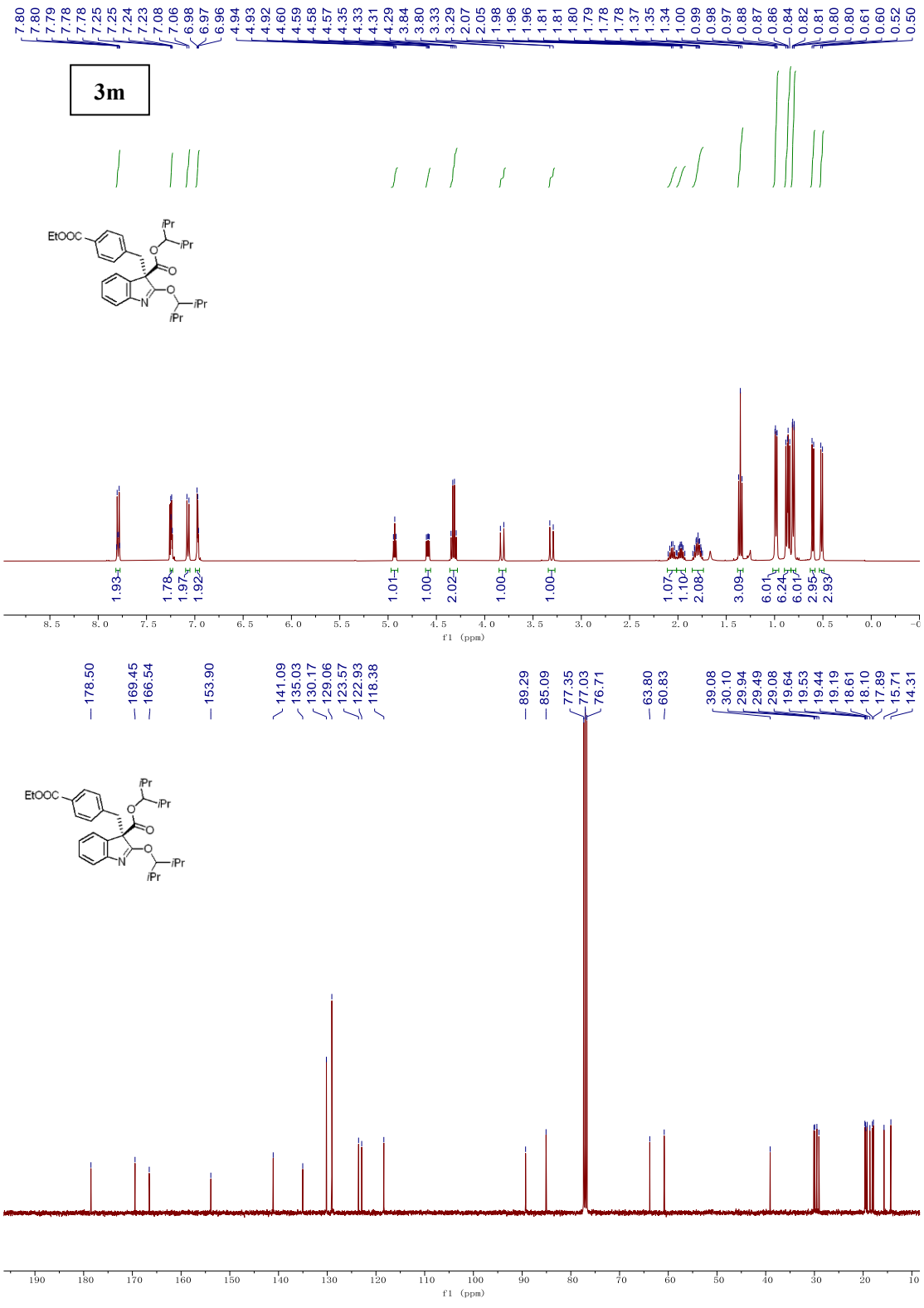
18.03
17.84
15.48
f1 (ppm)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iPr
iPr
iPr
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1.78
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1.92
1.01
1.00
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1.00
1.00
1.07
1.10
2.08
3.09
6.01
6.24
6.01
2.95
2.93
f1 (ppm)
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169.45
166.54
153.90
141.09
135.03
130.17
129.06
123.57
122.93
118.38
89.29
85.09
77.35
77.03
76.71
63.80
60.83
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30.10
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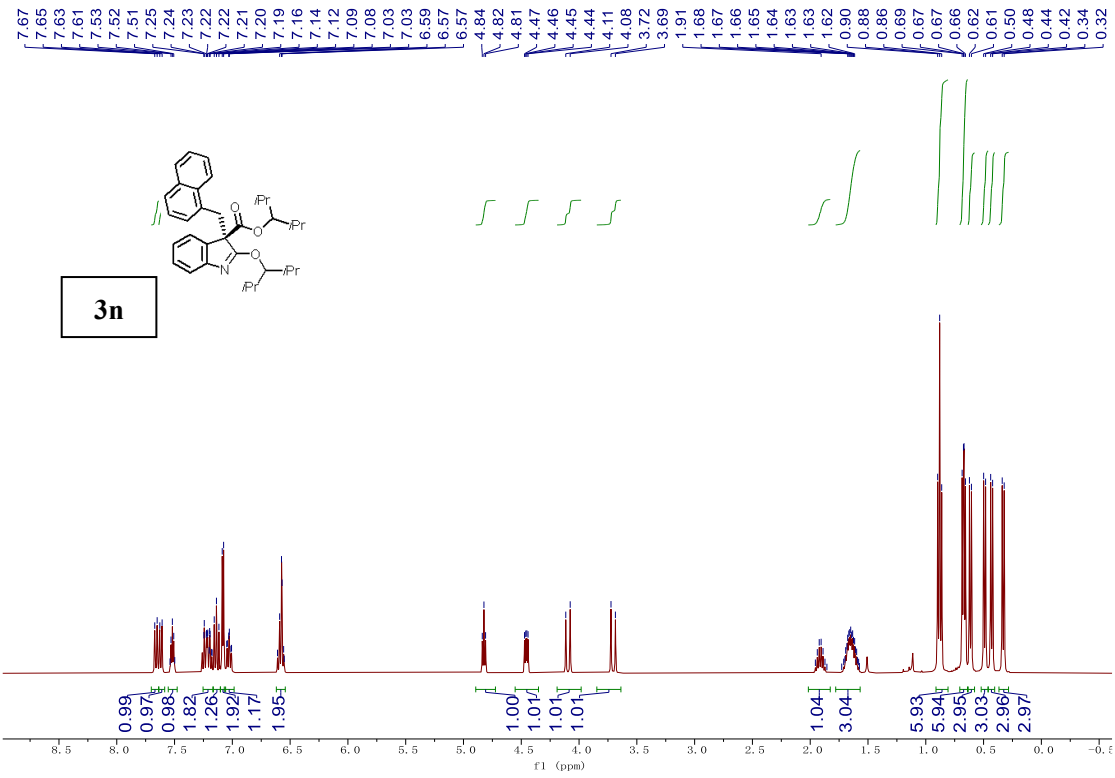
f1 (ppm)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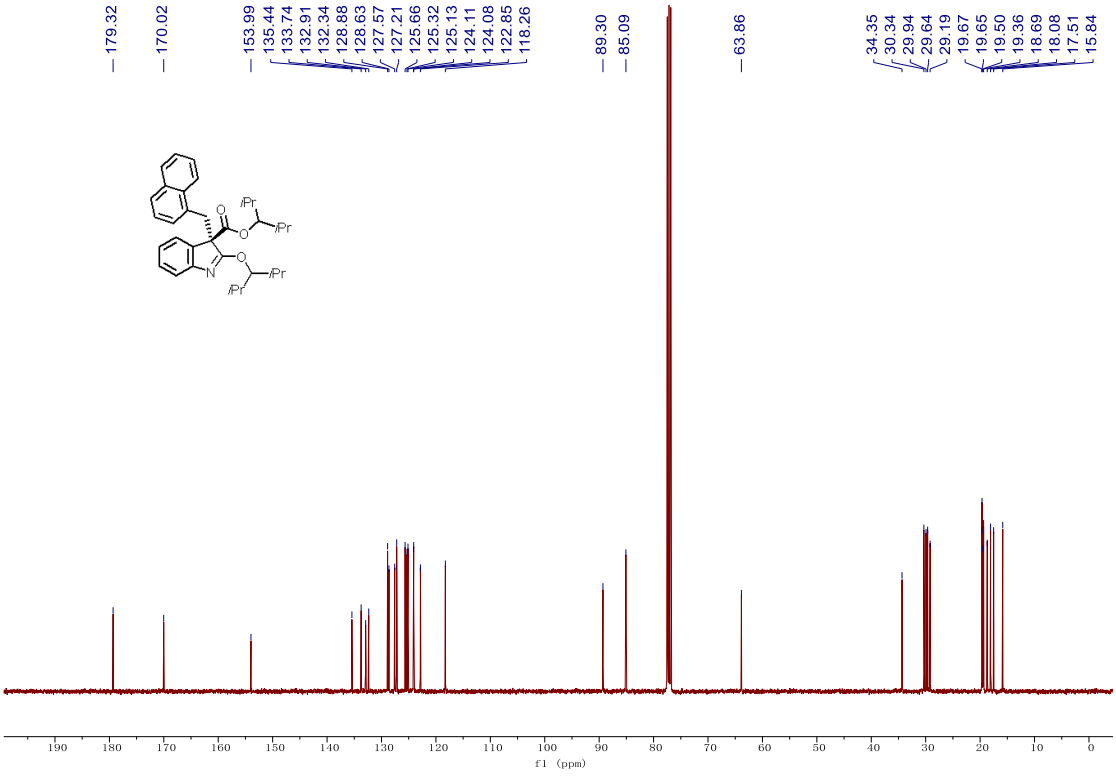
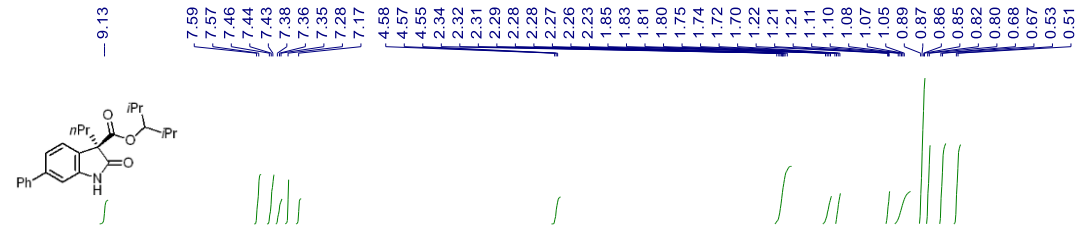
4.84 4.82 4.81 4.47 4.46 4.45 4.44 4.11 4.08 3.72 3.69
1.91 1.68 1.67 1.66 1.65 1.64 1.63 1.63 1.62 0.90 0.88 0.86 0.69 0.67 0.67 0.66 0.62 0.61 0.50 0.48 0.44 0.42 0.34 0.32
3n
0.99 0.97 0.98 1.82 1.26 1.92 1.17 1.95 1.00 1.01 1.01 1.01 1.04 3.04 5.93 5.94 2.95 3.03 2.96 2.97
f1 (ppm)


179.32 170.02 153.99 135.44 133.74 132.91 132.34 128.88 128.63 127.57 127.21 125.66 125.32 125.13 124.11 124.08 122.85 118.26 89.30 85.09 63.86 34.35 30.34 29.94 29.64 29.19 19.67 19.65 19.50 19.36 18.69 18.08 17.51 15.84
f1 (ppm)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4.58
4.57
4.55
2.34
2.32
2.31
2.29
2.28
2.28
2.27
2.26
2.23
1.85
1.83
1.81
1.80
1.75
1.74
1.72
1.70
1.22
1.21
1.21
1.11
1.10
1.08
1.07
1.05
0.89
0.87
0.86
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0.51
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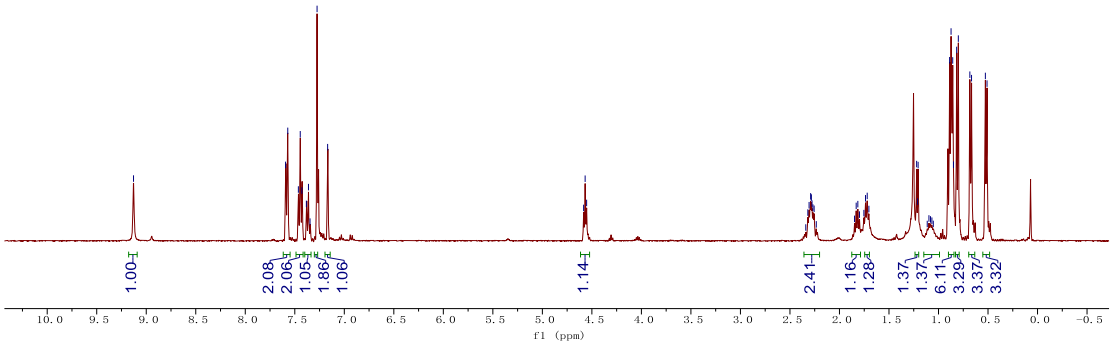
nPr
iPr
Ph
N
H

4o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3.37
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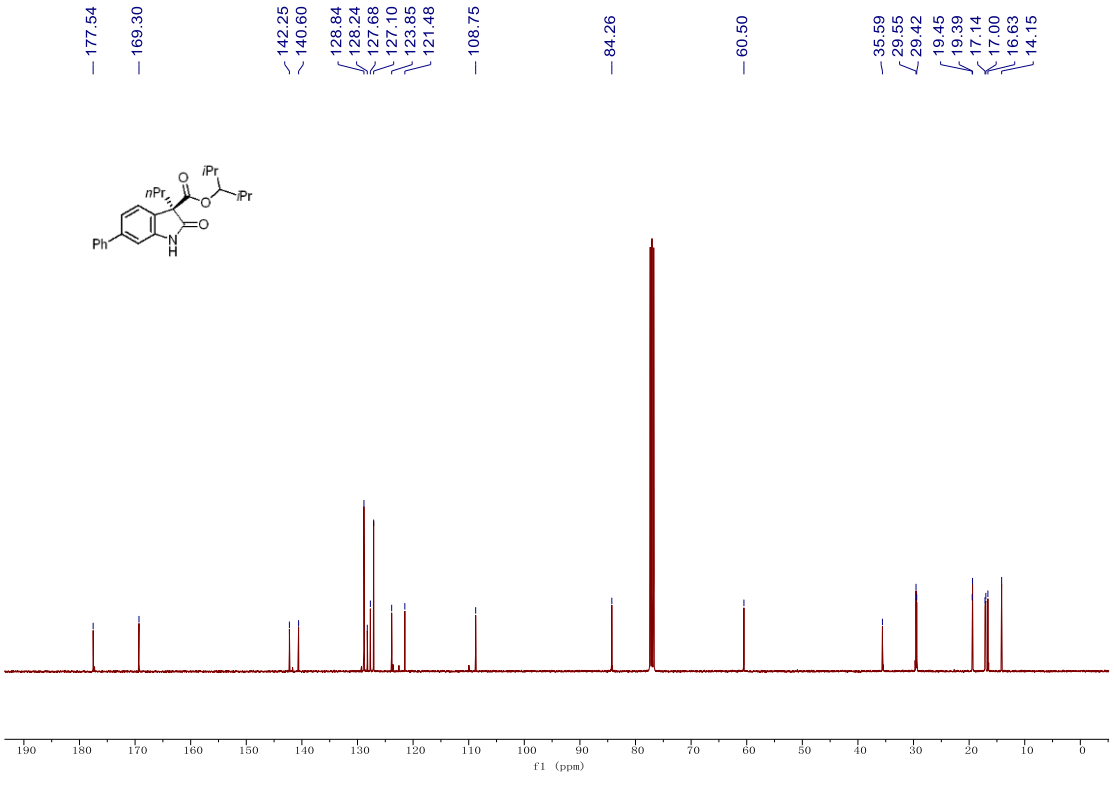
f1 (ppm)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35.59
29.55
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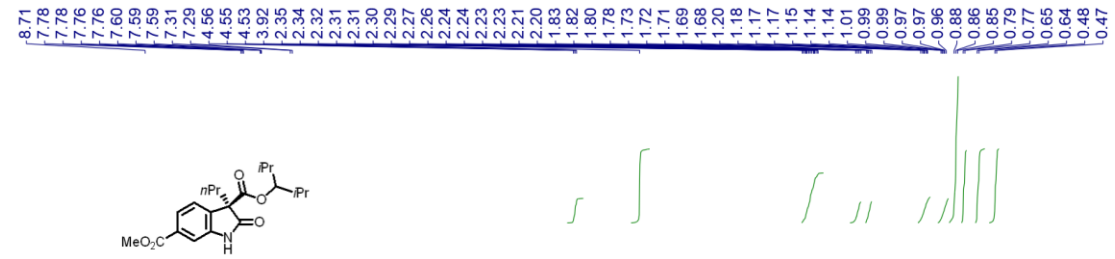
nPr
iPr
Ph
N
H
f1 (ppm)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3.92
2.35
2.34
2.32
2.31
2.31
2.30
2.29
2.27
2.26
2.24
2.24
2.23
2.23
2.21
2.20
1.83
1.82
1.80
1.78
1.73
1.72
1.71
1.69
1.68
1.20
1.18
1.17
1.17
1.15
1.14
1.14
1.01
0.99
0.99
0.97
0.97
0.96
0.88
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0.64
0.48
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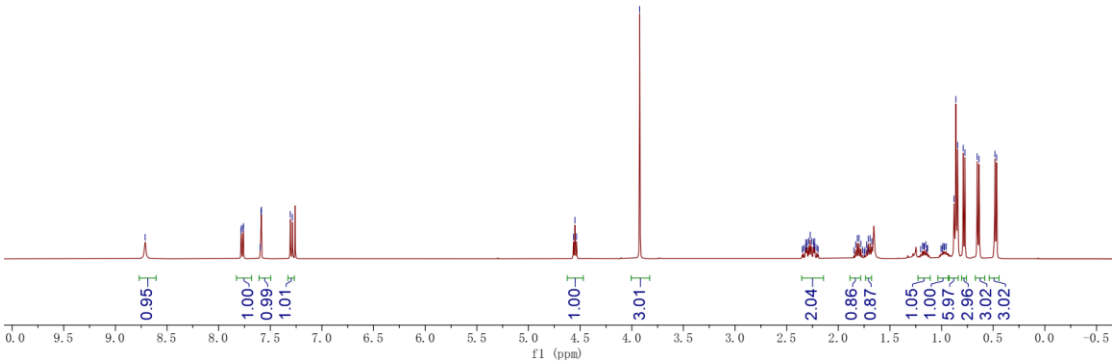
nPr
iPr
iPr
MeO2C

4p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0.99
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1.00
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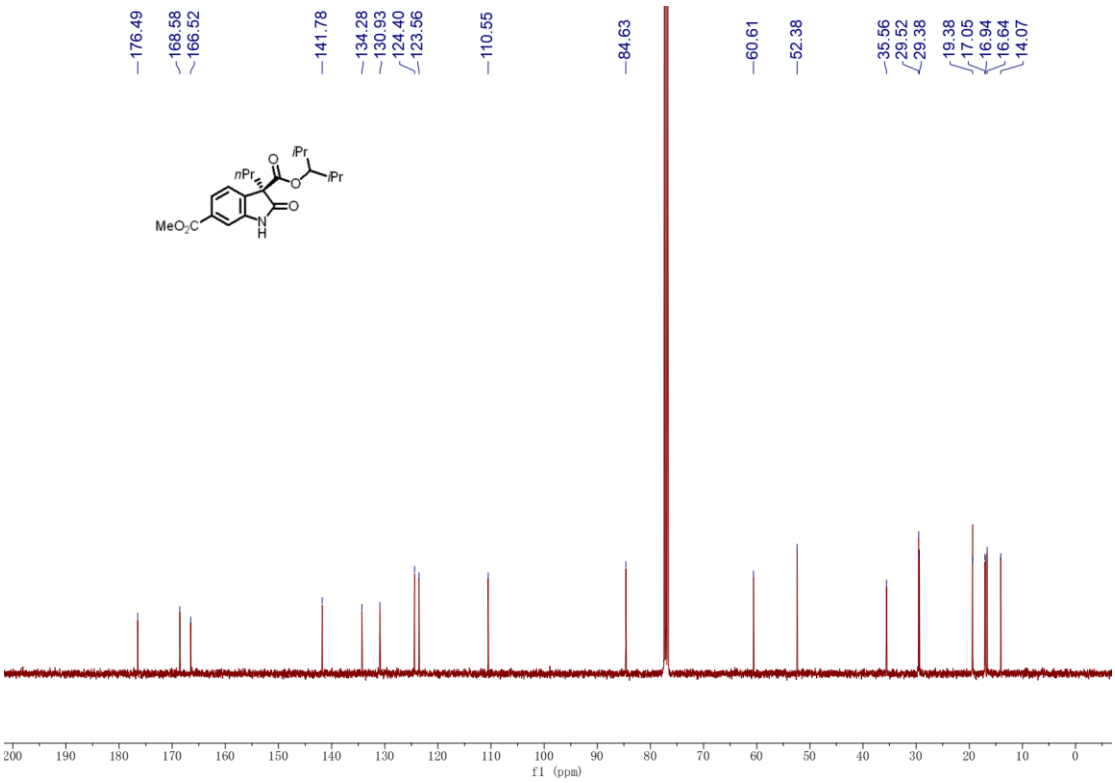
1.05
1.00
5.97
2.96
3.02
3.02
f1 (ppm)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124.40
123.56
110.55
84.63
60.61
52.38
35.56
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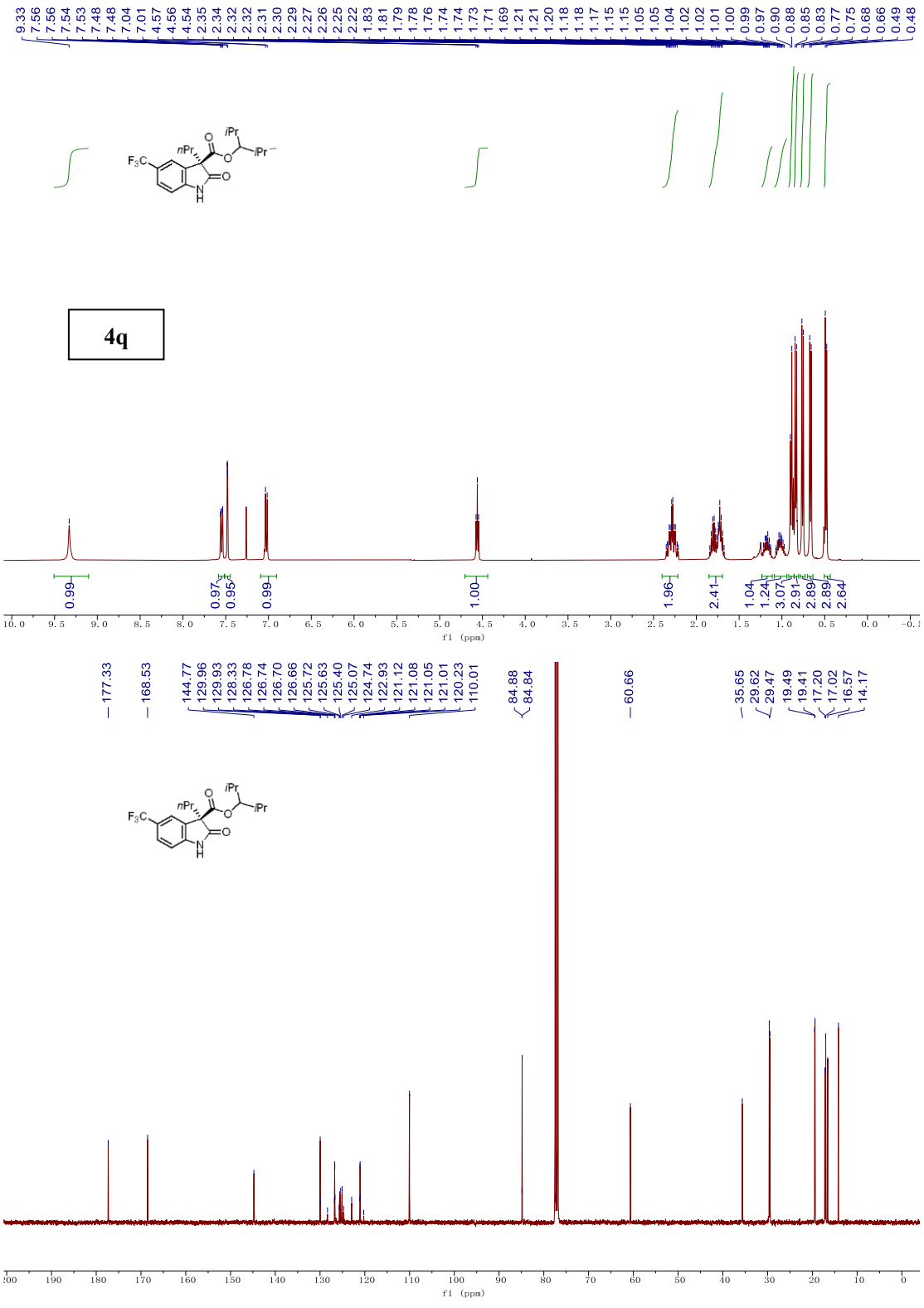
19.38
17.05
16.94
16.64
14.07
nPr
iPr
iPr
MeO2C
f1 (ppm)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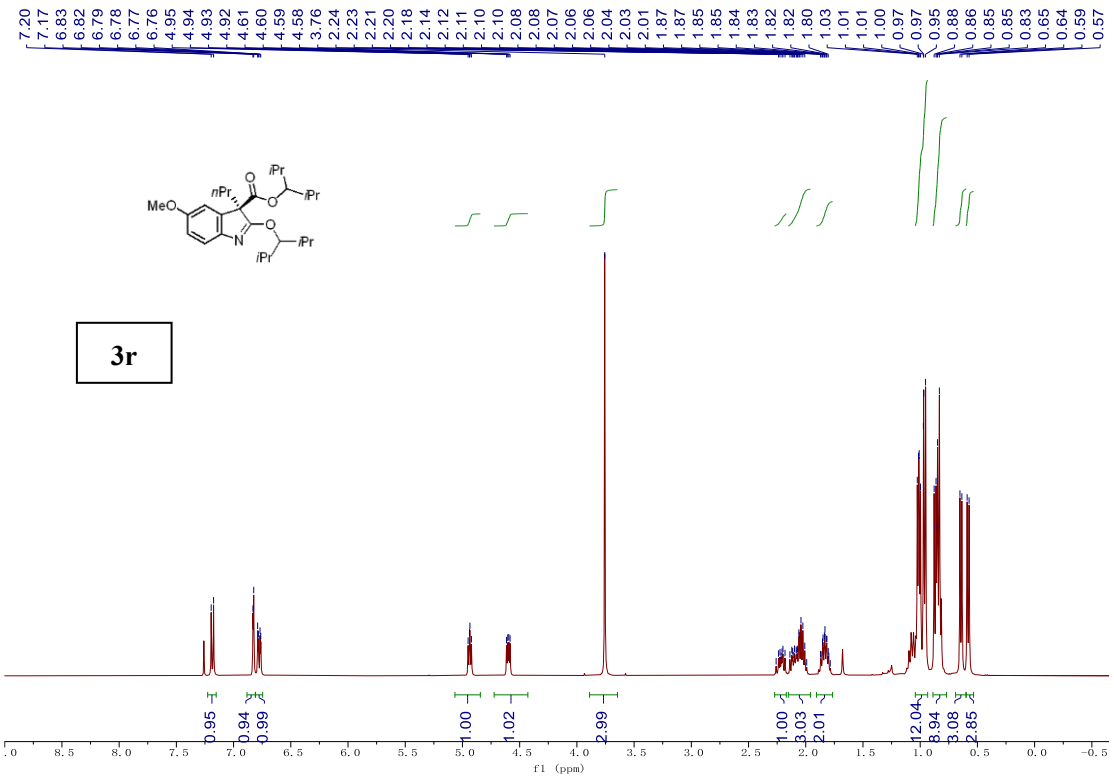
4q
0.99 0.97 0.95 0.99 1.00 1.96 2.41 1.04 1.24 3.07 2.91 2.89 2.89 2.64
f1 (ppm)
177.33 168.53 144.77 129.96 129.93 128.33 126.78 126.74 126.70 126.66 125.72 125.63 125.40 125.07 124.74 122.93 121.12 121.08 121.05 121.01 120.23 110.01 84.88 84.84 60.66 35.65 29.62 29.47 19.49 19.41 17.20 17.02 16.57 14.17
f1 (ppm)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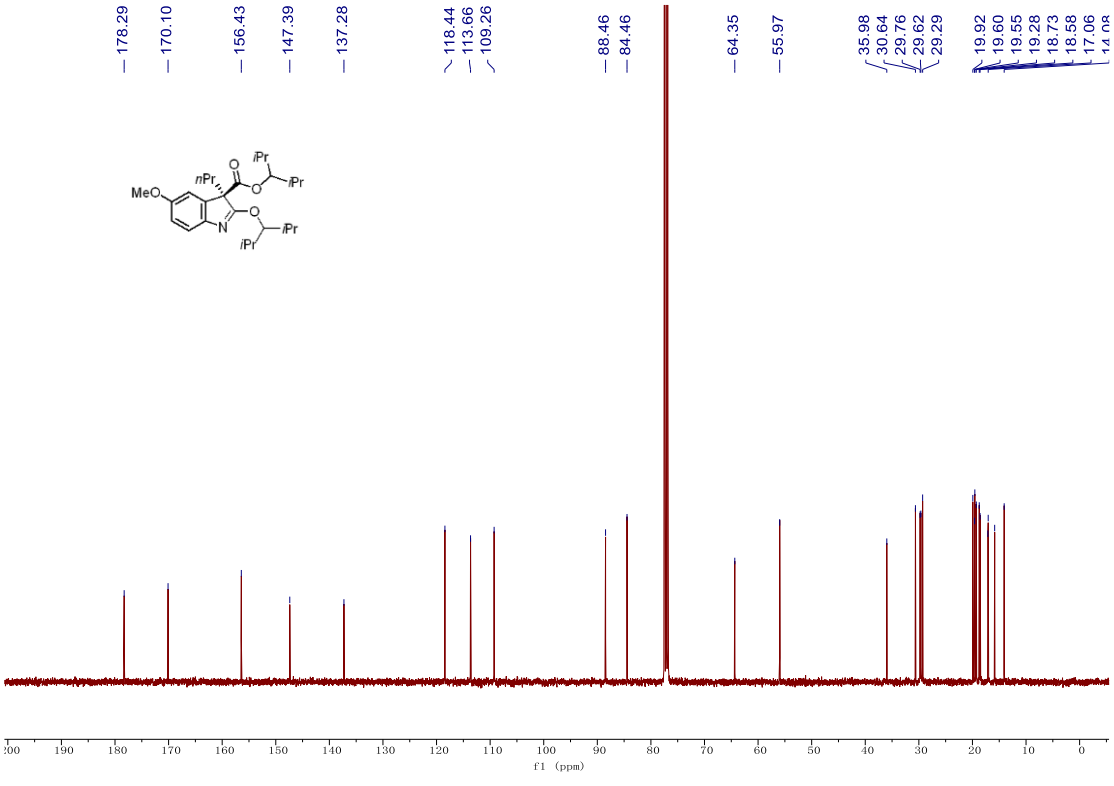
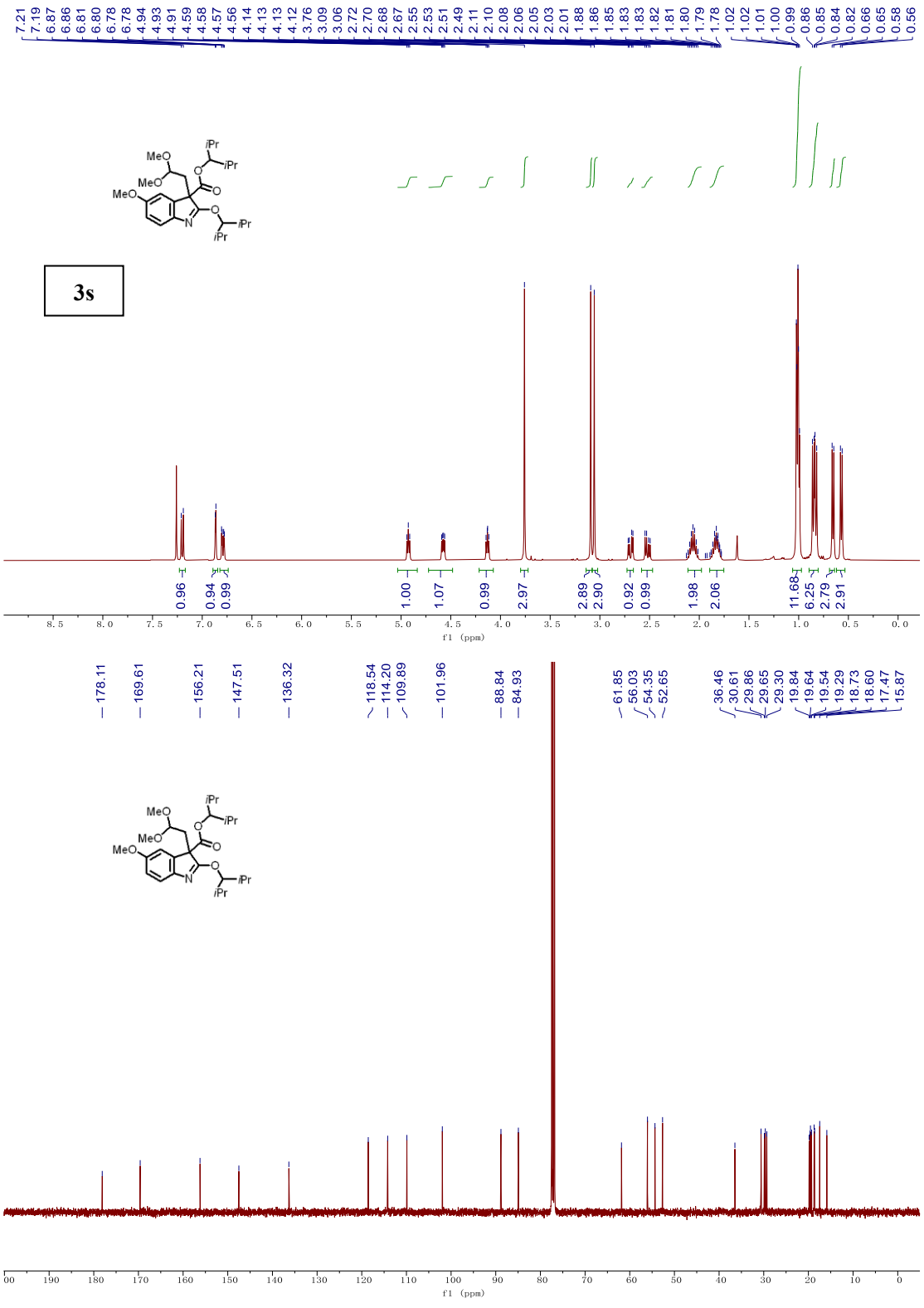
MeO
nPr
iPr
iPr
iPr
iPr
iPr
3r
0.95 0.94 0.99 1.00 1.02 2.99 1.00 3.03 2.01 12.04 8.94 3.08 2.85
f1 (ppm)


178.29 170.10 156.43 147.39 137.28 118.44 113.66 109.26 88.46 84.46 64.35 55.97 35.98 30.64 29.76 29.62 29.29 19.92 19.60 19.55 19.28 18.73 18.58 17.06
MeO
nPr
iPr
iPr
iPr
iPr
iPr
f1 (ppm)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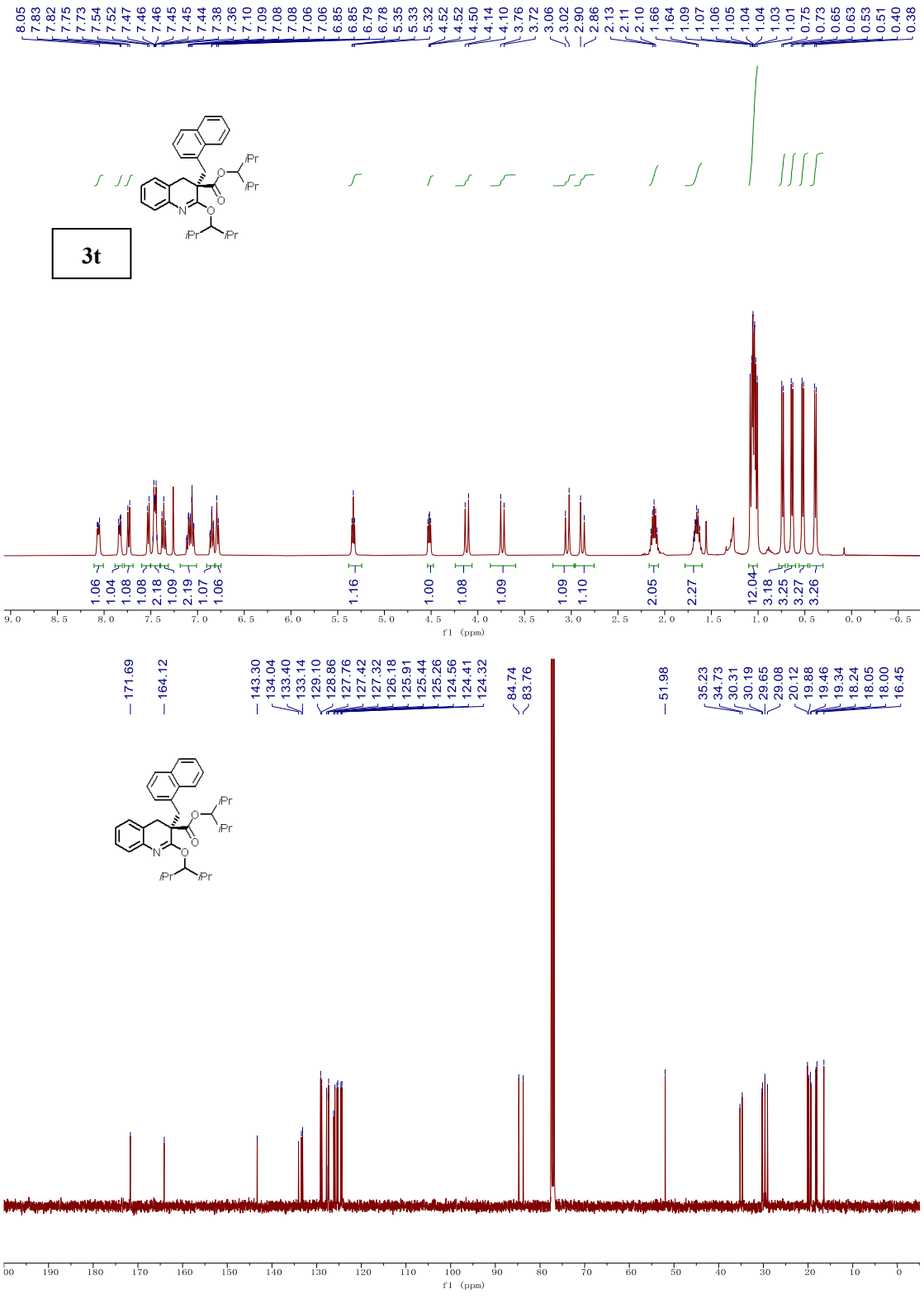
3s
0.96 0.94 0.99 1.00 1.07 0.99 2.97 2.89 2.90 0.92 0.99 1.98 2.06 11.68 6.25 2.79 2.91
f1 (ppm)
178.11 169.61 156.21 147.51 136.32 118.54 114.20 109.89 101.96 88.84 84.93 61.85 56.03 54.35 52.65 36.46 30.61 29.86 29.65 29.30 19.84 19.64 19.54 19.29 18.73 18.60 17.47 15.87
f1 (ppm)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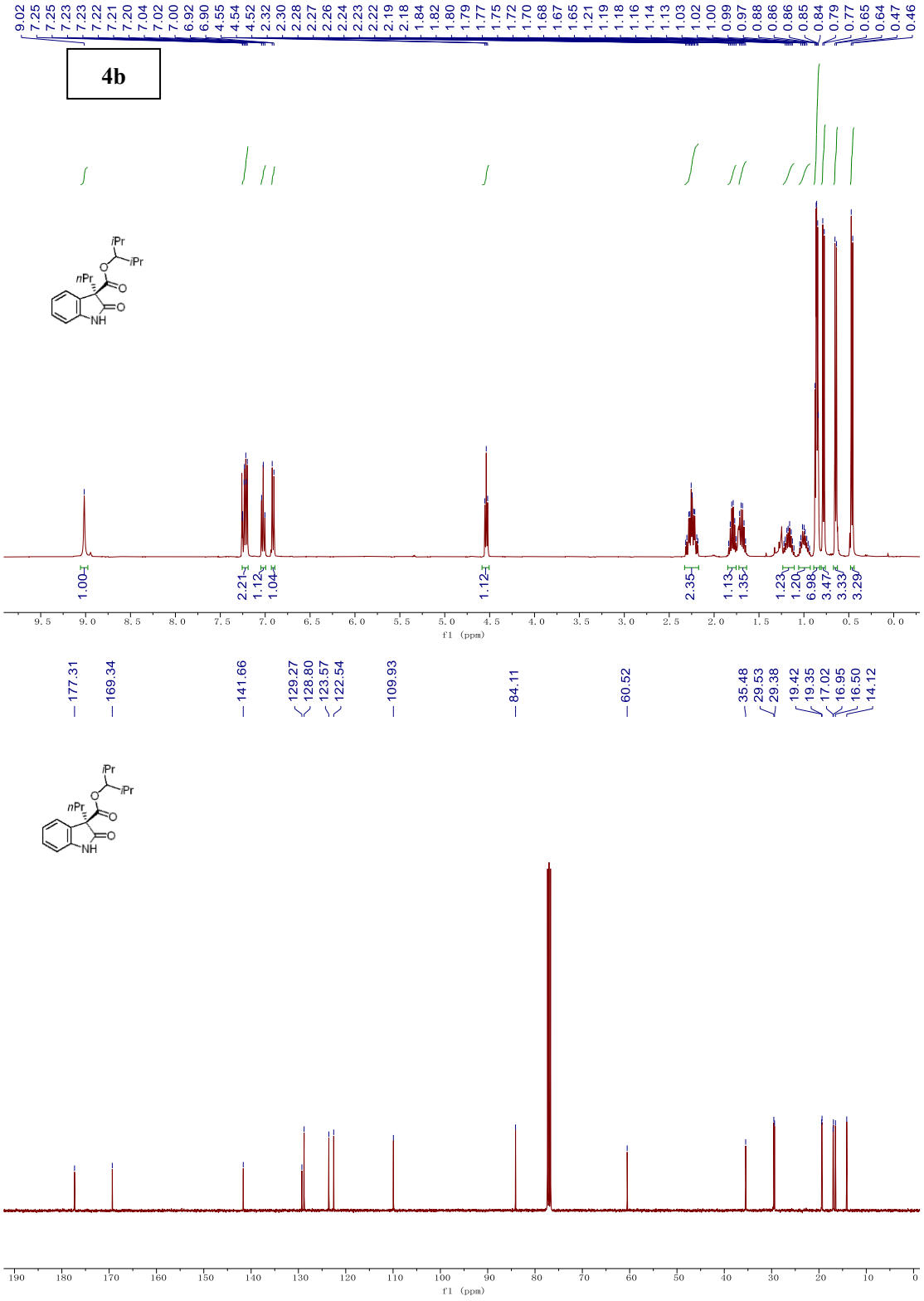
3t
1.06 1.04 1.08 1.08 2.18 1.09 2.19 1.07 1.06 1.16 1.00 1.08 1.09 1.09 1.10 2.05 2.27 12.04 3.18 3.25 3.27 3.26
f1 (ppm)
171.69 164.12 143.30 134.04 133.40 133.14 129.10 128.86 127.76 127.42 127.32 126.18 125.91 125.44 125.26 124.56 124.41 124.32 84.74 83.76 51.98 35.23 34.73 30.31 30.19 29.65 29.08 20.12 19.88 19.46 19.34 18.24 18.05 18.00 16.45
f1 (ppm)


4b
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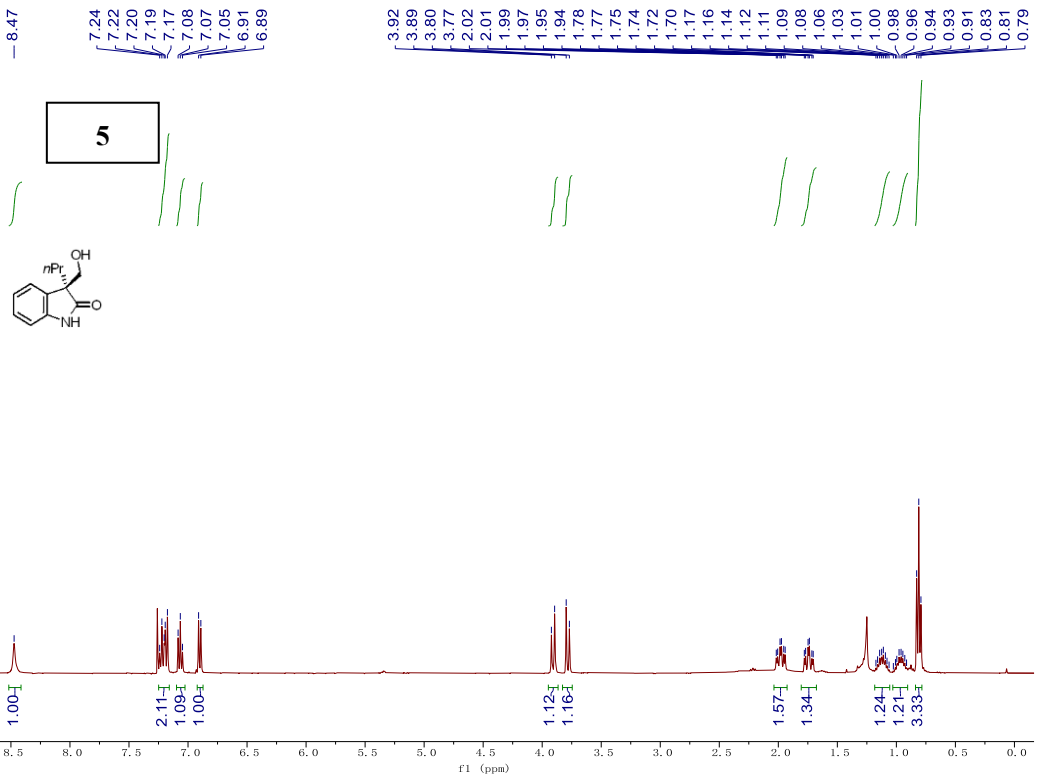
iPr
iPr
nPr
O
O
O
NH
1.00
2.21
1.12
1.04
1.12
2.35
1.13
1.35
1.23
1.20
6.98
3.47
3.33
3.29
f1 (ppm)
177.31
169.34
141.66
129.27
128.80
123.57
122.54
109.93
84.11
60.52
35.48
29.53
29.38
19.42
19.35
17.02
16.95
16.50
14.12
f1 (ppm)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7.17
7.08
7.07
7.05
6.91
6.89
3.92
3.89
3.80
3.77
2.02
2.01
1.99
1.97
1.95
1.94
1.78
1.77
1.75
1.74
1.72
1.70
1.17
1.16
1.14
1.12
1.11
1.09
1.08
1.06
1.03
1.01
1.00
0.98
0.96
0.94
0.93
0.91
0.83
0.81
0.79
5
OH
nPr
O
NH
1.00
2.11
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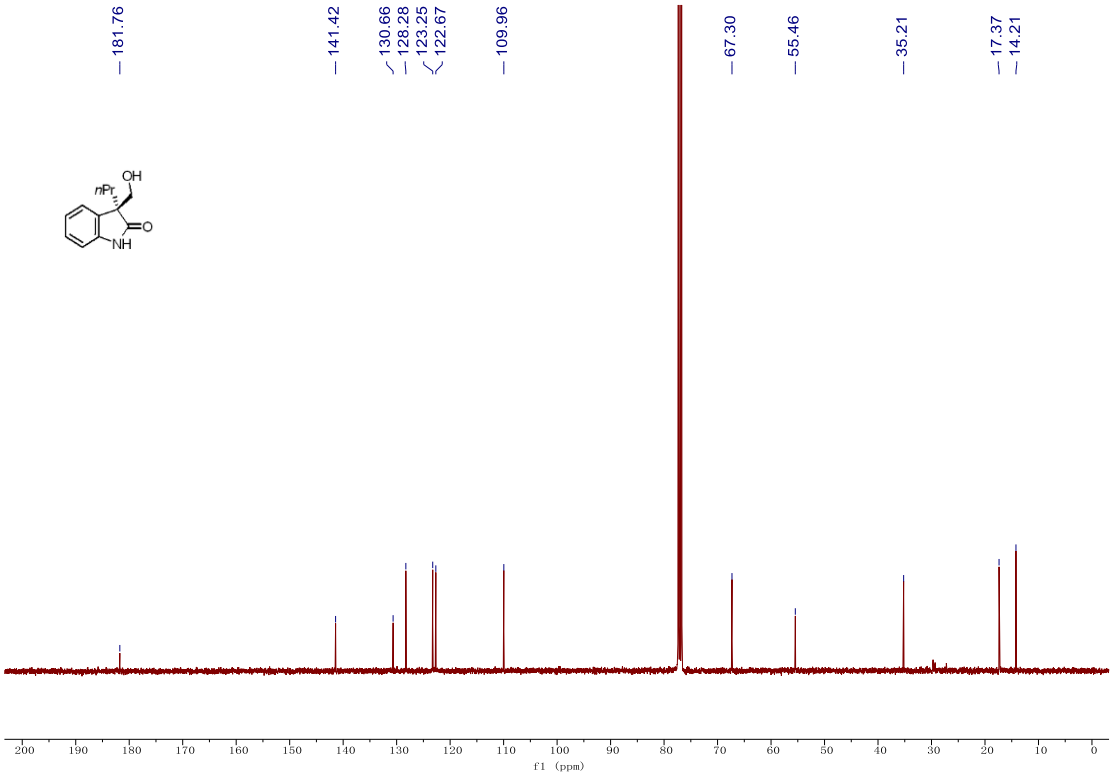
1.00
1.12
1.16
1.57
1.34
1.24
1.21
3.33
f1 (ppm)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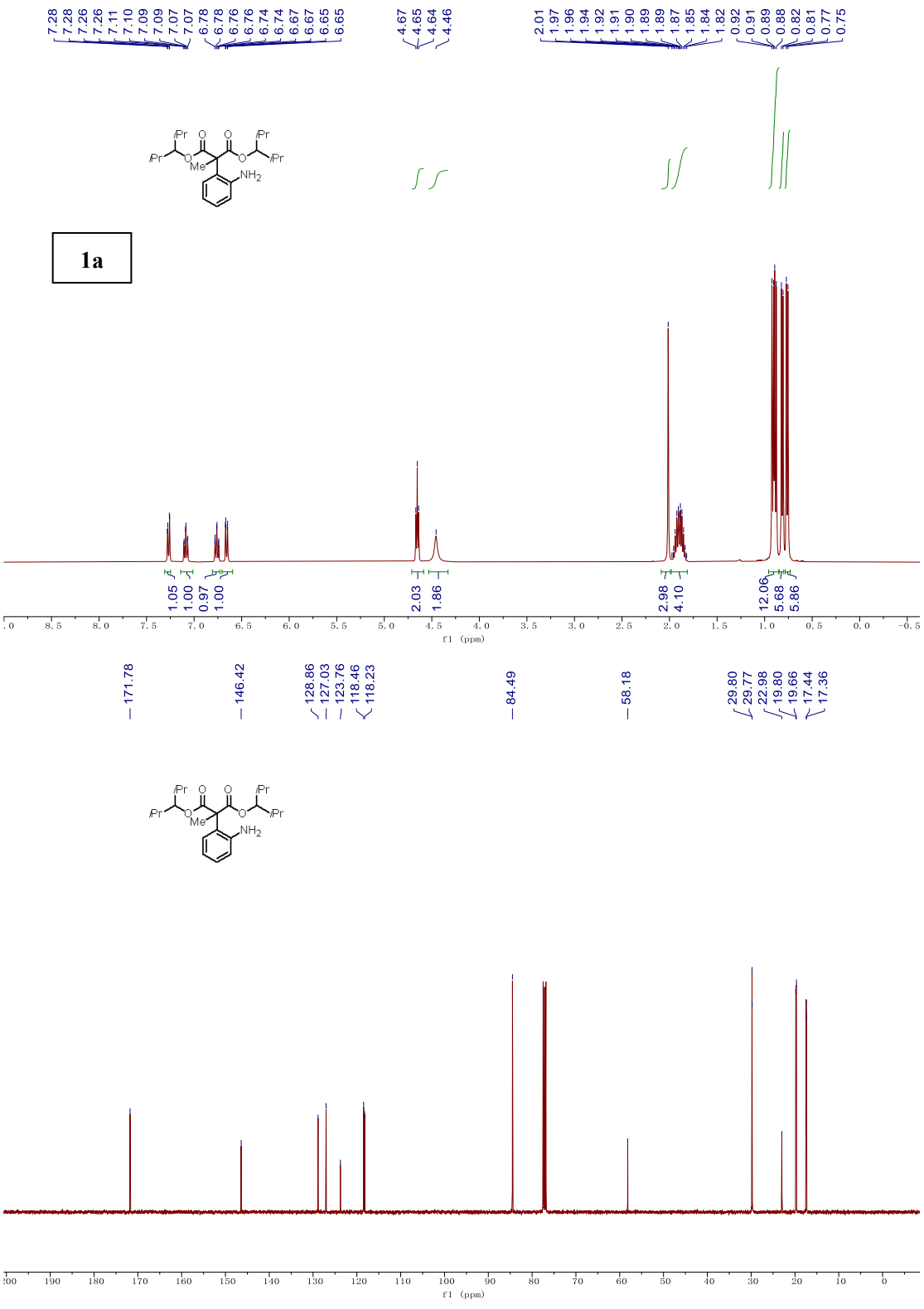
109.96
67.30
55.46
35.21
17.37
14.21
OH
nPr
O
NH
f1 (ppm)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7.09
7.09
7.07
7.07
6.78
6.78
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6.76
6.74
6.74
6.67
6.67
6.65
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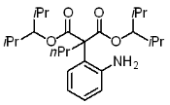
1.96
1.94
1.92
1.91
1.90
1.89
1.89
1.87
1.85
1.84
1.82
0.92
0.91
0.89
0.88
0.82
0.81
0.77
0.75
iPr
iPr
O
O
iPr
iPr
O
O
Me
NH2
1a
1.05
1.00
0.97
1.00
2.03
1.86
2.98
4.10
12.06
5.68
5.86
f1 (ppm)
171.78
146.42
128.86
127.03
123.76
118.46
118.23
84.49
58.18
29.80
29.77
22.98
19.80
19.66
17.44
17.36
f1 (ppm)

1b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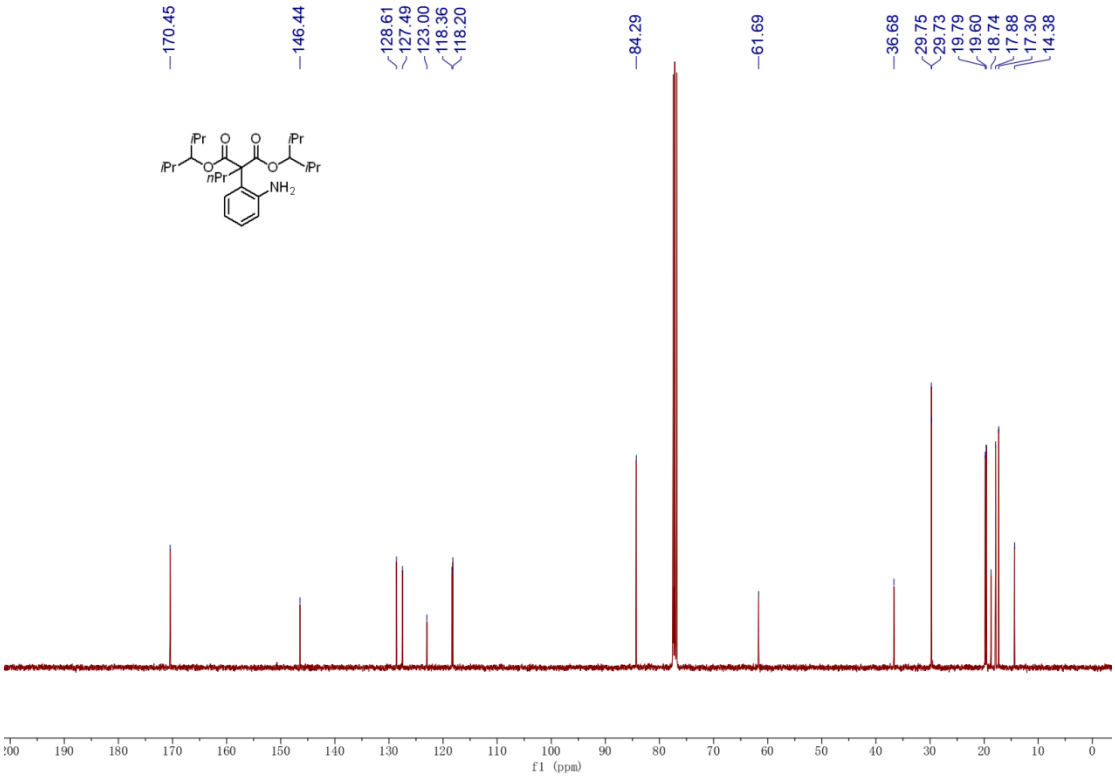
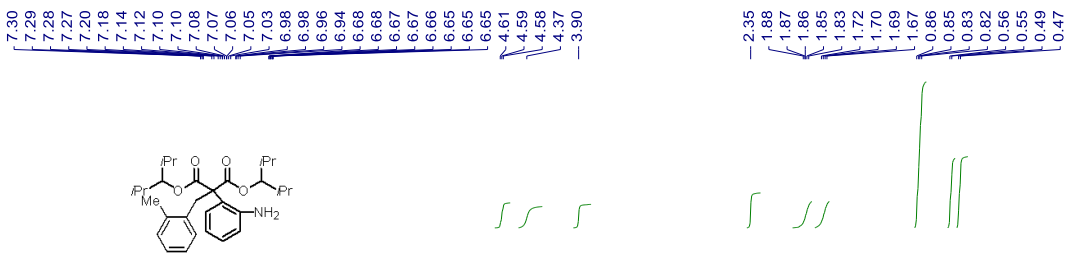
iPr
O
O
iPr
iPr
O
nPr
NH2

7.28 7.27 7.26 7.08 7.07 7.06 7.06 7.04 7.04 6.77 6.76 6.75 6.75 6.74 6.73 6.73 6.63 6.63 6.61 6.61
4.63 4.62 4.60 4.40
2.45 2.44 2.43 2.42 2.41 1.93 1.92 1.90 1.89 1.88 1.87 1.87 1.85 1.85
1.43 1.41 1.41 1.01 0.99 0.97 0.90 0.88 0.87 0.86 0.78 0.76 0.71
0.84 1.00 1.00 1.02 2.03 2.01 1.99 4.18 2.07 3.07 12.39 5.84 5.83
f1 (ppm)


170.45 146.44 128.61 127.49 123.00 118.36 118.20 84.29 61.69 36.68 29.75 29.73 19.79 19.60 18.74 17.88 17.30 14.38
f1 (ppm)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7.12
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7.03
6.98
6.98
6.96
6.94
6.68
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4.59
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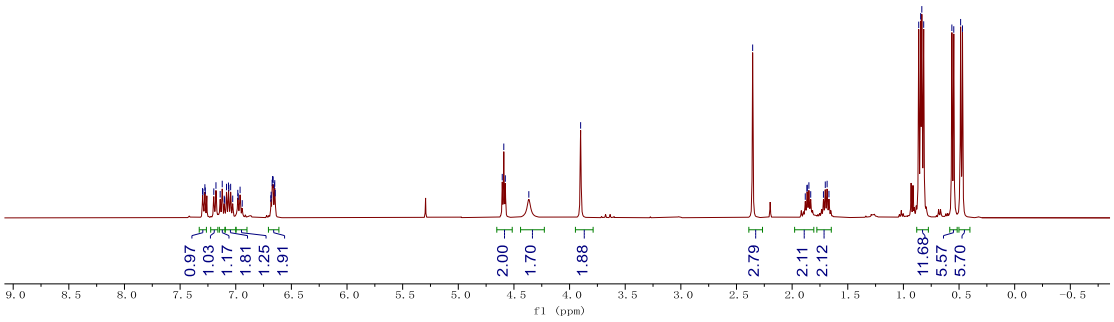
3.90
2.35
1.88
1.87
1.86
1.85
1.83
1.72
1.70
1.69
1.67
0.86
0.85
0.83
0.82
0.56
0.55
0.49
0.47
iPr
iPr
Me
NH2

1d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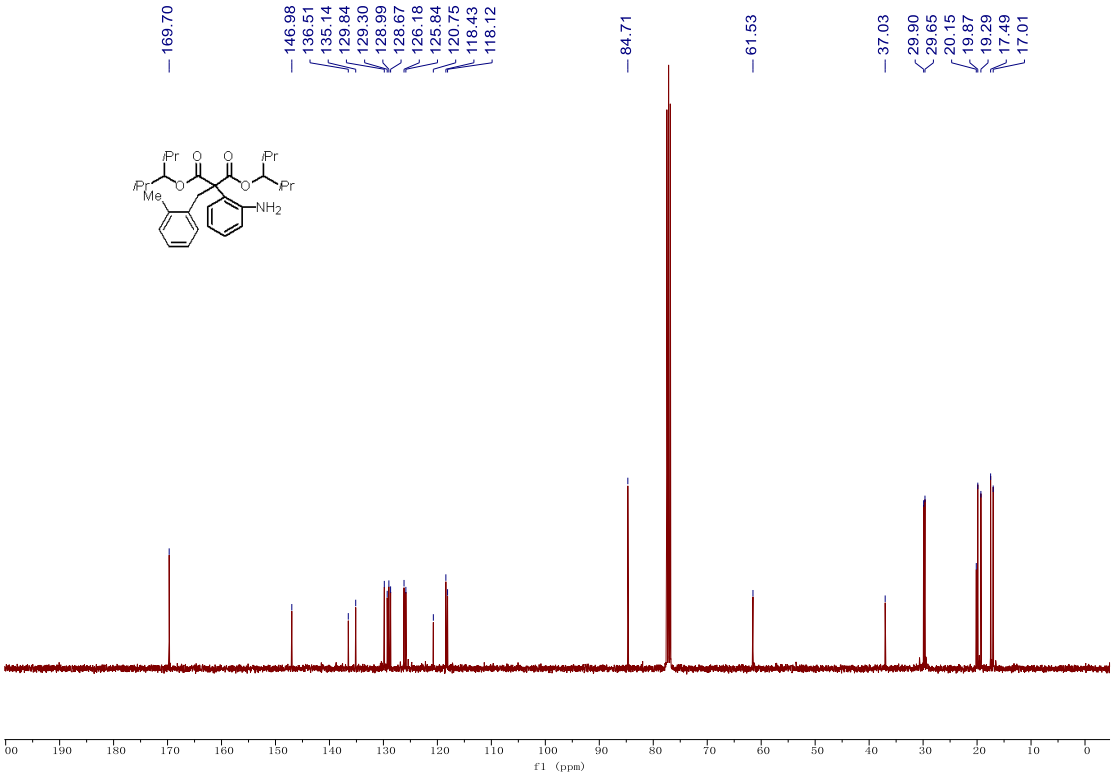
1.03
1.17
1.81
1.25
1.91
2.00
1.70
1.88
2.79
2.11
2.12
11.68
5.57
5.70
f1 (ppm)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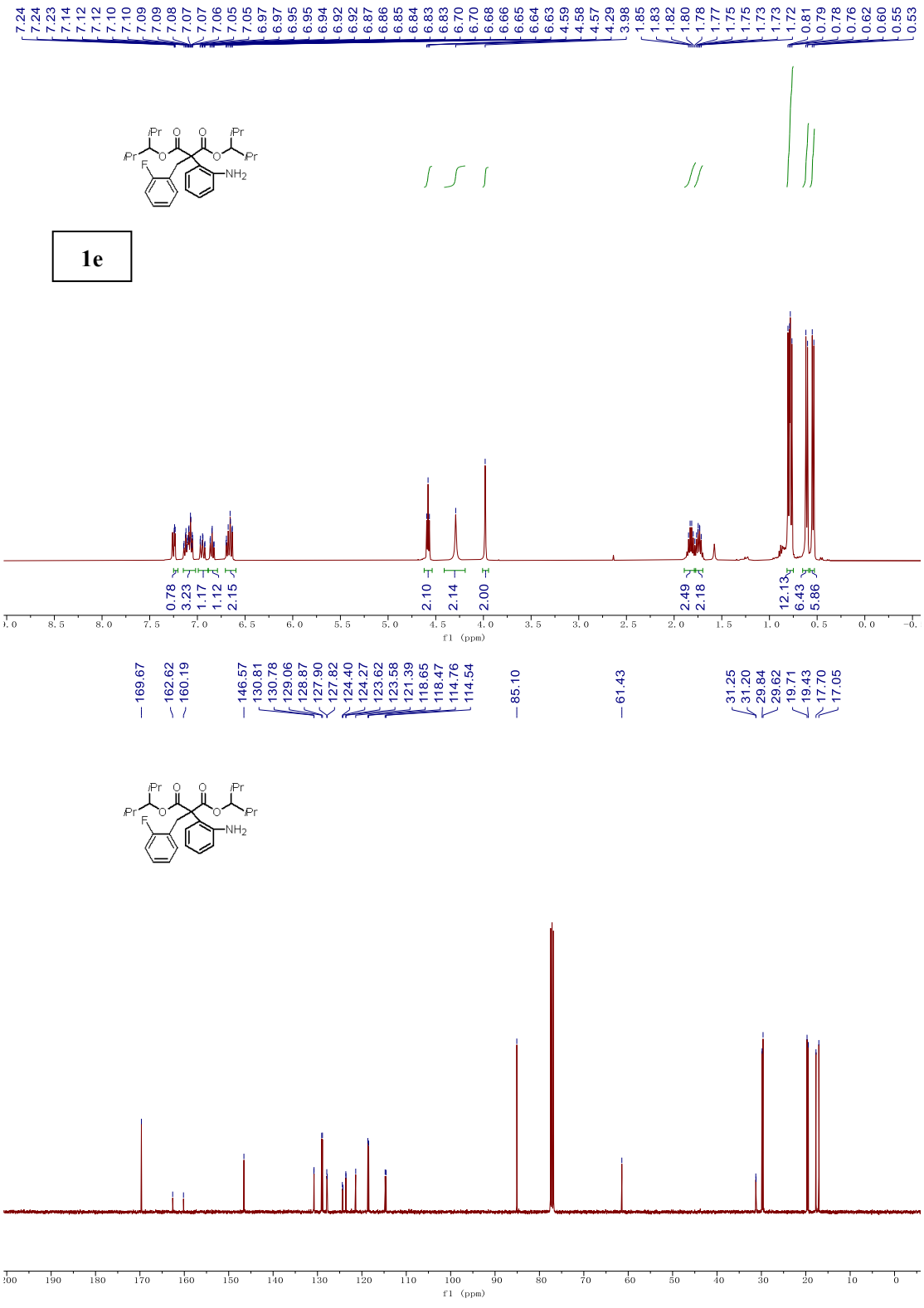
125.84
120.75
118.43
118.12
84.71
61.53
37.03
29.90
29.65
20.15
19.87
19.29
17.49
17.01
iPr
iPr
Me
NH2
f1 (ppm)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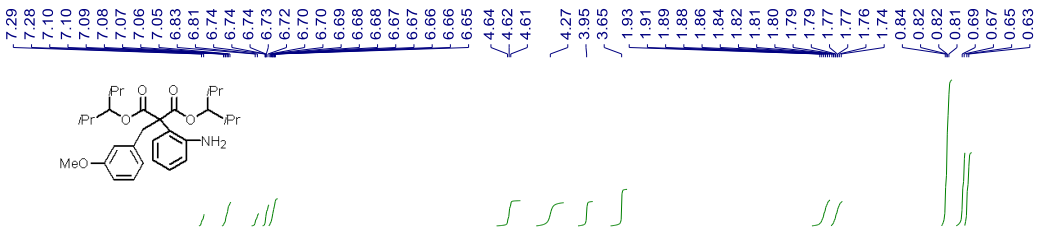
iPr
iPr
iPr
iPr
F
NH2
1e
0.78 3.23 1.17 1.12 2.15 2.10 2.14 2.00 2.49 2.18 12.13 6.43 5.86
f1 (ppm)
169.67 162.62 160.19 146.57 130.81 130.78 129.06 128.87 127.90 127.82 124.40 124.27 123.62 123.58 121.39 118.65 118.47 114.76 114.54 85.10 61.43 31.25 31.20 29.84 29.62 19.71 19.43 17.70 17.05
f1 (ppm)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7.06
7.05
6.83
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1.77
1.77
1.76
1.74
0.84
0.82
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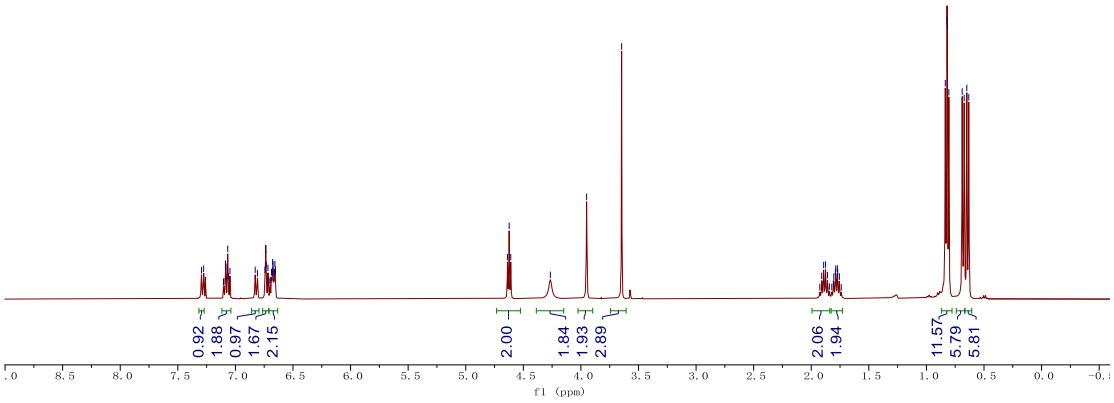
0.69
0.67
0.65
0.63
iPr
iPr
iPr
iPr
NH2
MeO

1f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1.93
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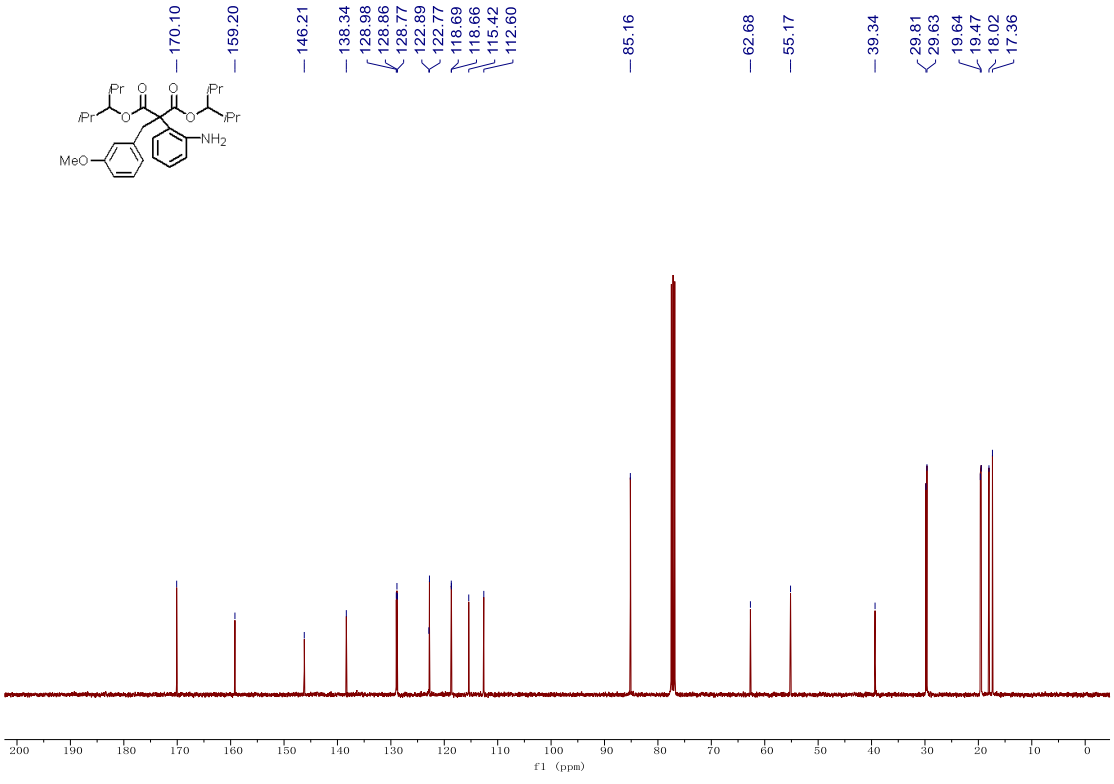
2.06
1.94
11.57
5.79
5.81
f1 (ppm)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118.66
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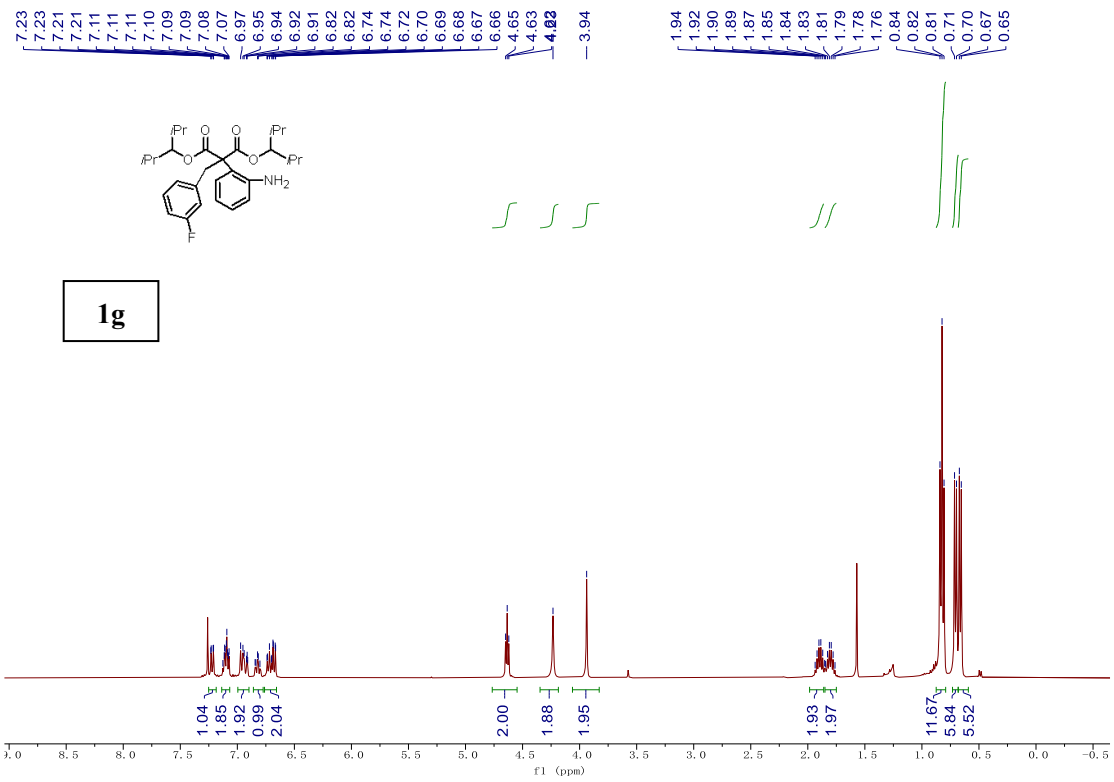
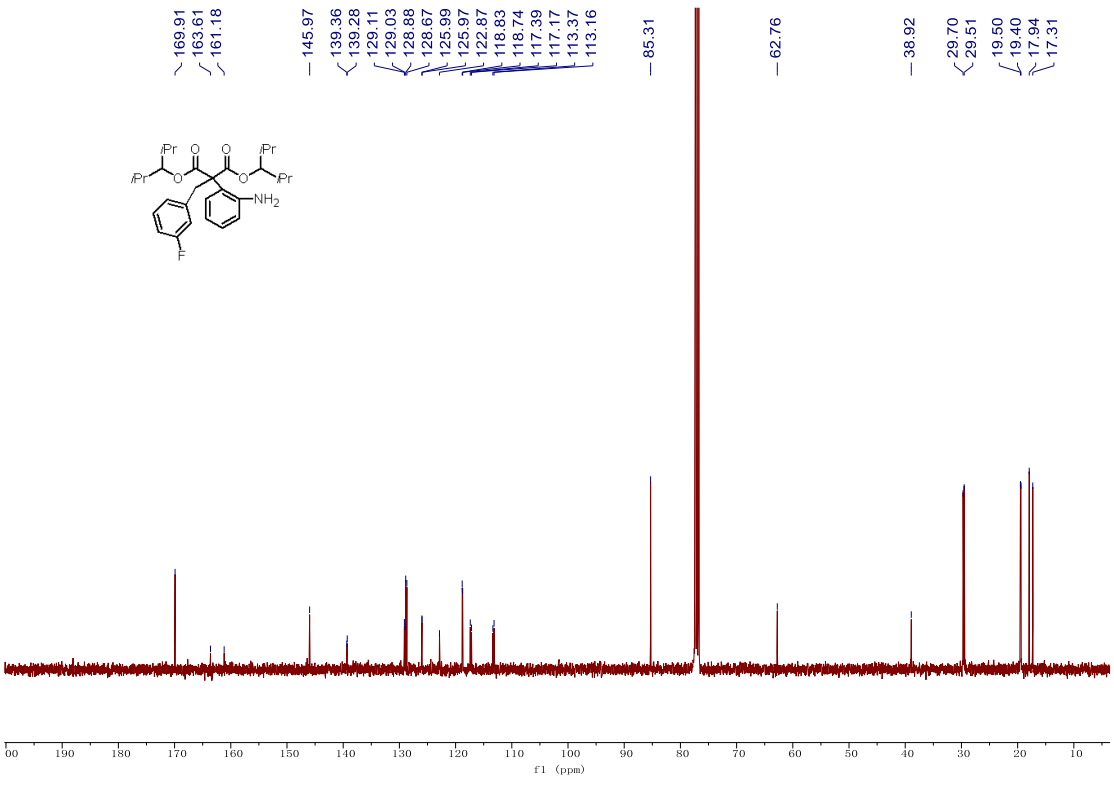
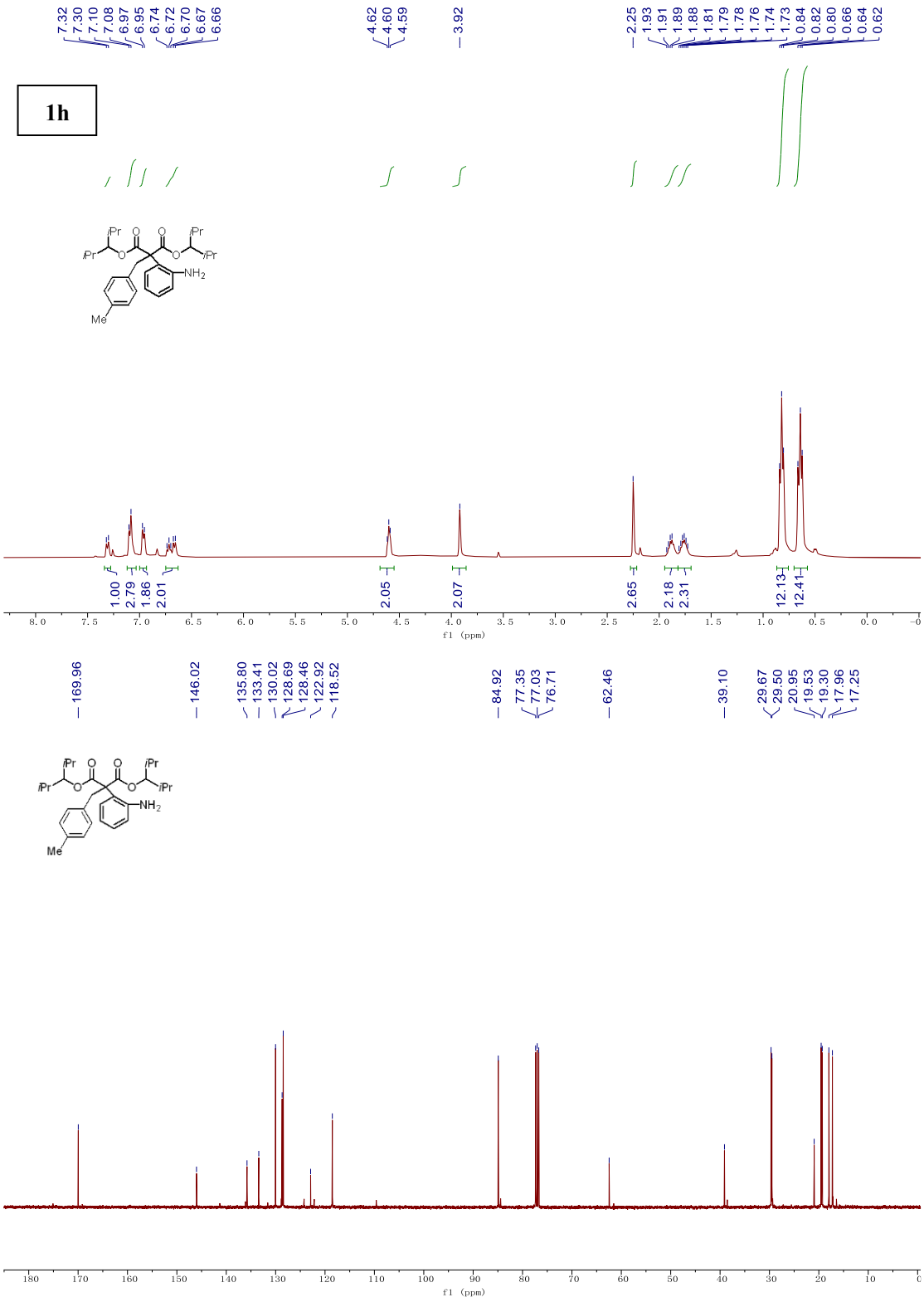
85.16
62.68
55.17
39.34
29.81
29.63
19.64
19.47
18.02
17.36
iPr
iPr
iPr
iPr
NH2
MeO
f1 (ppm)


7.23
7.23
7.21
7.21
7.11
7.11
7.10
7.09
7.09
7.08
7.07
6.97
6.95
6.94
6.92
6.91
6.82
6.82
6.74
6.74
6.72
6.70
6.69
6.68
6.67
6.66
4.65
4.63
3.94
1.94
1.92
1.90
1.89
1.87
1.85
1.84
1.83
1.81
1.79
1.78
1.76
0.84
0.82
0.81
0.71
0.70
0.67
0.65
iPr
iPr
iPr
iPr
NH2
F
1g
1.04
1.85
1.92
0.99
2.04
2.00
1.88
1.95
1.93
1.97
11.67
5.84
5.52
f1 (ppm)


169.91
163.61
161.18
145.97
139.36
139.28
129.11
129.03
128.88
128.67
125.99
125.97
122.87
118.83
118.74
117.39
117.17
113.37
113.16
85.31
62.76
38.92
29.70
29.51
19.50
19.40
17.94
17.31
iPr
iPr
iPr
iPr
NH2
F
f1 (ppm)

1h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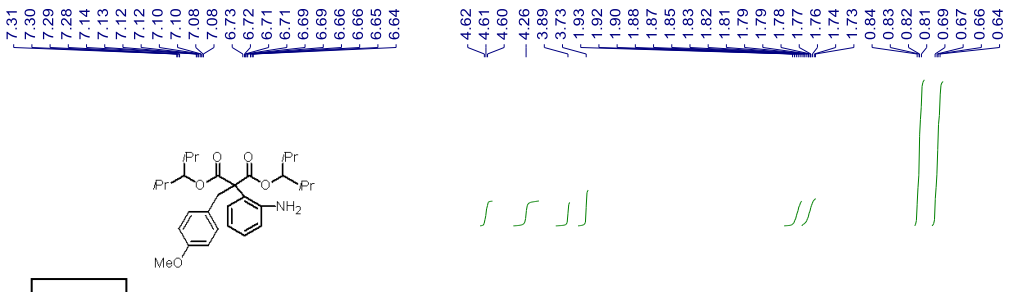
7.30
7.10
7.08
6.97
6.95
6.74
6.72
6.70
6.67
6.66
4.62
4.60
4.59
3.92
2.25
1.93
1.91
1.89
1.88
1.81
1.79
1.78
1.76
1.74
1.73
0.84
0.82
0.80
0.66
0.64
0.62
iPr
iPr
iPr
iPr
NH2
Me
1.00
2.79
1.86
2.01
2.05
2.07
2.65
2.18
2.31
12.13
12.41
f1 (ppm)
169.96
146.02
135.80
133.41
130.02
128.69
128.46
122.92
118.52
84.92
77.35
77.03
76.71
62.46
39.10
29.67
29.50
20.95
19.53
19.30
17.96
17.25
f1 (ppm)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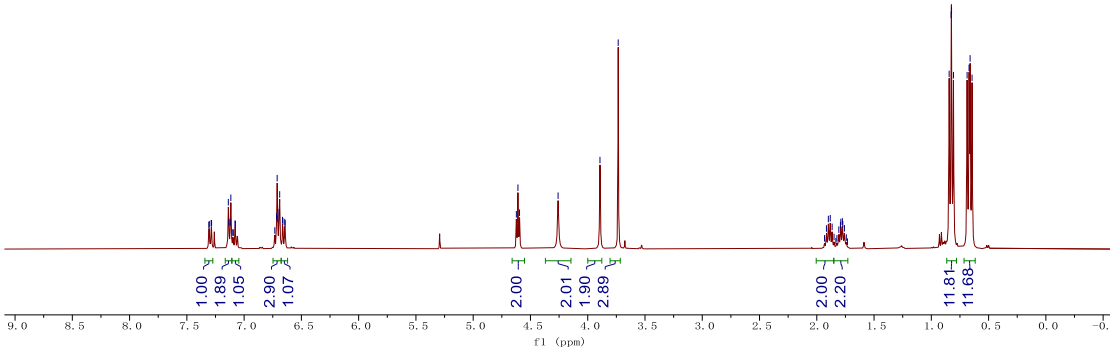
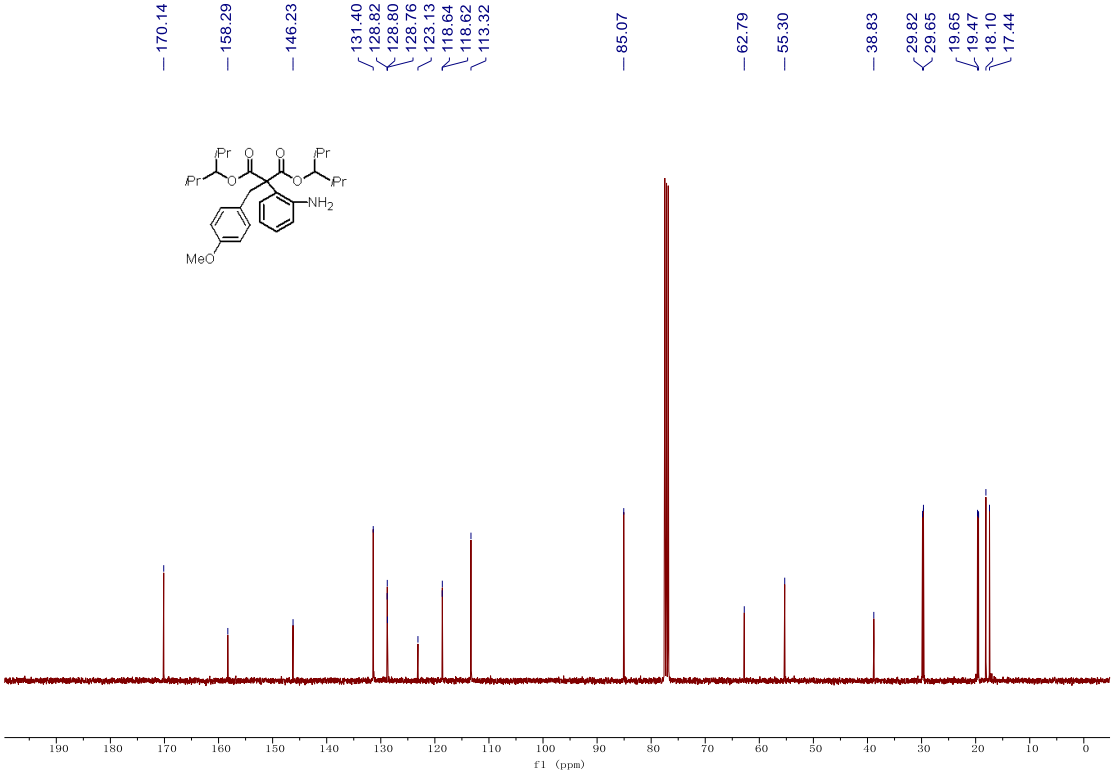
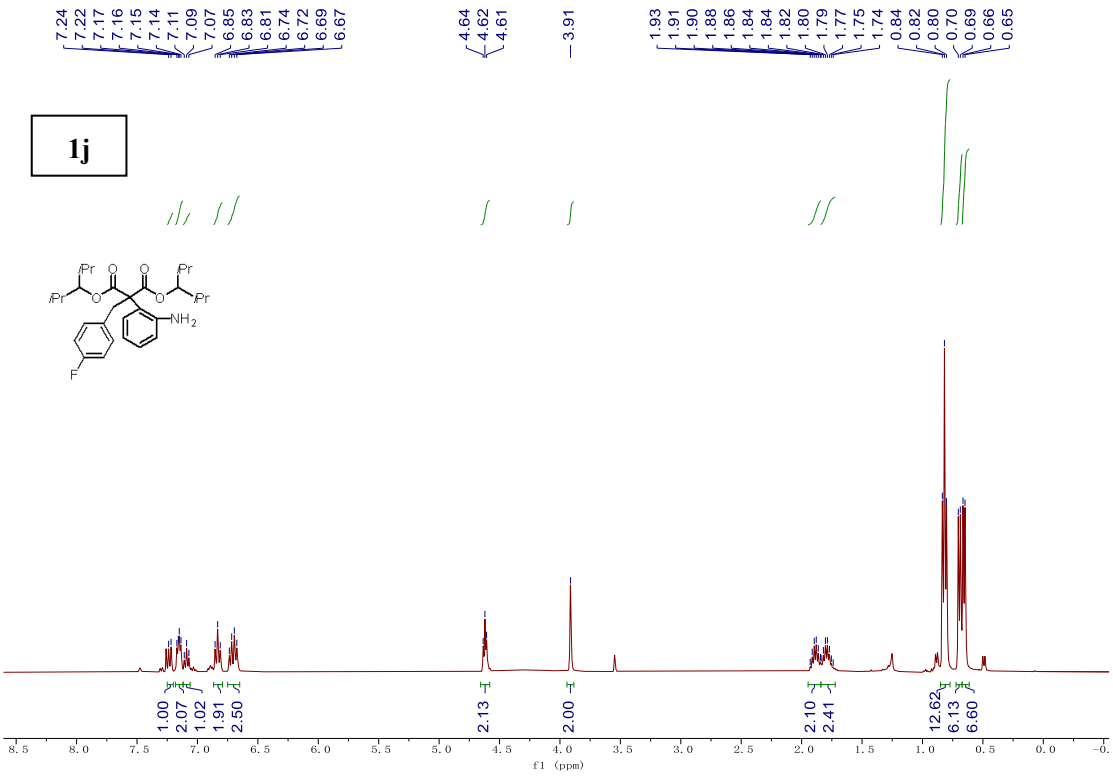
7.30
7.29
7.28
7.14
7.13
7.12
7.12
7.10
7.10
7.08
7.08
6.73
6.72
6.71
6.71
6.69
6.69
6.66
6.66
6.65
6.64
4.62
4.61
4.60
4.26
3.89
3.73
1.93
1.92
1.90
1.88
1.87
1.85
1.83
1.82
1.81
1.79
1.79
1.78
1.77
1.76
1.74
1.73
0.84
0.83
0.82
0.81
0.69
0.67
0.66
0.64
iPr
iPr
iPr
iPr
NH2
MeO

1i


1.00
1.89
1.05
2.90
1.07
2.00
2.01
1.90
2.89
2.00
2.20
11.81
11.68
f1 (ppm)


170.14
158.29
146.23
131.40
128.82
128.80
128.76
123.13
118.64
118.62
113.32
85.07
62.79
55.30
38.83
29.82
29.65
19.65
19.47
18.10
17.44
iPr
iPr
iPr
iPr
NH2
MeO
f1 (ppm)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7.22
7.17
7.16
7.15
7.14
7.11
7.09
7.07
6.85
6.83
6.81
6.74
6.72
6.69
6.67
4.64
4.62
4.61
3.91
1.93
1.91
1.90
1.88
1.86
1.84
1.84
1.82
1.80
1.79
1.77
1.75
1.74
0.84
0.82
0.80
0.70
0.69
0.66
0.65
1j
iPr
iPr
iPr
iPr
NH2
F
1.00
2.07
1.02
1.91
2.50
2.13
2.00
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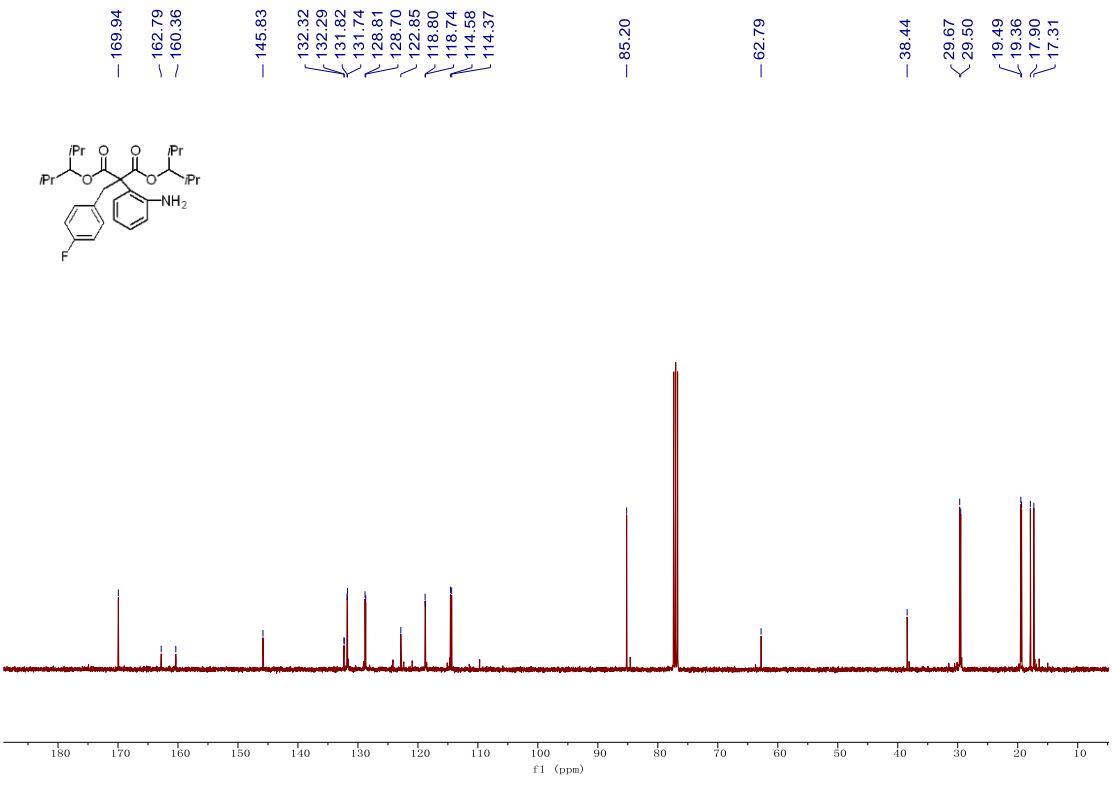
2.41
12.62
6.13
6.60
f1 (ppm)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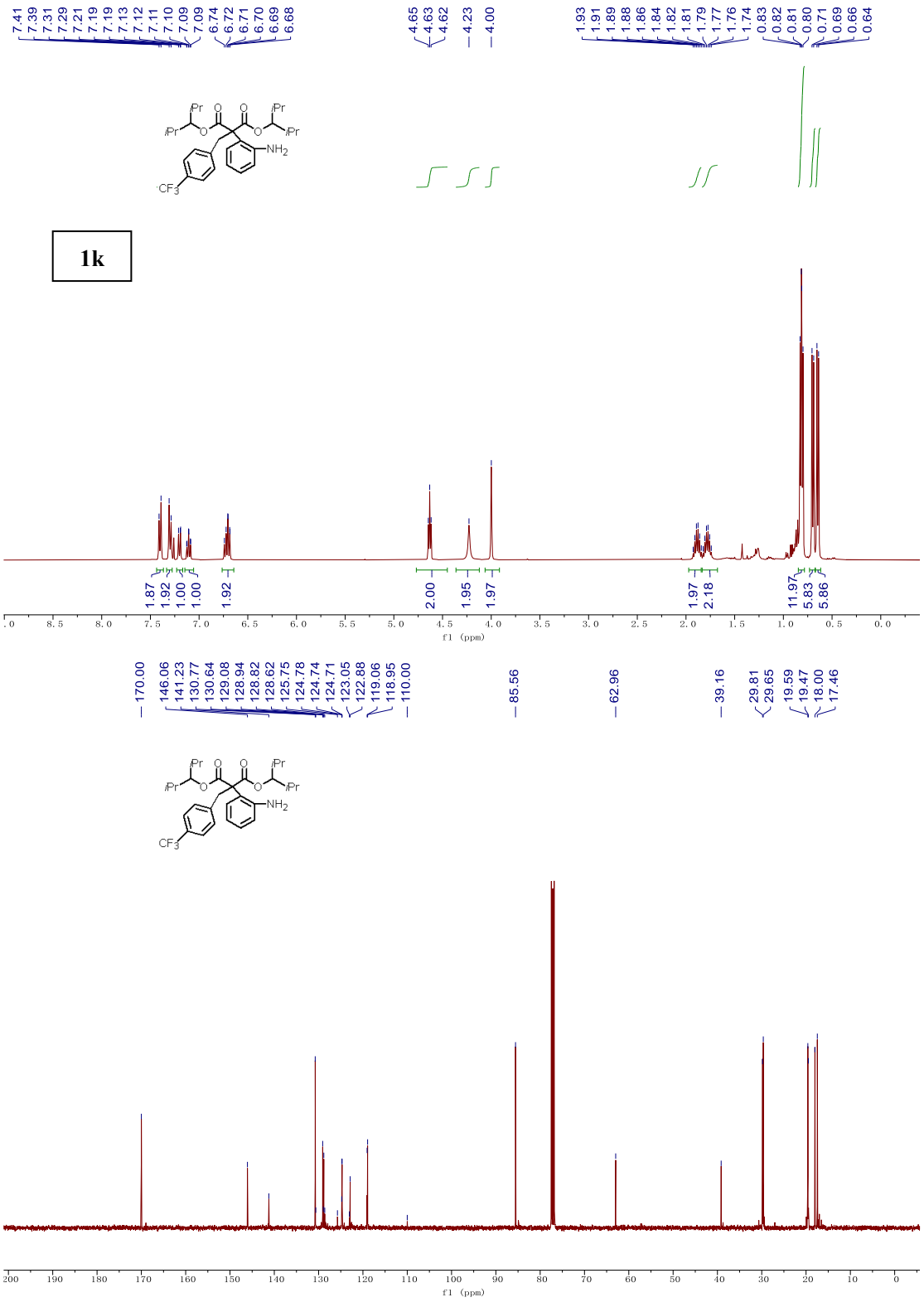
162.79
160.36
145.83
132.32
132.29
131.82
131.74
128.81
128.70
122.85
118.80
118.74
114.58
114.37
85.20
62.79
38.44
29.67
29.50
19.49
19.36
17.90
17.31
iPr
iPr
iPr
iPr
NH2
F
f1 (ppm)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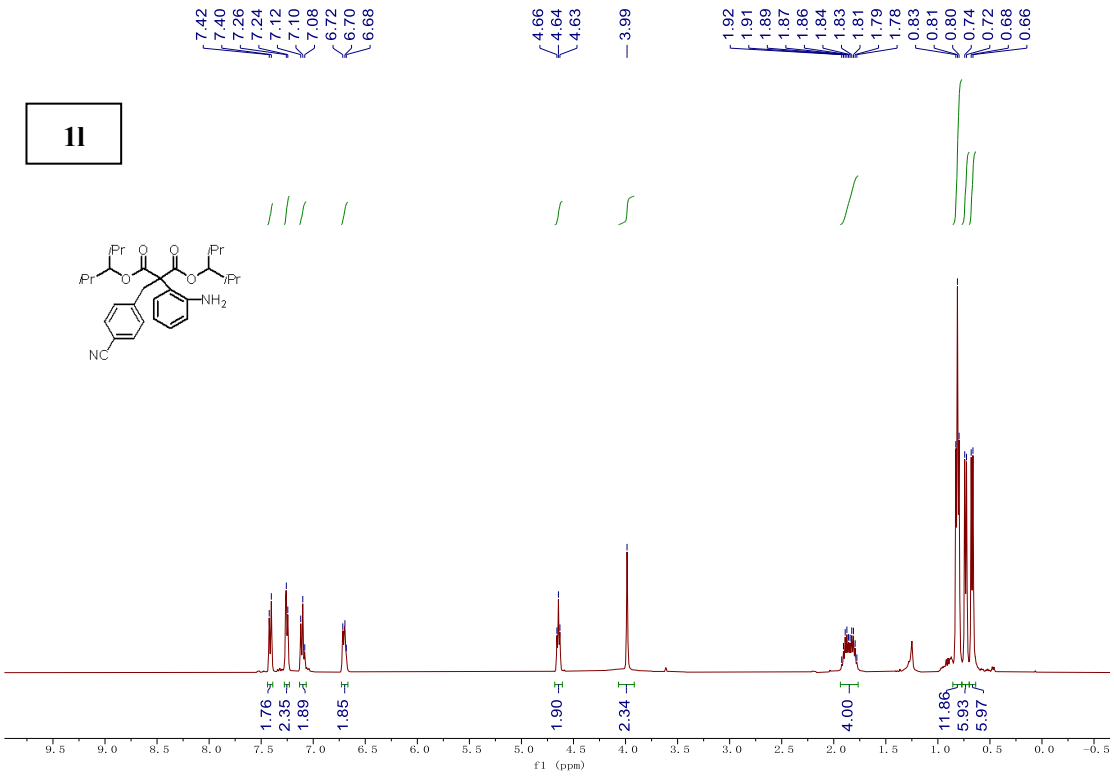
7.39
7.31
7.29
7.21
7.19
7.13
7.12
7.11
7.10
7.09
7.09
6.74
6.72
6.71
6.70
6.69
6.68
4.65
4.63
4.62
4.23
4.00
1.93
1.91
1.89
1.88
1.86
1.84
1.82
1.81
1.79
1.77
1.76
1.74
0.83
0.82
0.81
0.80
0.71
0.69
0.66
0.64
iPr
iPr
iPr
iPr
NH2
CF3
1k
1.87
1.92
1.00
1.00
1.92
2.00
1.95
1.97
1.97
2.18
11.97
5.83
5.86
f1 (ppm)
170.00
146.06
141.23
130.77
130.64
129.08
128.94
128.82
128.62
125.75
124.78
124.74
124.71
123.05
122.88
119.06
118.95
110.00
85.56
62.96
39.16
29.81
29.65
19.59
19.47
18.00
17.46
f1 (ppm)

1l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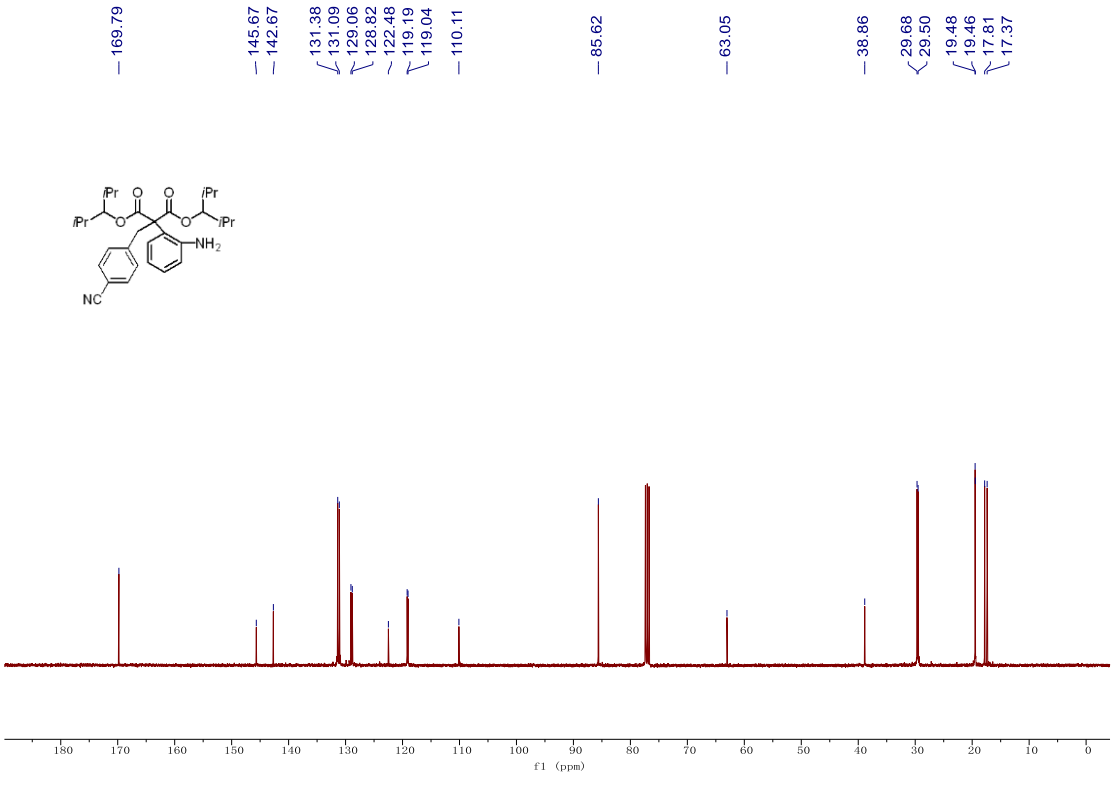
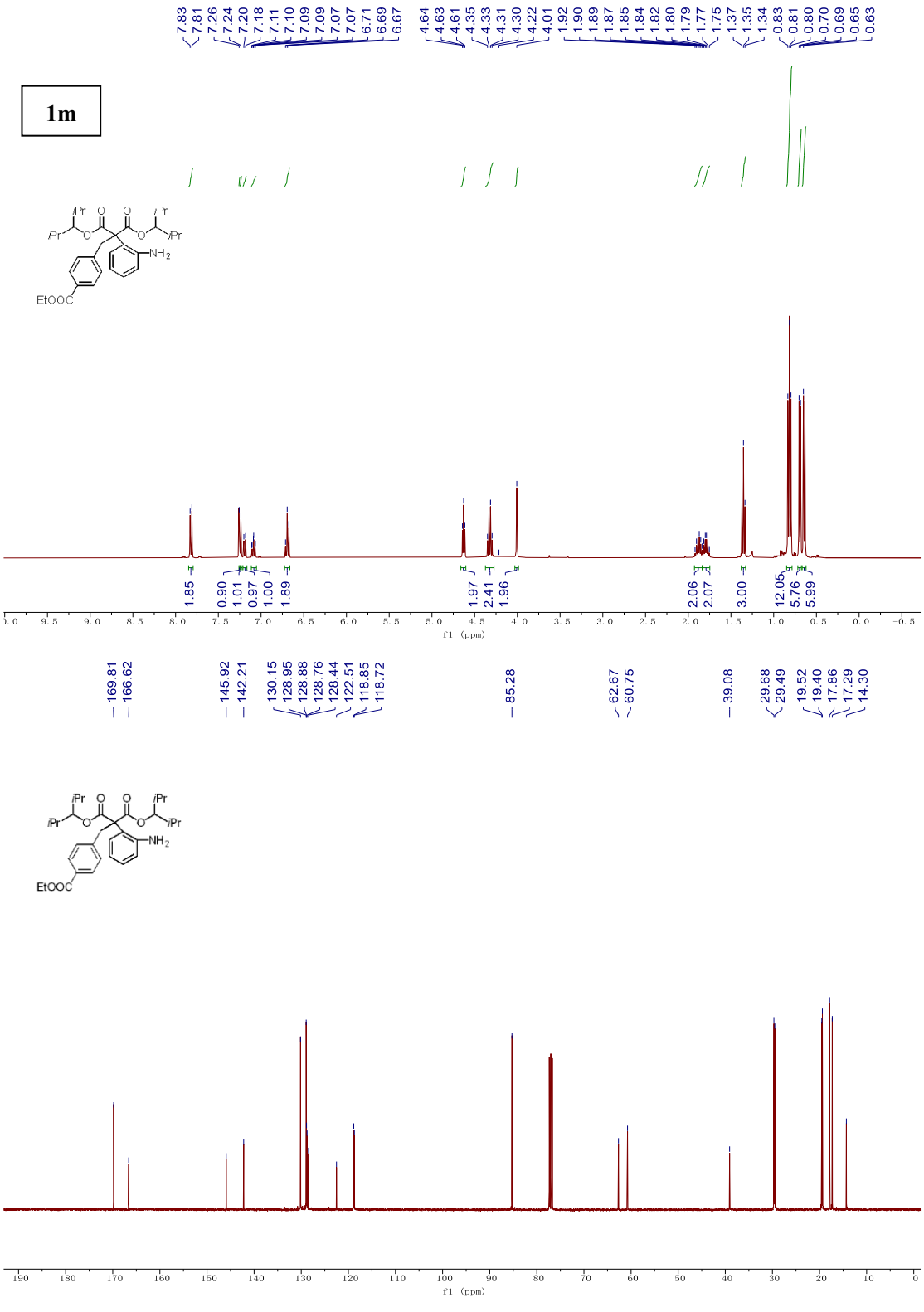
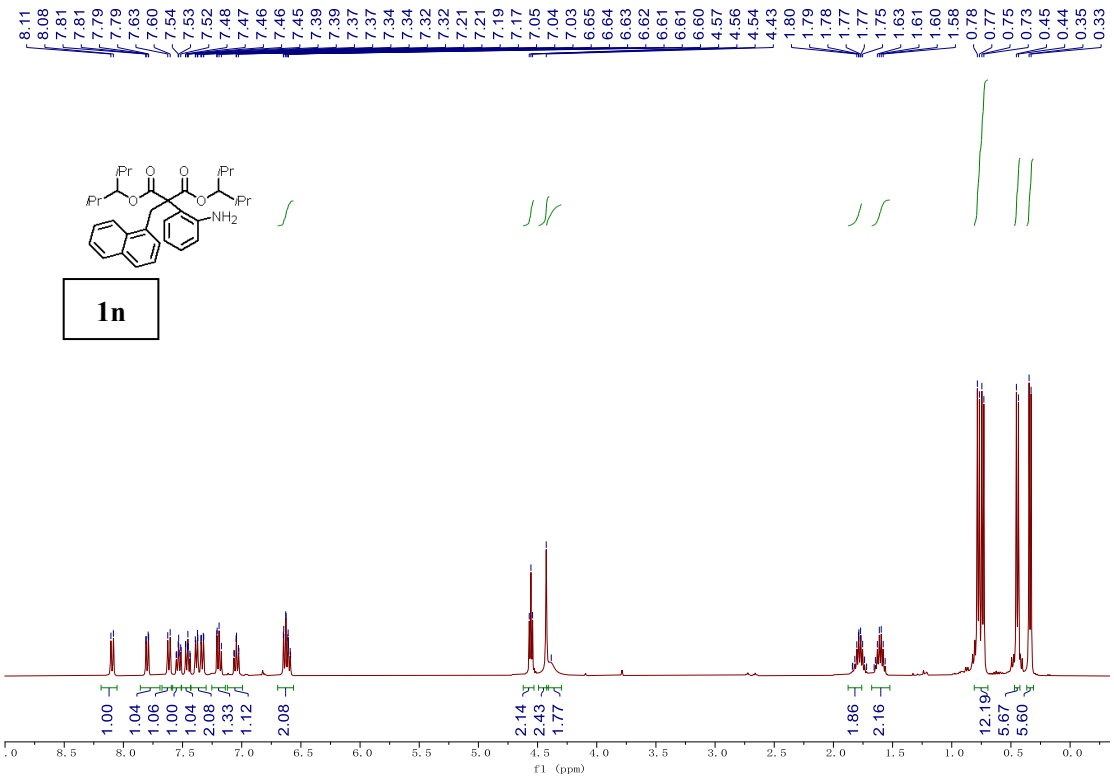
7.40
7.26
7.24
7.12
7.10
7.08
6.72
6.70
6.68
4.66
4.64
4.63
3.99
1.92
1.91
1.89
1.87
1.86
1.84
1.83
1.81
1.79
1.78
0.83
0.81
0.80
0.74
0.72
0.68
0.66
iPr
iPr
iPr
iPr
NH2
NC
1.76
2.35
1.89
1.85
1.90
2.34
4.00
11.86
5.93
5.97
f1 (ppm)

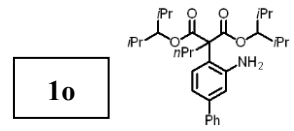

169.79
145.67
142.67
131.38
131.09
129.06
128.82
122.48
119.19
119.04
110.11
85.62
63.05
38.86
29.68
29.50
19.48
19.46
17.81
17.37
iPr
iPr
iPr
iPr
NH2
NC
f1 (ppm)

1m


7.83 7.81 7.26 7.24 7.20 7.18 7.11 7.10 7.09 7.09 7.07 7.07 6.71 6.69 6.67
4.64 4.63 4.61 4.35 4.33 4.31 4.30 4.22 4.01
1.92 1.90 1.89 1.87 1.85 1.84 1.82 1.80 1.79 1.77 1.75 1.37 1.35 1.34 0.83 0.81 0.80 0.70 0.69 0.65 0.63
iPr
iPr
O
O
O
O
iPr
iPr
NH2
EtOOC
1.85 0.90 1.01 0.97 1.00 1.89 1.97 2.41 1.96 2.06 2.07 3.00 12.05 5.76 5.99
f1 (ppm)
169.81 166.62 145.92 142.21 130.15 128.95 128.88 128.76 128.44 122.51 118.85 118.72 85.28 62.67 60.75 39.08 29.68 29.49 19.52 19.40 17.86 17.29 14.30
f1 (ppm)

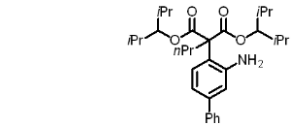

8.11 8.08 7.81 7.81 7.79 7.79 7.63 7.60 7.54 7.53 7.52 7.48 7.47 7.46 7.46 7.45 7.39 7.39 7.37 7.37 7.34 7.34 7.32 7.32 7.21 7.21 7.19 7.17 7.05 7.04 7.03 6.65 6.64 6.63 6.62 6.61 6.61 6.60 4.57 4.56 4.54 4.43 1.80 1.79 1.78 1.77 1.77 1.75 1.63 1.61 1.60 1.58 0.78 0.77 0.75 0.73 0.45 0.44 0.35 0.33
iPr
iPr
O
O
O
O
iPr
iPr
NH2
1n
1.00 1.04 1.06 1.00 1.04 2.08 1.33 1.12 2.08 2.14 2.43 1.77 1.86 2.16 12.19 5.67 5.60
f1 (ppm)
169.68 147.00 133.63 132.46 131.91 129.33 129.10 129.05 127.04 126.67 126.16 125.45 125.34 122.67 120.52 118.46 118.12 84.78 61.37 36.34 29.84 29.57 19.82 19.23 17.50 16.87
f1 (ppm)

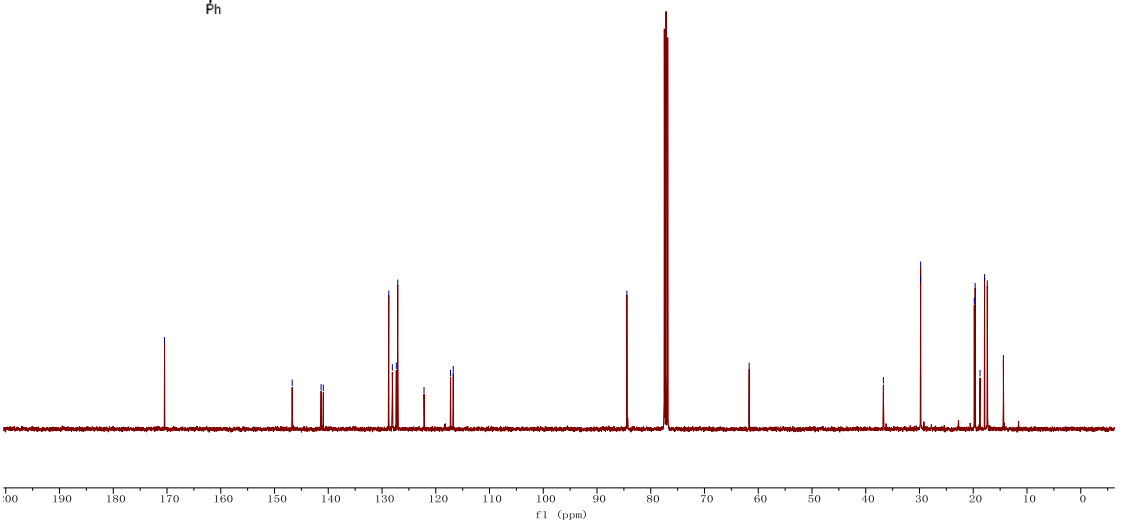
1o

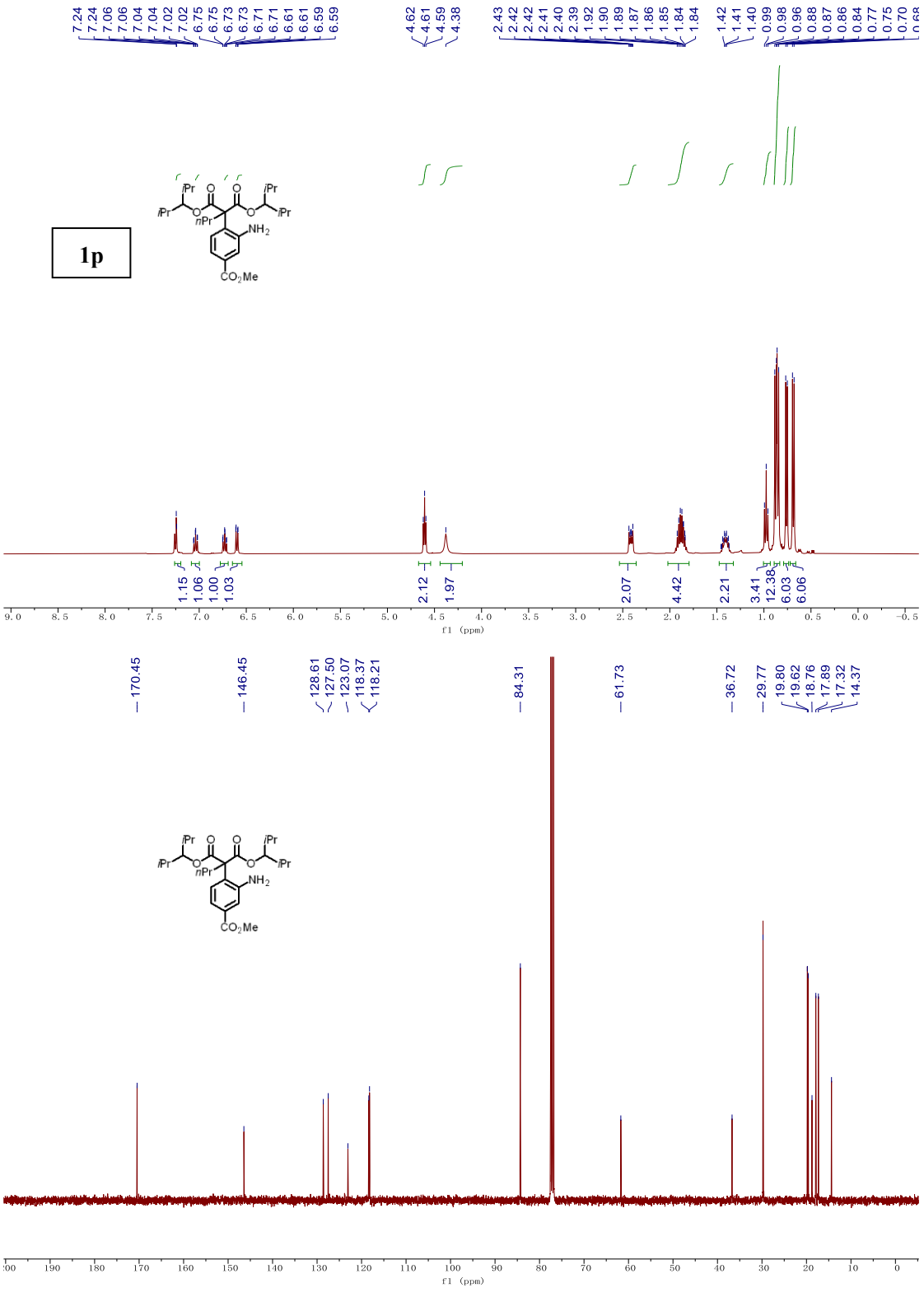

iPr
iPr
O
O
iPr
iPr
O
O
nPr
NH2
Ph

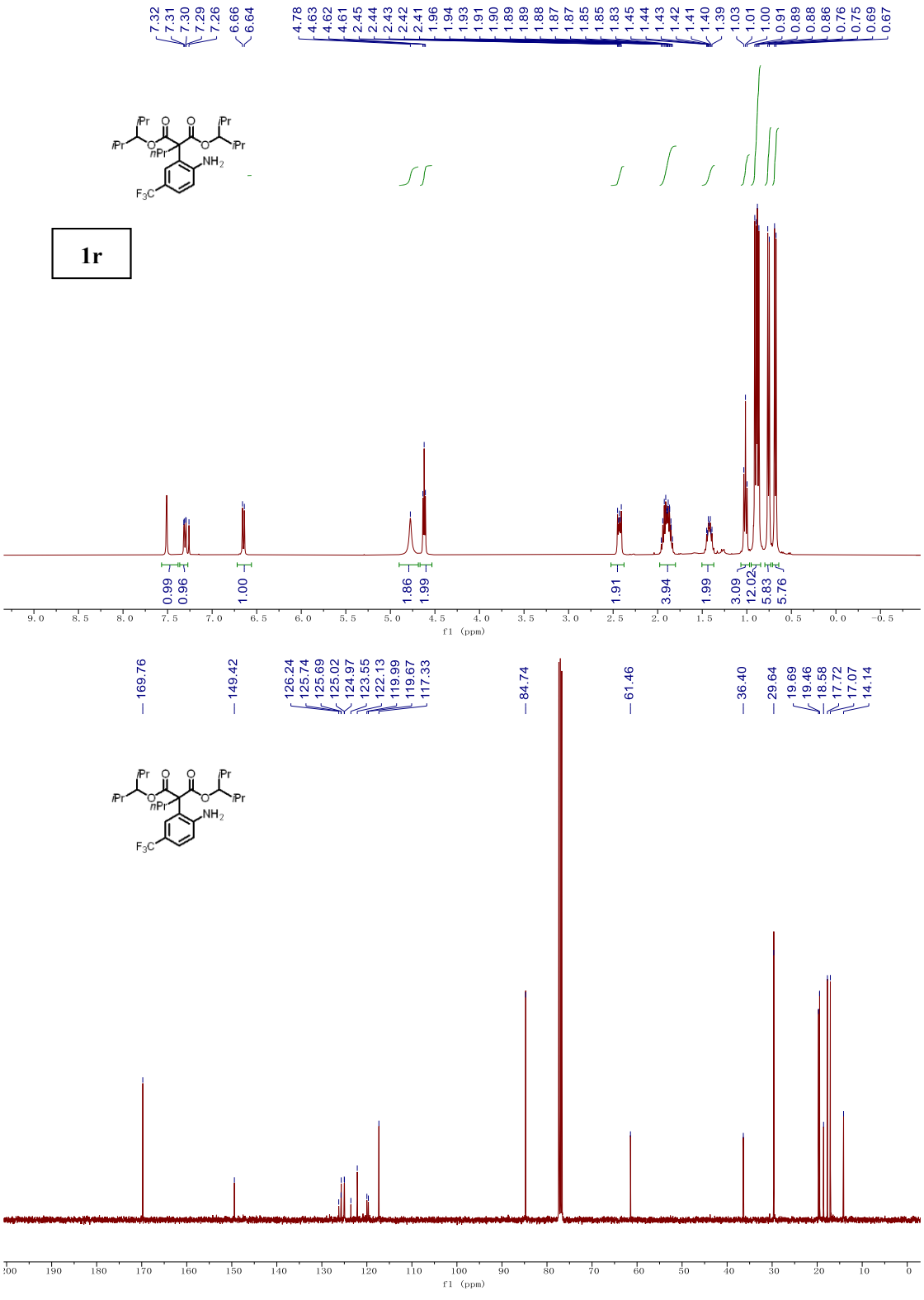
7.58
7.58
7.56
7.56
7.42
7.42
7.40
7.40
7.38
7.34
7.33
7.33
7.32
7.31
7.30
7.29
7.29
7.28
7.01
7.01
6.99
6.99
6.87
6.87
4.67
4.66
4.64
4.49
2.49
2.48
2.47
2.46
2.45
1.96
1.95
1.93
1.91
1.90
1.90
1.88
1.87
1.47
1.46
1.45
1.43
1.43
1.04
1.02
1.00
0.92
0.91
0.89
0.81
0.80
0.75
1.81
1.83
1.89
0.90
0.90
2.00
1.90
2.00
4.22
2.18
2.94
12.45
5.87
5.74
f1 (ppm)

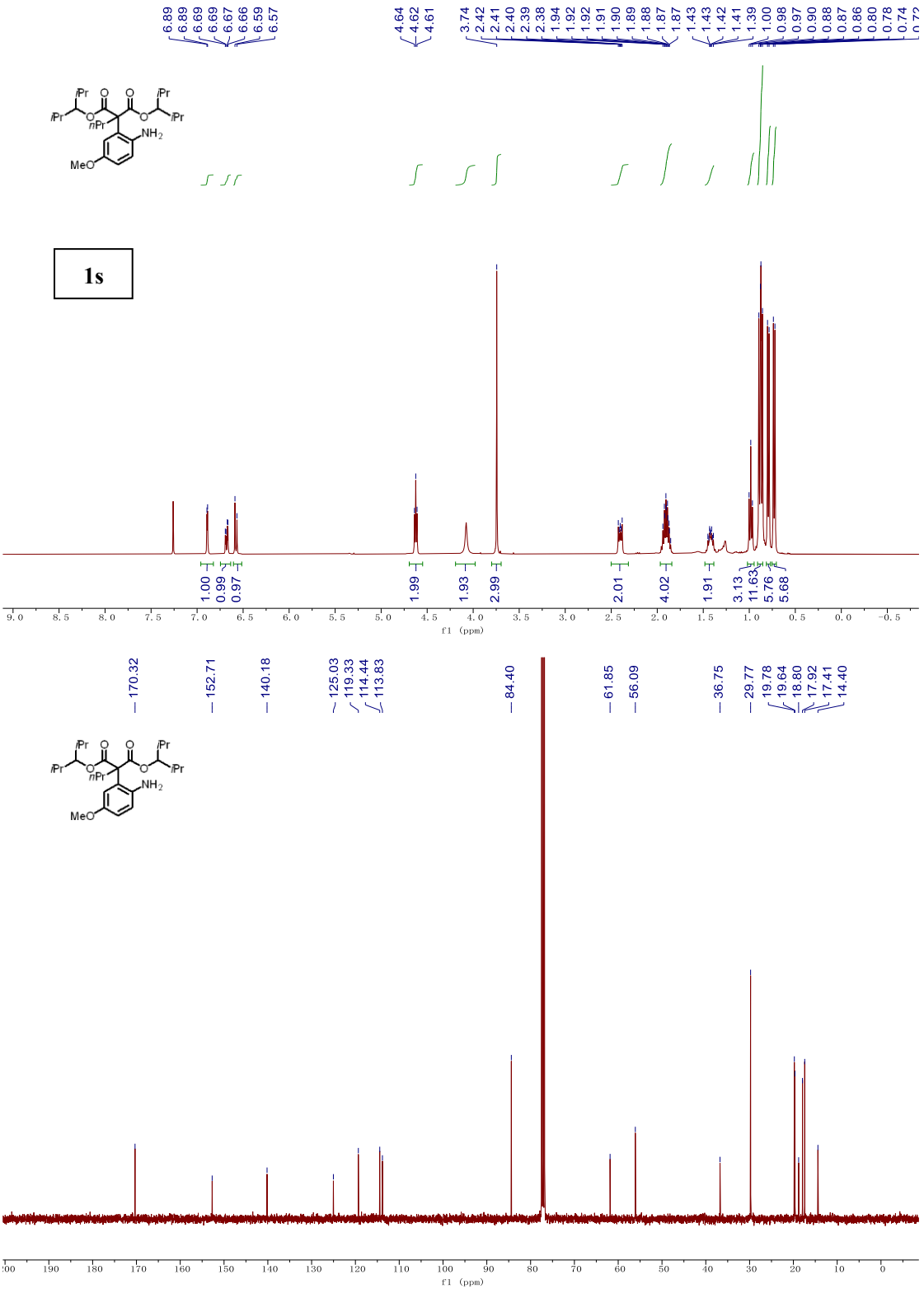

170.47
146.72
141.34
140.92
128.74
128.08
127.34
127.07
122.19
117.26
116.75
84.44
61.69
36.71
29.80
29.79
19.81
19.65
18.74
17.89
17.39
14.40

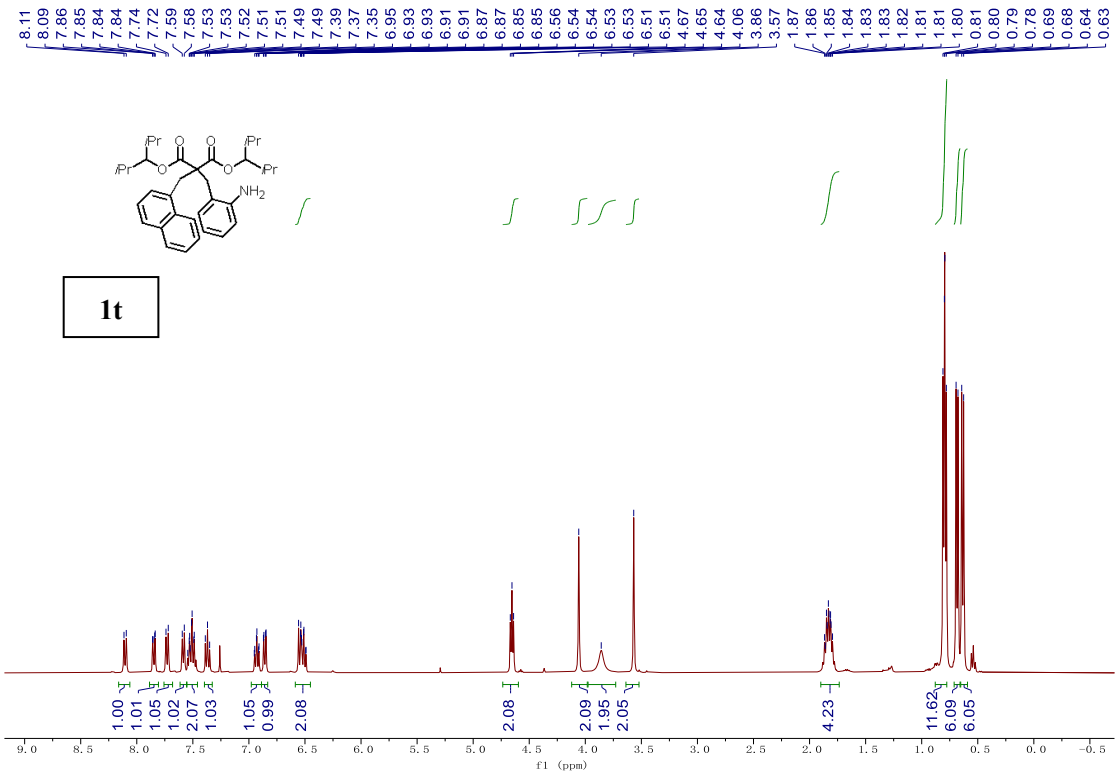

iPr
iPr
O
O
iPr
iPr
O
O
nPr
NH2
Ph

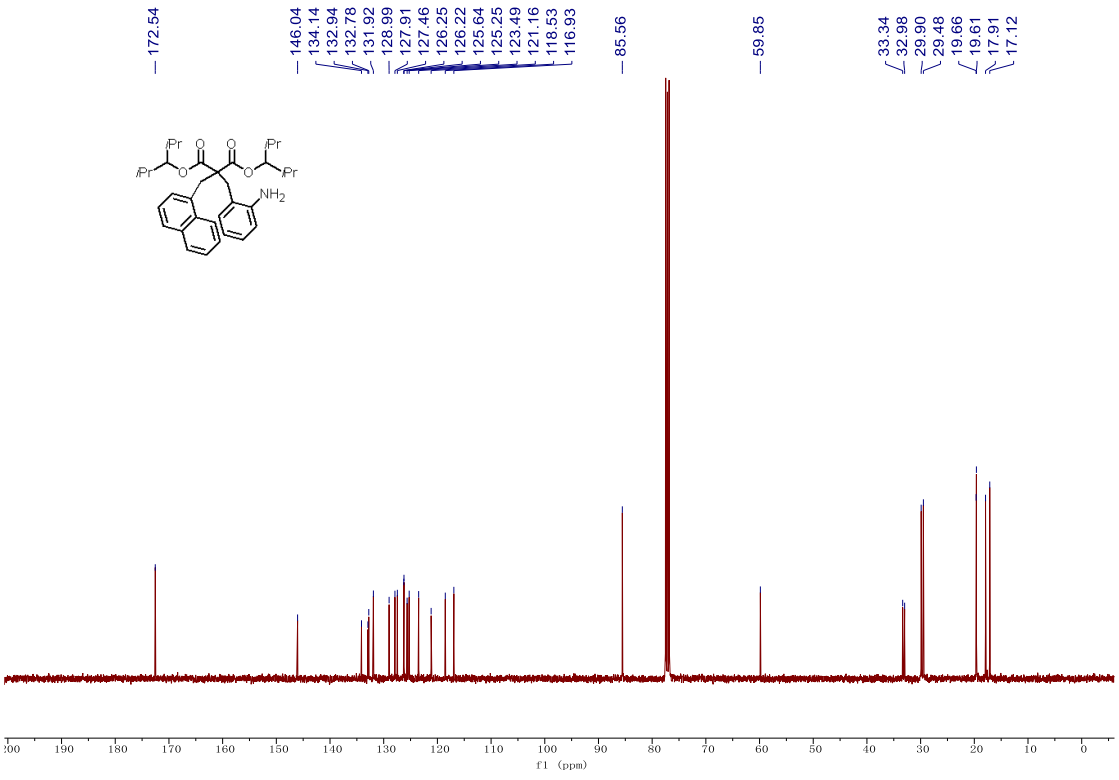

f1 (ppm)


7.24 7.24 7.06 7.06 7.04 7.04 7.02 7.02 6.75 6.75 6.73 6.73 6.71 6.71 6.61 6.61 6.59 6.59
4.62 4.61 4.59 4.38
2.43 2.42 2.42 2.41 2.40 2.39 1.92 1.90 1.89 1.87 1.86 1.85 1.84 1.84
1.42 1.41 1.40 0.99 0.98 0.96 0.88 0.87 0.86 0.84 0.77 0.75 0.70
1p
NH2
CO2Me
1.15 1.06 1.00 1.03 2.12 1.97 2.07 4.42 2.21 3.41 12.38 6.03 6.06
f1 (ppm)
170.45 146.45 128.61 127.50 123.07 118.37 118.21 84.31 61.73 36.72 29.77 19.80 19.62 18.76 17.89 17.32 14.37
f1 (ppm)

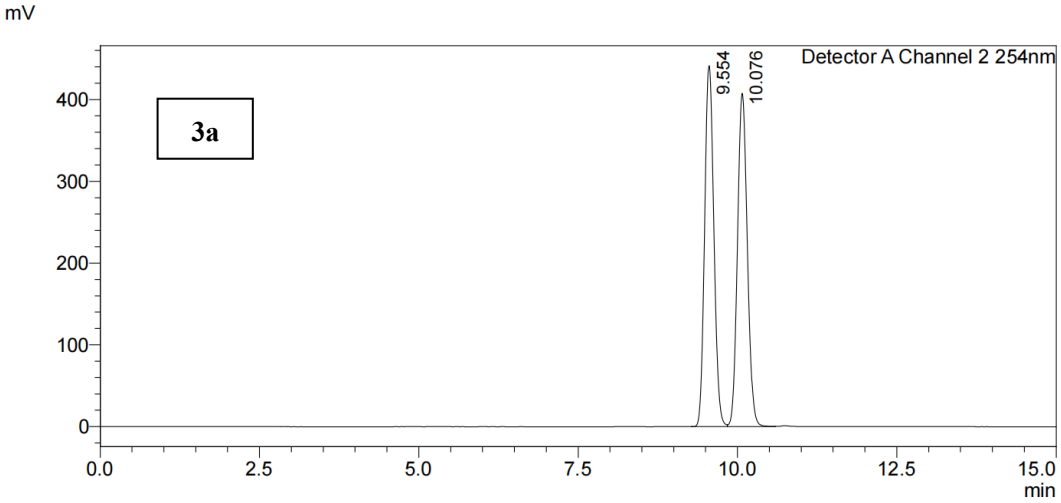

7.32
7.31
7.30
7.29
7.26
6.66
6.64
4.78
4.63
4.62
4.61
2.45
2.44
2.43
2.42
2.41
1.96
1.94
1.93
1.91
1.90
1.89
1.89
1.88
1.87
1.87
1.85
1.85
1.83
1.45
1.44
1.43
1.42
1.41
1.40
1.39
1.03
1.01
1.00
0.91
0.89
0.88
0.86
0.76
0.75
0.69
0.67
1r
0.99
0.96
1.00
1.86
1.99
1.91
3.94
1.99
3.09
12.02
5.83
5.76
f1 (ppm)
169.76
149.42
126.24
125.74
125.69
125.02
124.97
123.55
122.13
119.99
119.67
117.33
84.74
61.46
36.40
29.64
19.69
19.46
18.58
17.72
17.07
14.14
f1 (ppm)


1s
6.89
6.89
6.69
6.69
6.67
6.66
6.59
6.57
4.64
4.62
4.61
3.74
2.42
2.41
2.40
2.39
2.38
1.94
1.92
1.92
1.91
1.90
1.89
1.88
1.87
1.87
1.43
1.43
1.42
1.41
1.39
1.00
0.98
0.97
0.90
0.88
0.87
0.86
0.80
0.78
0.74
1.00
0.99
0.97
1.99
1.93
2.99
2.01
4.02
1.91
3.13
11.63
5.76
5.68
f1 (ppm)
170.32
152.71
140.18
125.03
119.33
114.44
113.83
84.40
61.85
56.09
36.75
29.77
19.78
19.64
18.80
17.92
17.41
14.40
f1 (ppm)


8.11 8.09 7.86 7.85 7.84 7.84 7.74 7.72 7.59 7.58 7.53 7.53 7.52 7.51 7.51 7.49 7.49 7.39 7.37 7.35 6.95 6.93 6.93 6.91 6.91 6.87 6.87 6.85 6.85 6.56 6.54 6.54 6.53 6.53 6.51 6.51 4.67 4.65 4.64 4.06 3.86 3.57 1.87 1.86 1.85 1.84 1.83 1.83 1.82 1.81 1.81 1.80 0.81 0.80 0.79 0.78 0.69 0.68 0.64 0.63
iPr
iPr
iPr
iPr
NH2
1t
1.00 1.01 1.05 1.02 2.07 1.03 1.05 0.99 2.08 2.08 2.09 1.95 2.05 4.23 11.62 6.09 6.05
f1 (ppm)

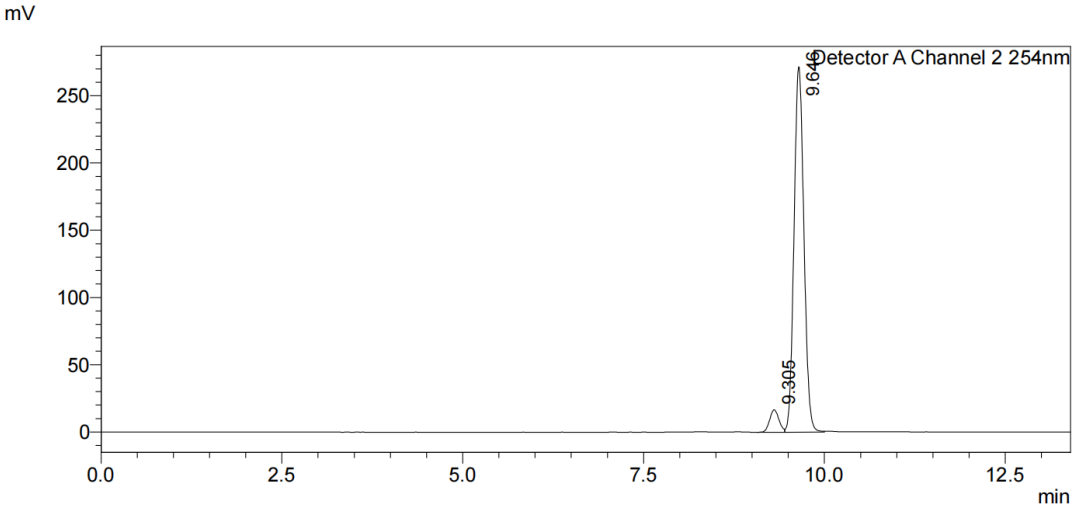

172.54
146.04 134.14 132.94 132.78 131.92 128.99 127.91 127.46 126.25 126.22 125.64 125.25 123.49 121.16 118.53 116.93
85.56
59.85
33.34 32.98 29.90 29.48 19.66 19.61 17.91 17.12
iPr
iPr
iPr
iPr
NH2
f1 (ppm)

10. Copies of HPLC chromatograms



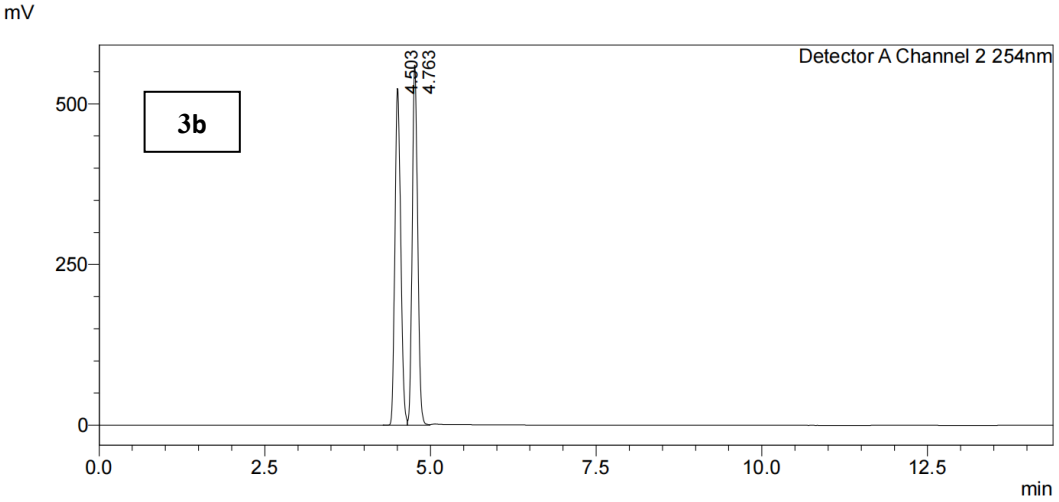
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.554	4365457	441143	49.846
2	10.076	4392377	407652	50.154
Total		8757833	848795	



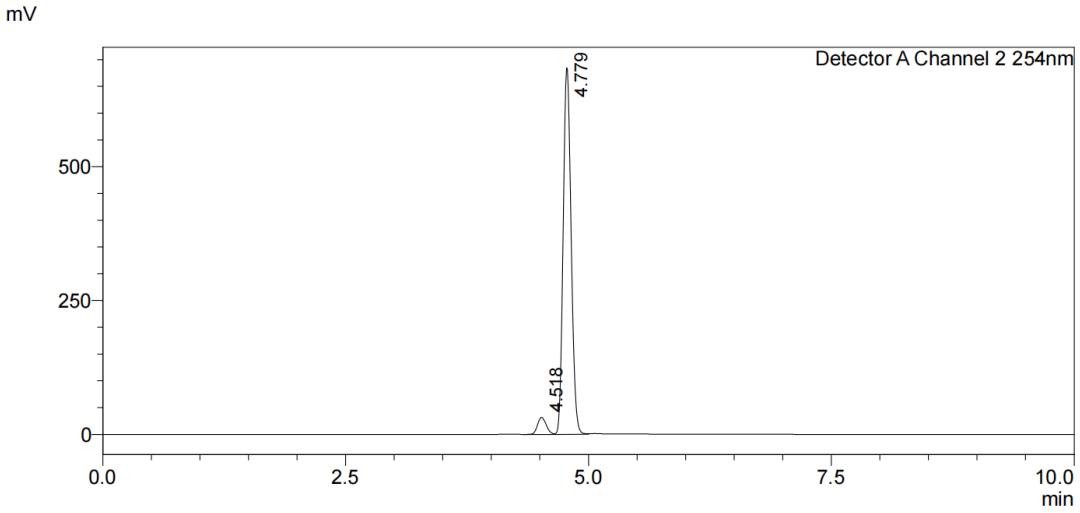
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.305	149140	16607	5.453
2	9.646	2585908	271585	94.547
Total		2735048	288192	



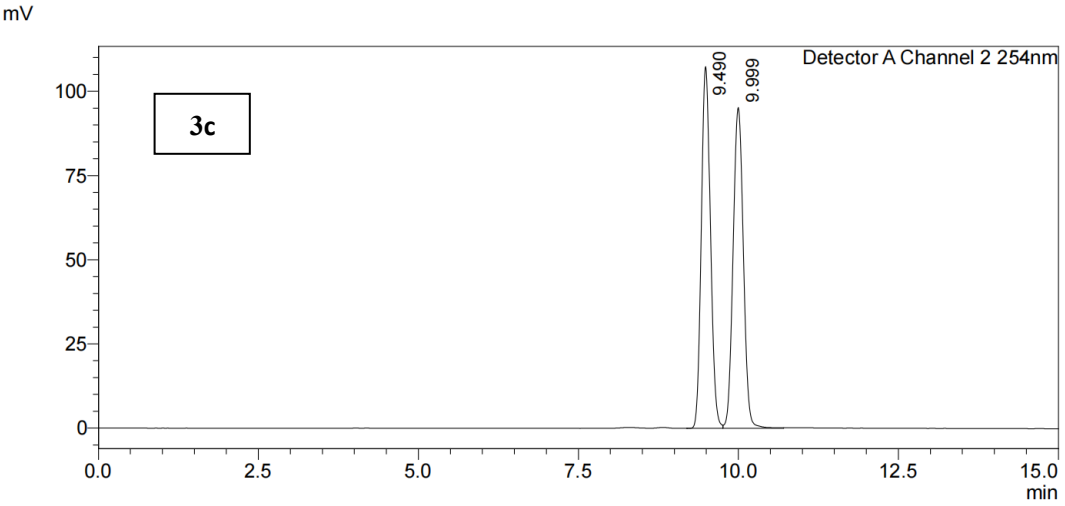
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	4.503	3196782	524117	49.899
2	4.763	3209728	560065	50.101
Total		6406511	1084181	



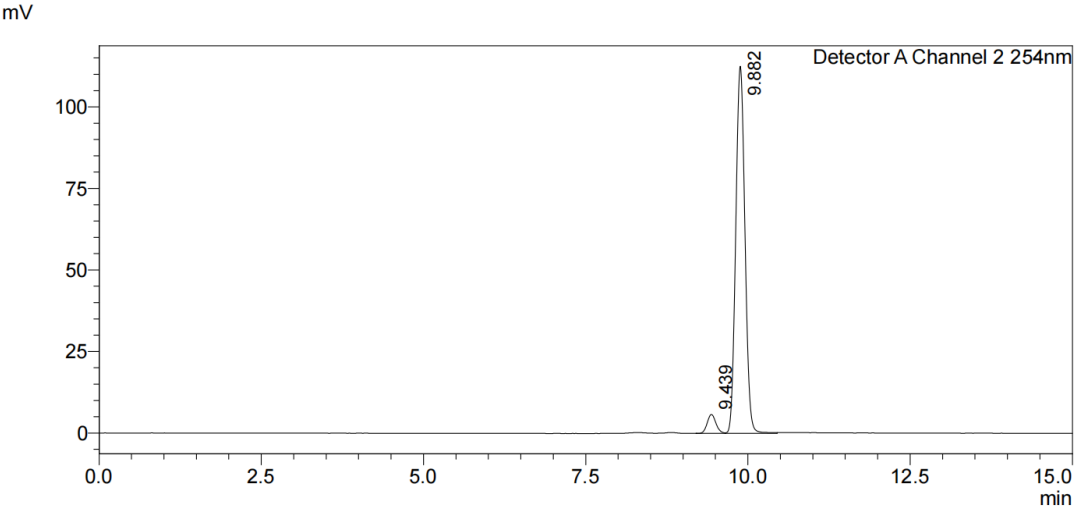
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	4.518	193843	31770	4.702
2	4.779	3928474	684638	95.298
Total		4122318	716408	



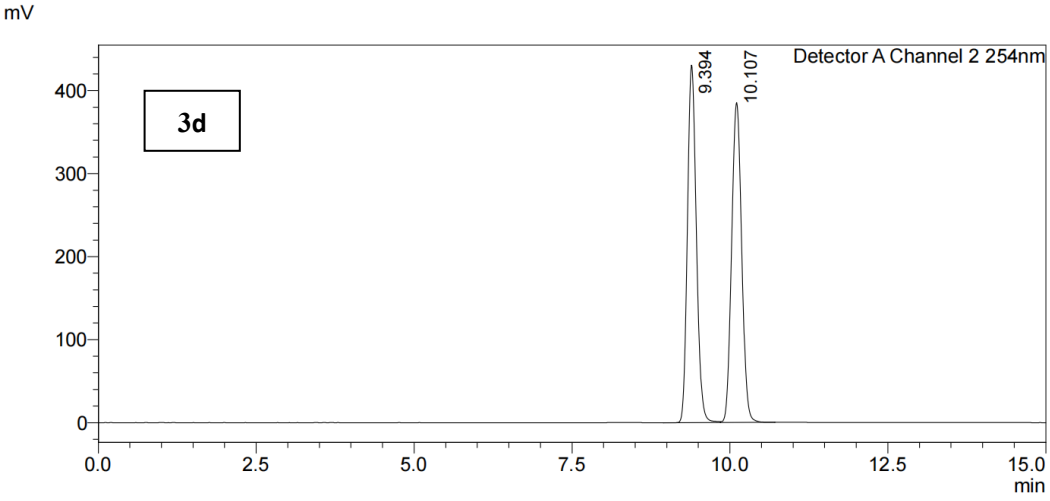
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.490	1056085	107436	49.594
2	9.999	1073394	95292	50.406
Total		2129479	202728	



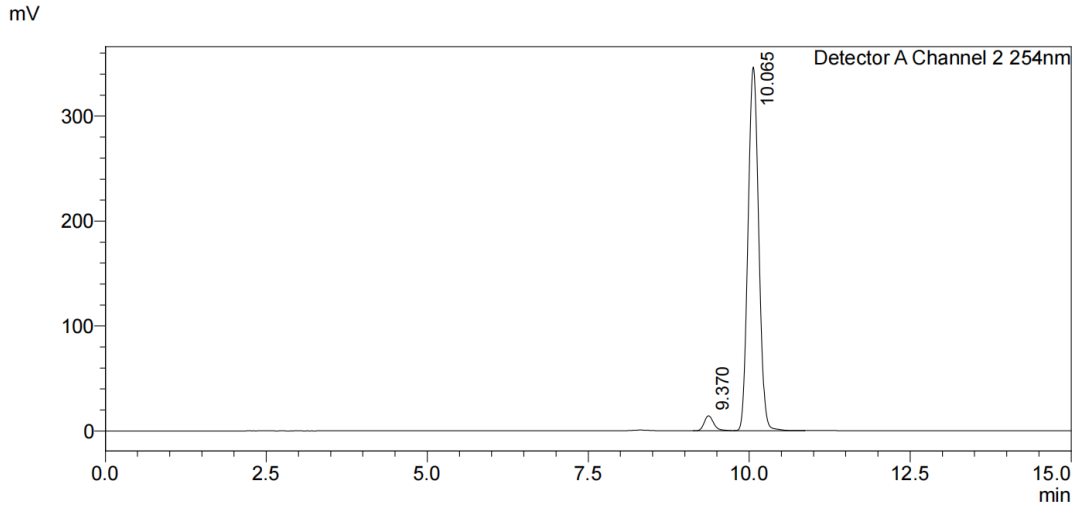
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.439	55191	5822	4.703
2	9.882	1118232	112578	95.297
Total		1173423	118399	



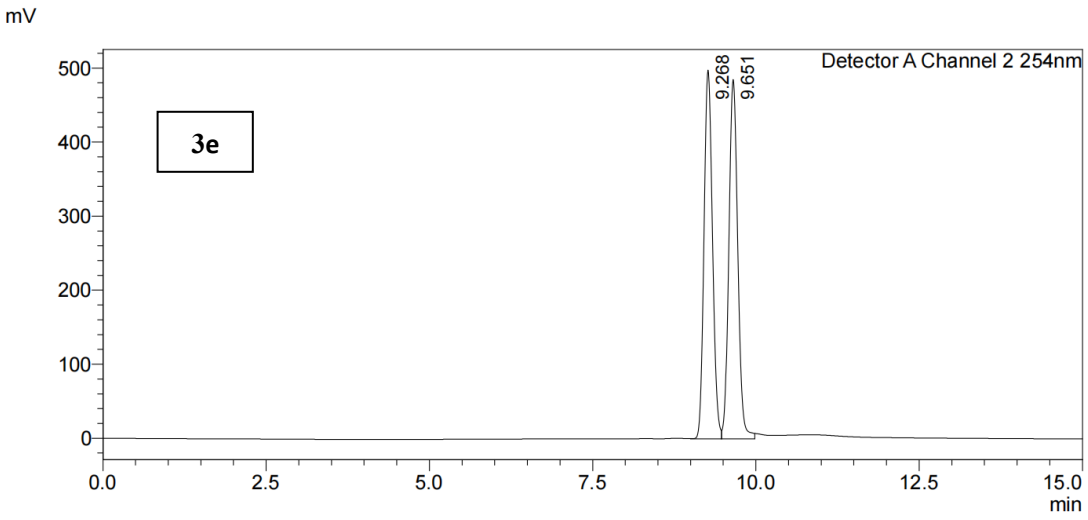
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.394	4243887	430561	49.912
2	10.107	4258777	385242	50.088
Total		8502664	815803	



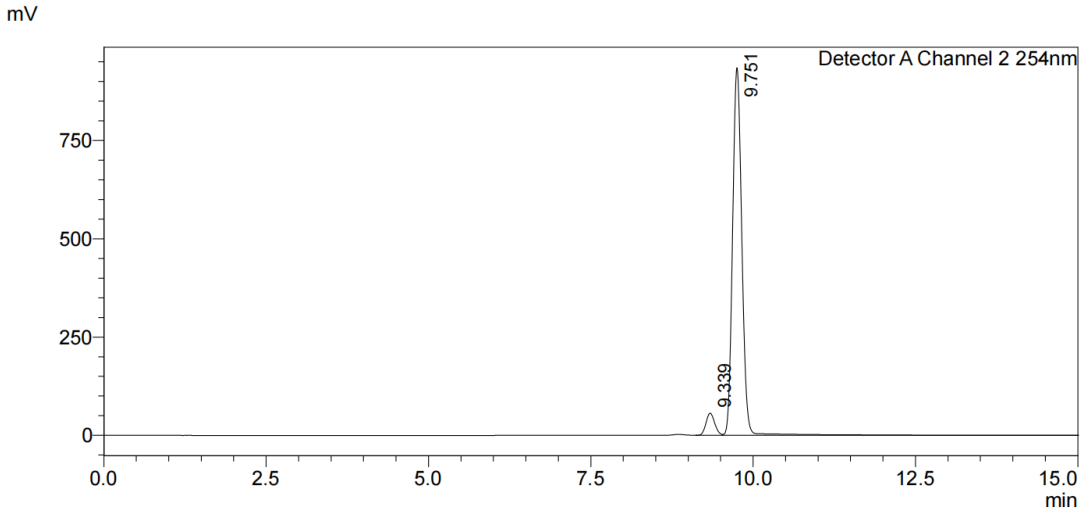
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.370	149183	14356	3.579
2	10.065	4019224	346705	96.421
Total		4168407	361061	



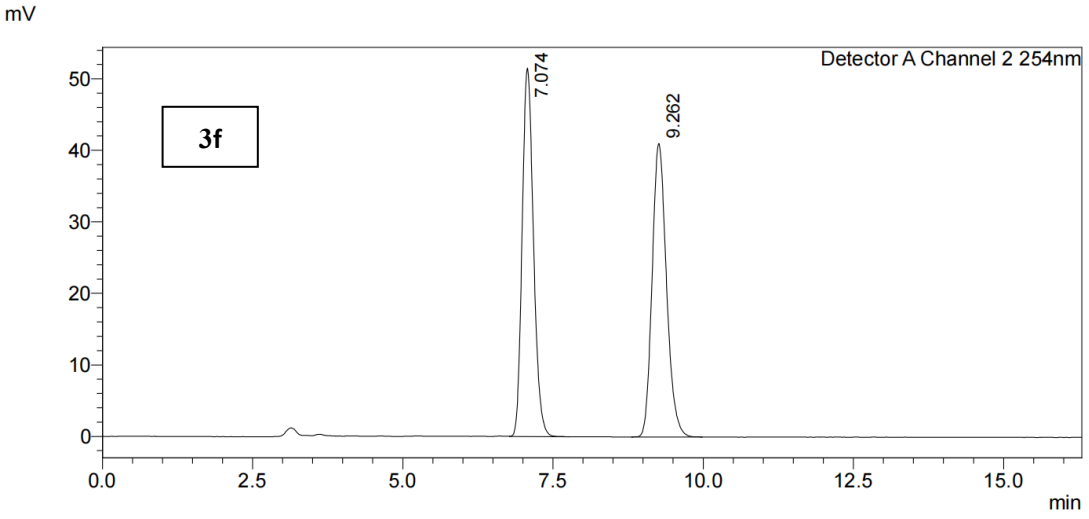
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.268	4528609	498099	49.544
2	9.651	4611967	485294	50.456
Total		9140576	983393	



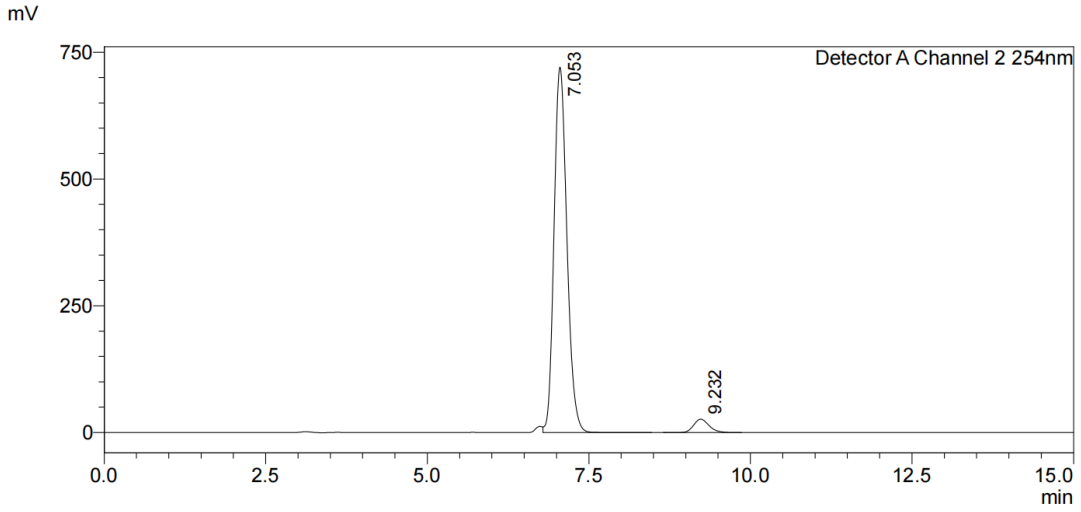
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.339	537375	56414	5.343
2	9.751	9520478	935072	94.657
Total		10057852	991486	



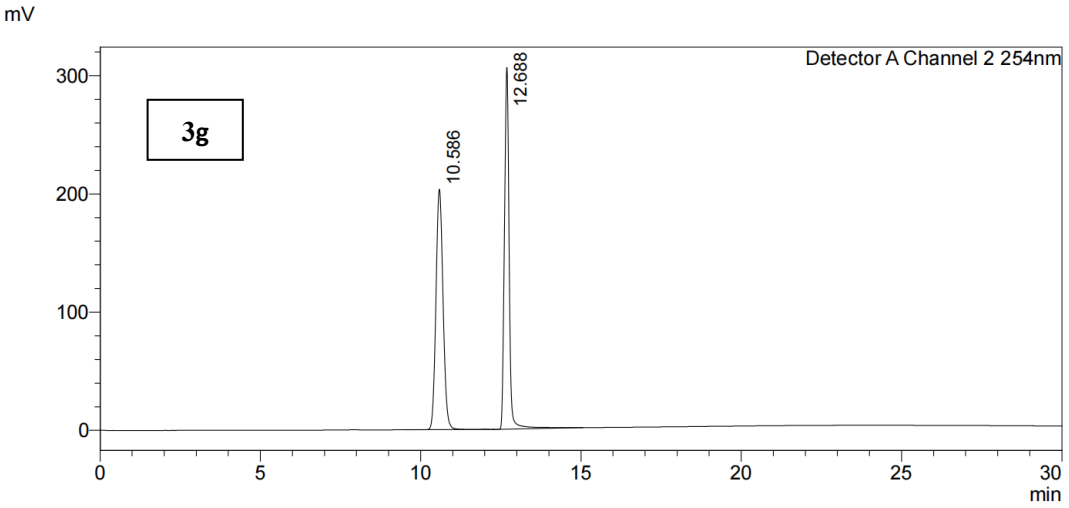
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	7.074	675759	51532	49.765
2	9.262	682134	41037	50.235
Total		1357893	92569	



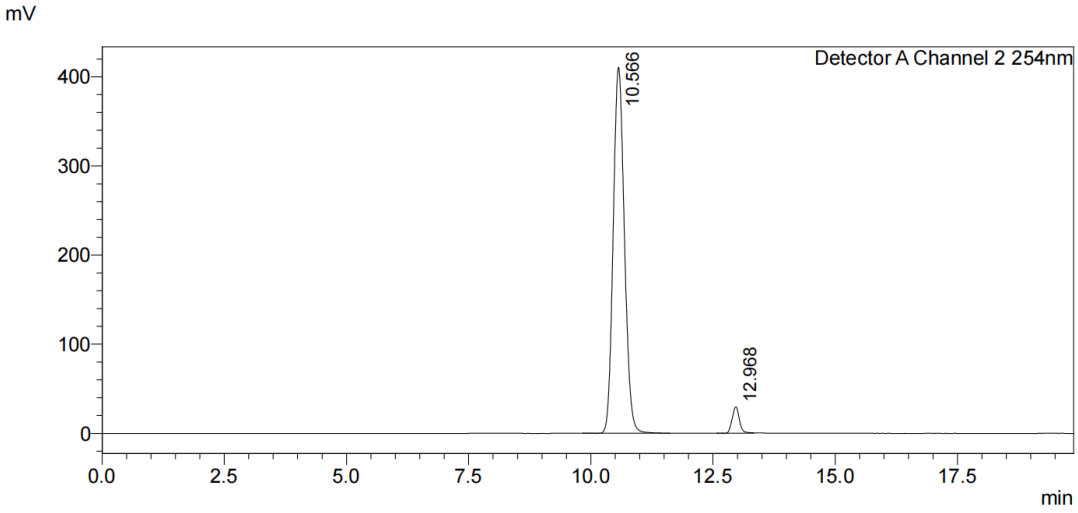
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	7.053	10038613	720609	95.790
2	9.232	441153	26420	4.210
Total		10479767	747029	



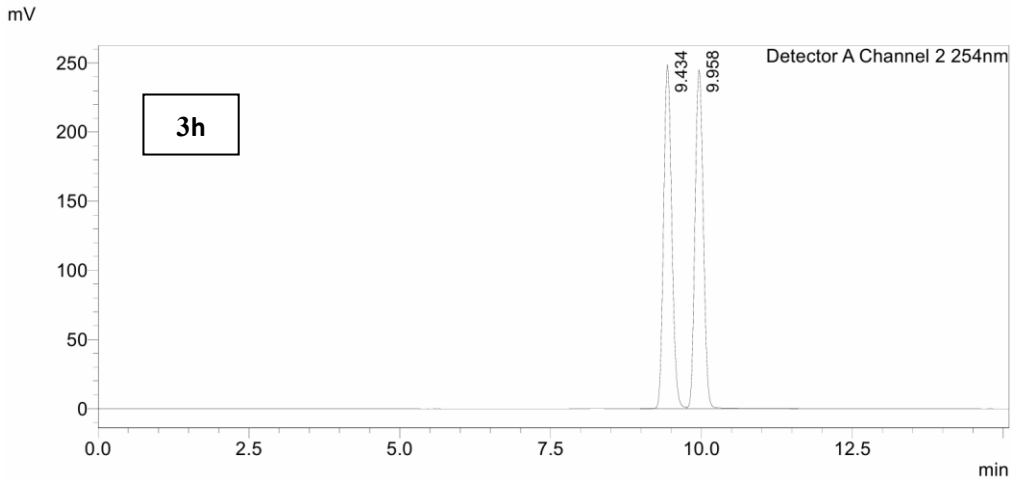
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.586	3146461	203369	50.102
2	12.688	3133611	305890	49.898
Total		6280072	509259	



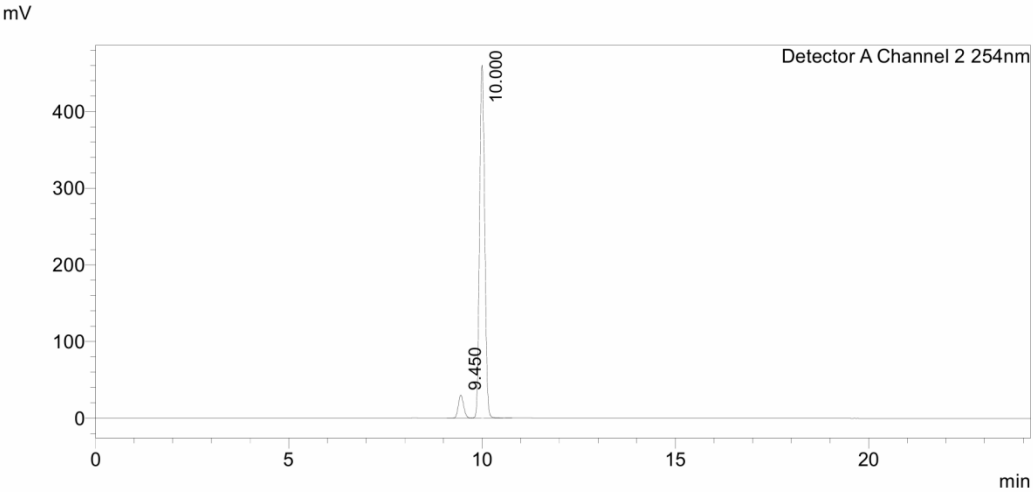
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.566	6557154	410703	95.544
2	12.968	305792	29662	4.456
Total		6862946	440365	



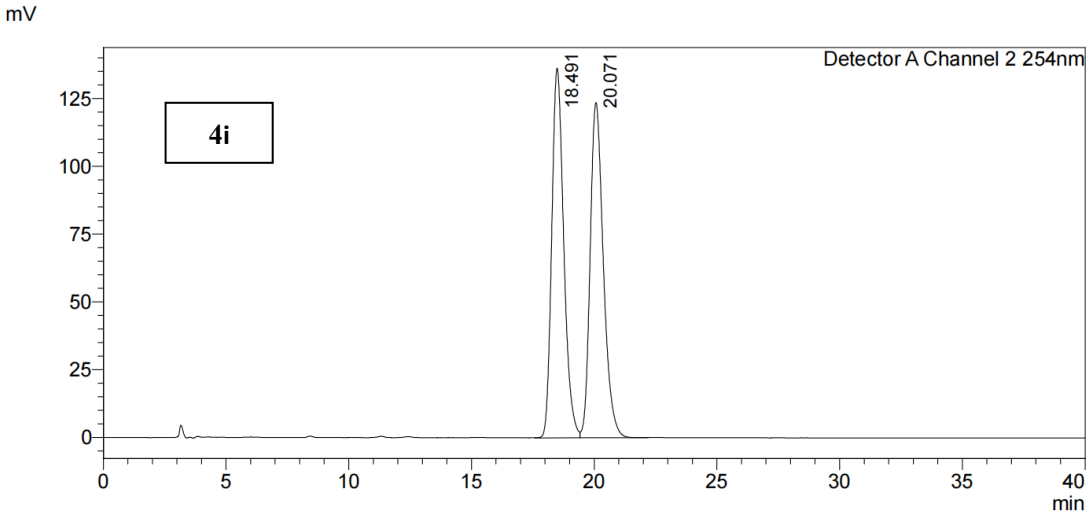
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.434	2348819	248754	50.059
2	9.958	2343269	245135	49.941
Total		4692088	493889	



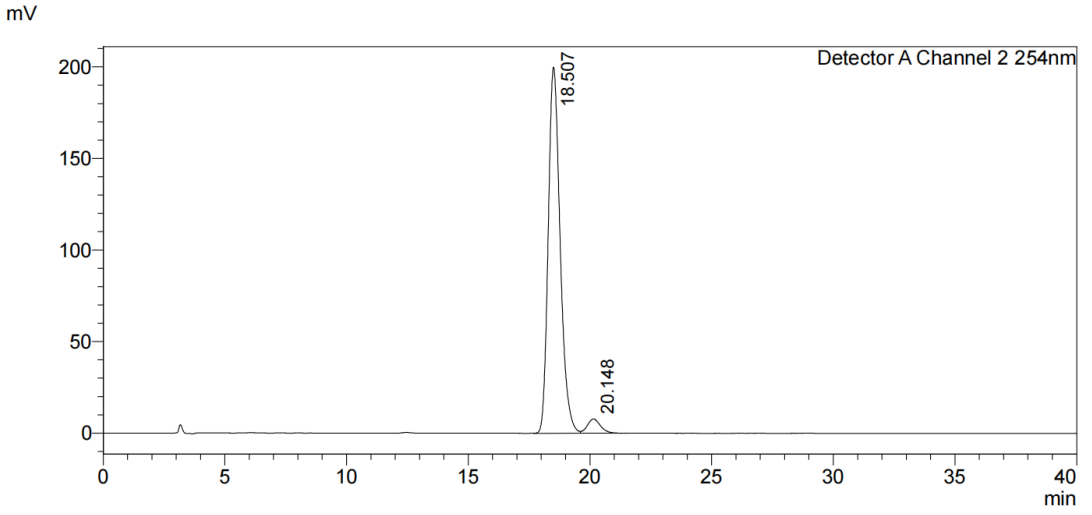
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.450	289944	30083	6.330
2	10.000	4290250	460508	93.670
Total		4580194	490591	



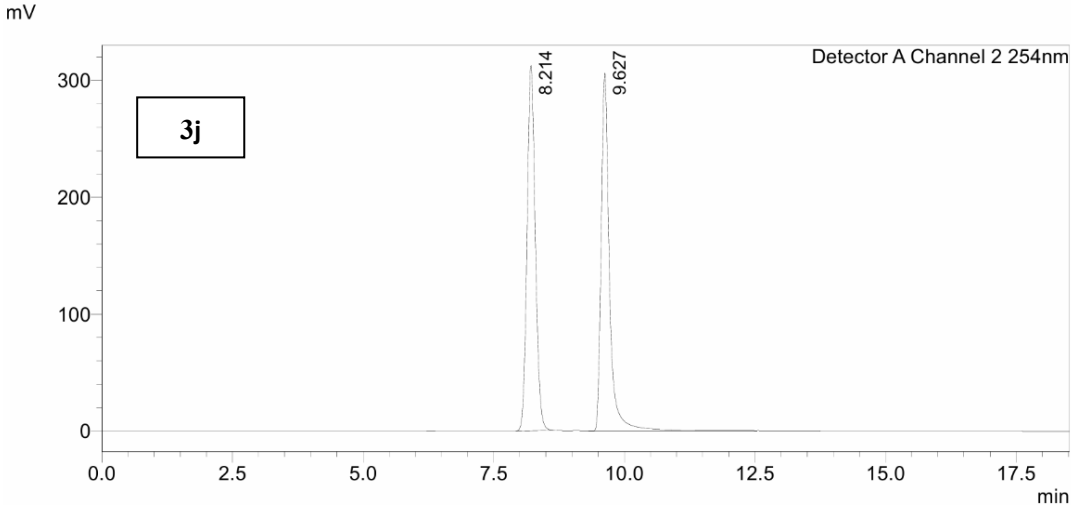
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	18.491	4640114	136332	50.133
2	20.071	4615528	123649	49.867
Total		9255642	259981	



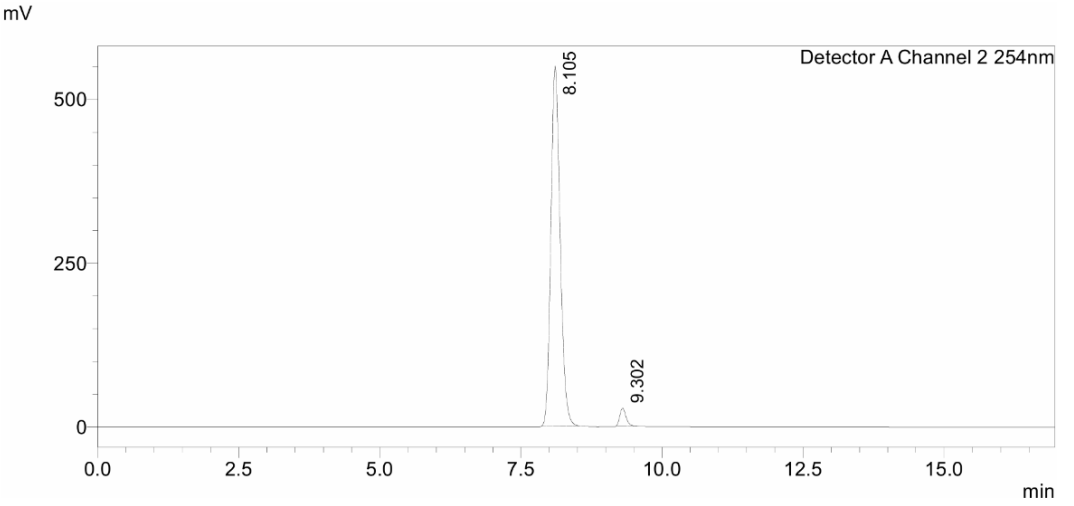
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	18.507	6796268	199950	95.872
2	20.148	292619	7803	4.128
Total		7088887	207753	



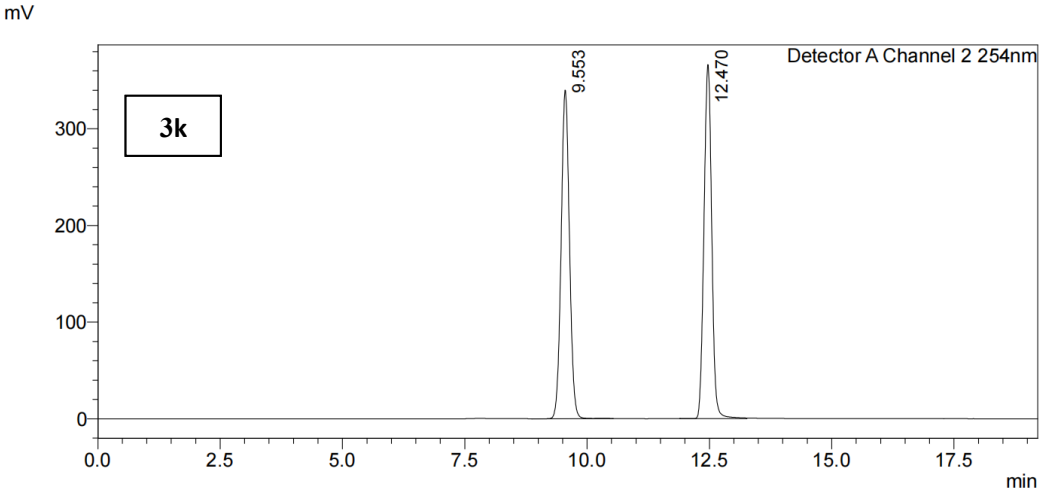
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	8.214	3431331	312292	50.231	
2	9.627	3399833	306038	49.769	
Total		6831164	618330		



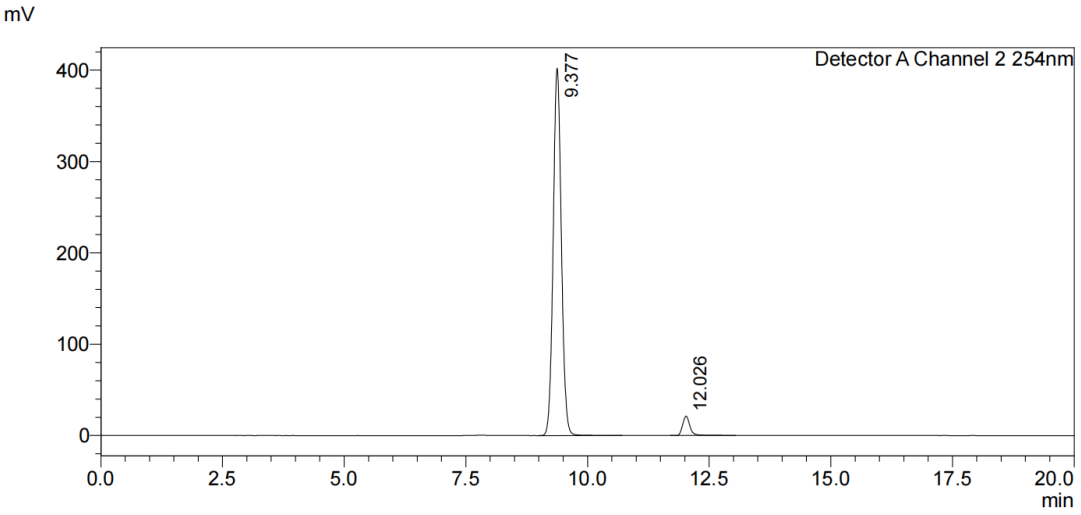
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	8.105	6271700	549512	96.806	
2	9.302	206947	27188	3.194	
Total		6478647	576700		



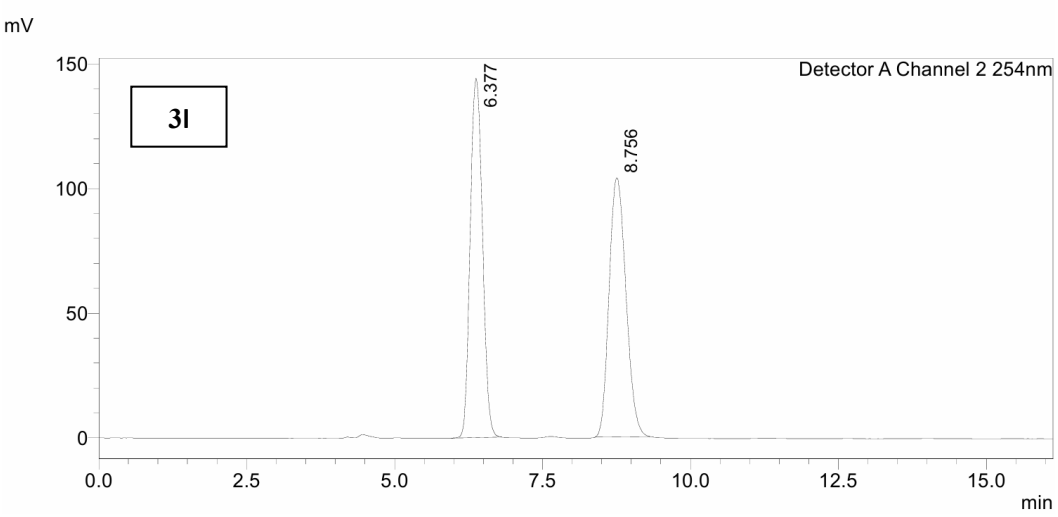
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.553	4044430	340124	49.939
2	12.470	4054347	366323	50.061
Total		8098777	706448	



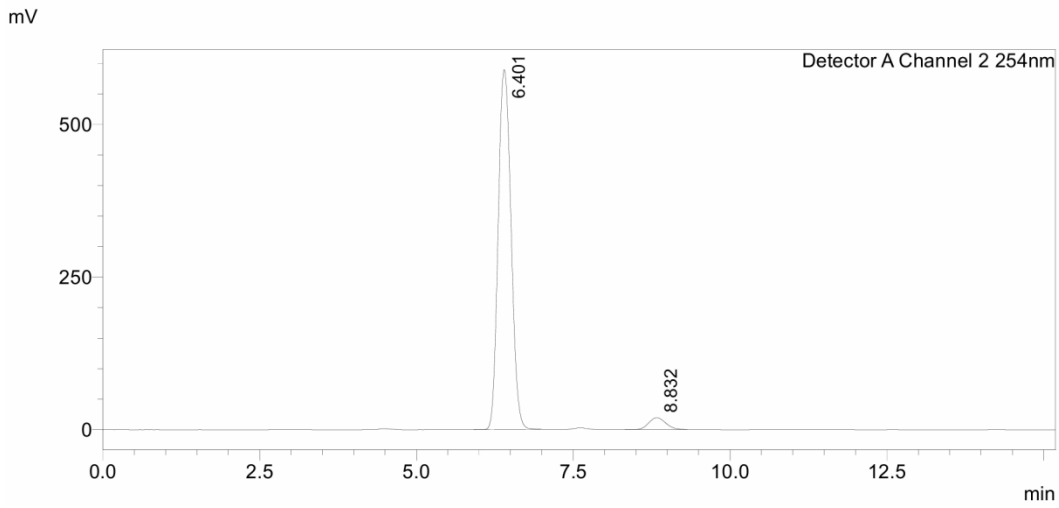
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.377	4723778	402108	95.414
2	12.026	227037	21226	4.586
Total		4950815	423333	



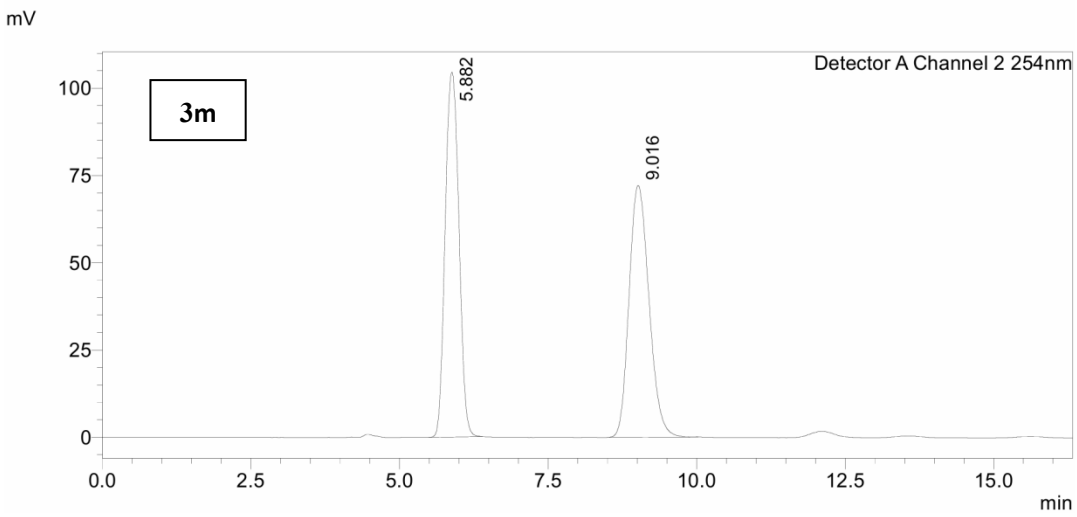
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.377	2079974	144073	50.244
2	8.756	2059786	103918	49.756
Total		4139760	247991	



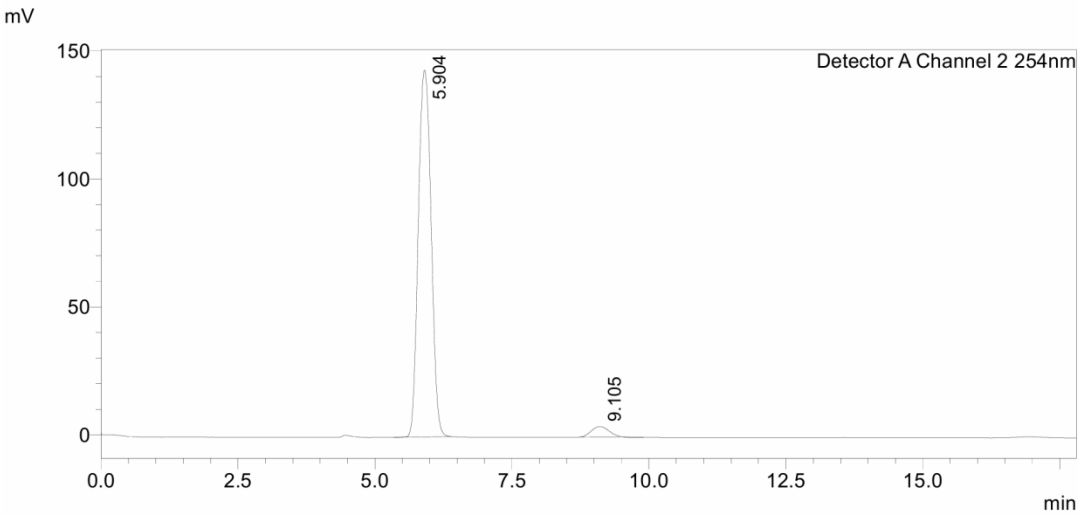
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.401	8462693	589643	95.829
2	8.832	368342	19417	4.171
Total		8831036	609059	



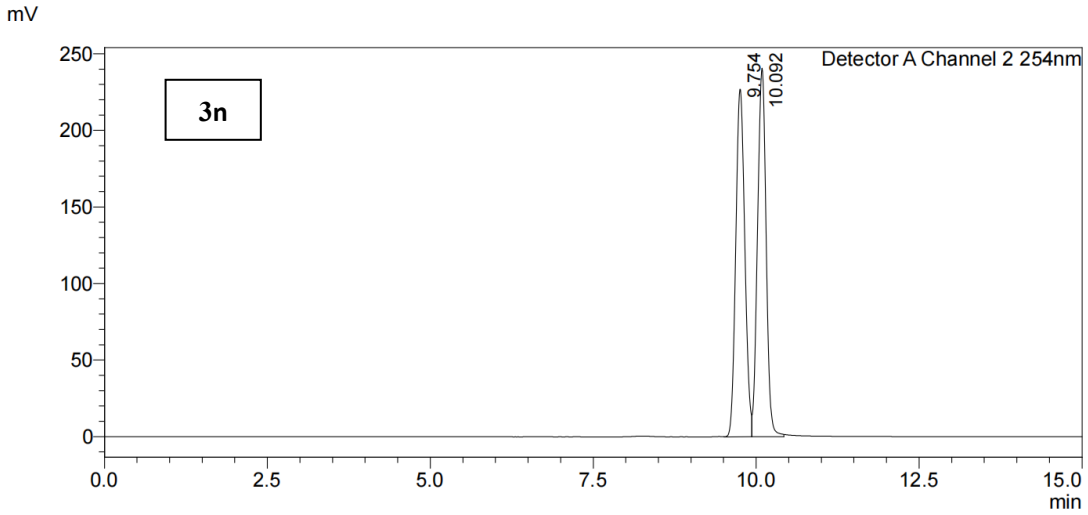
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	5.882	1684416	104535	49.996
2	9.016	1684697	72151	50.004
Total		3369113	176686	



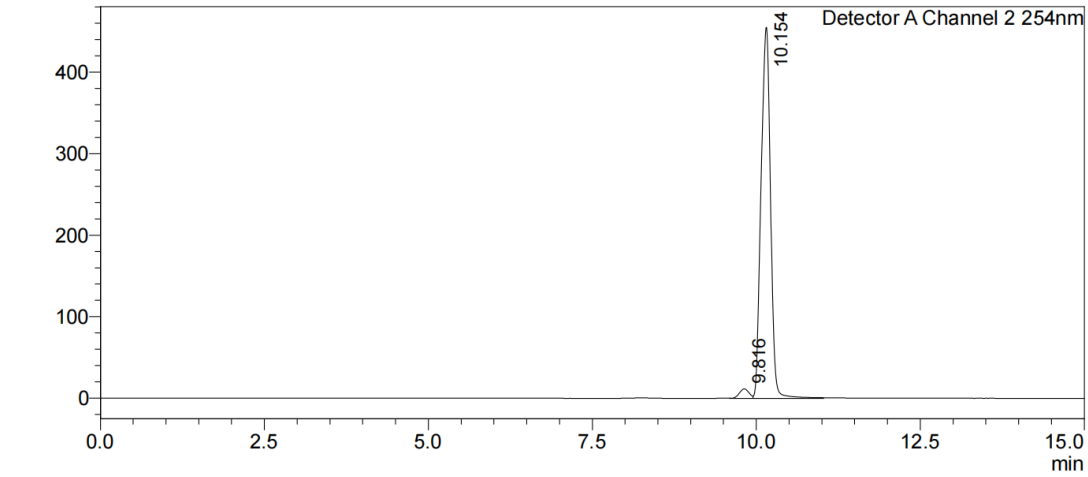
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	5.904	2339798	143286	95.985
2	9.105	97875	4201	4.015
Total		2437673	147486	



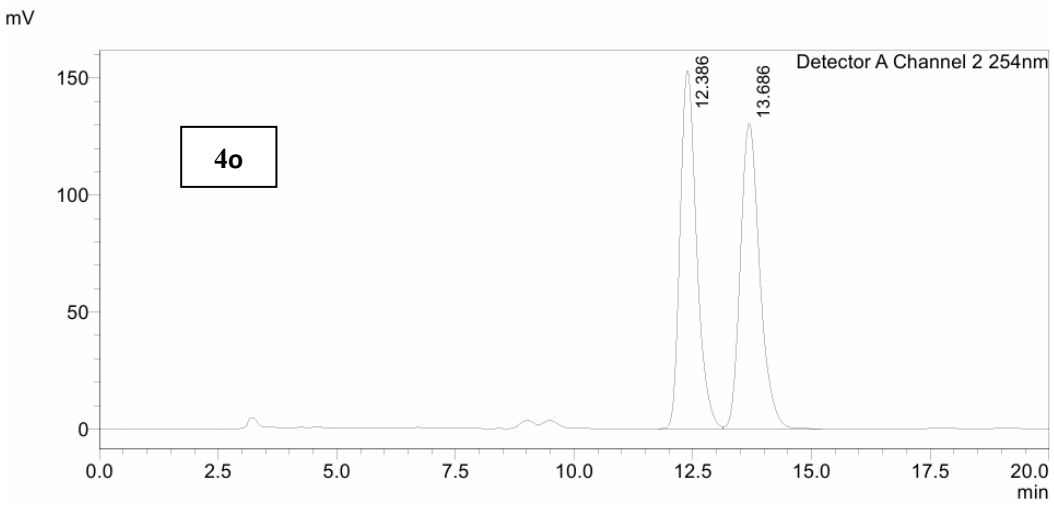
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.754	2205693	227075	49.883
2	10.092	2216044	240701	50.117
Total		4421737	467776	



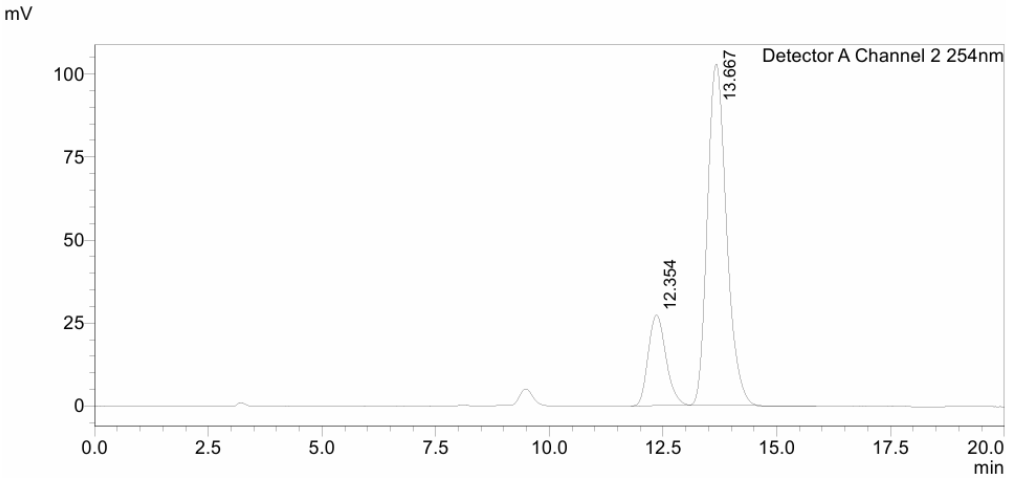
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.816	117491	11536	2.511
2	10.154	4561114	455102	97.489
Total		4678605	466638	



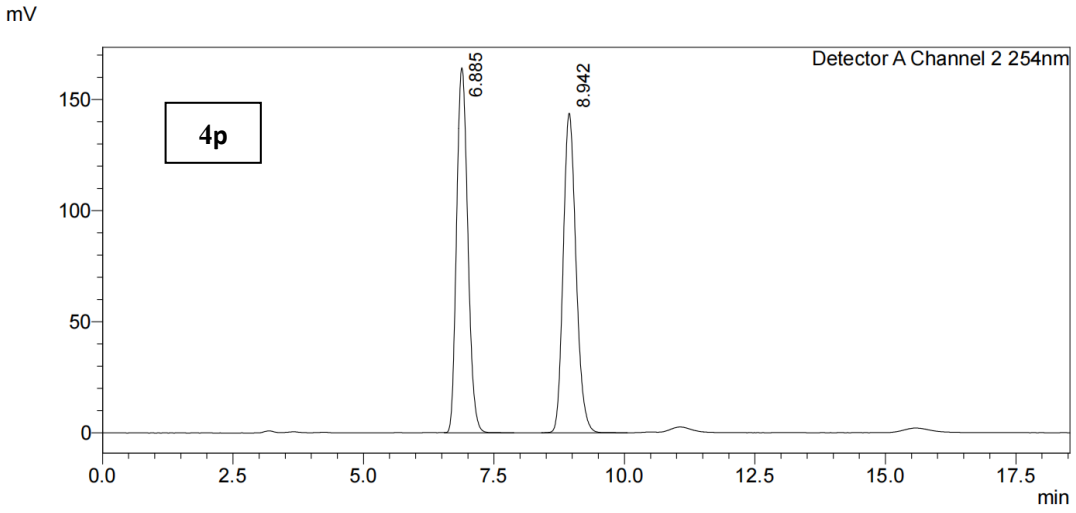
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	12.386	3700306	153109	49.987	
2	13.686	3702295	130449	50.013	
Total		7402601	283558		



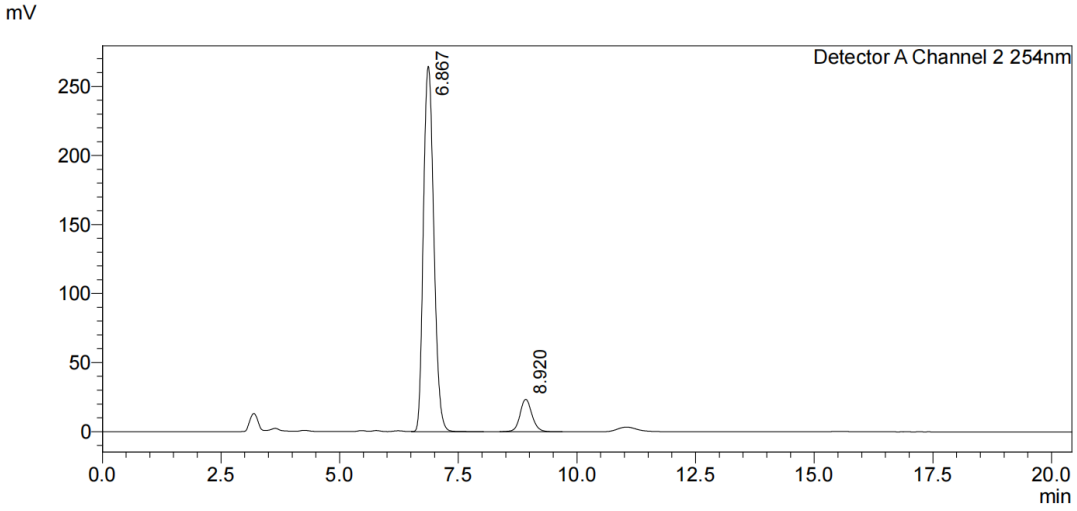
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	12.354	740421	27264	19.739	
2	13.667	3010722	102819	80.261	
Total		3751143	130083		



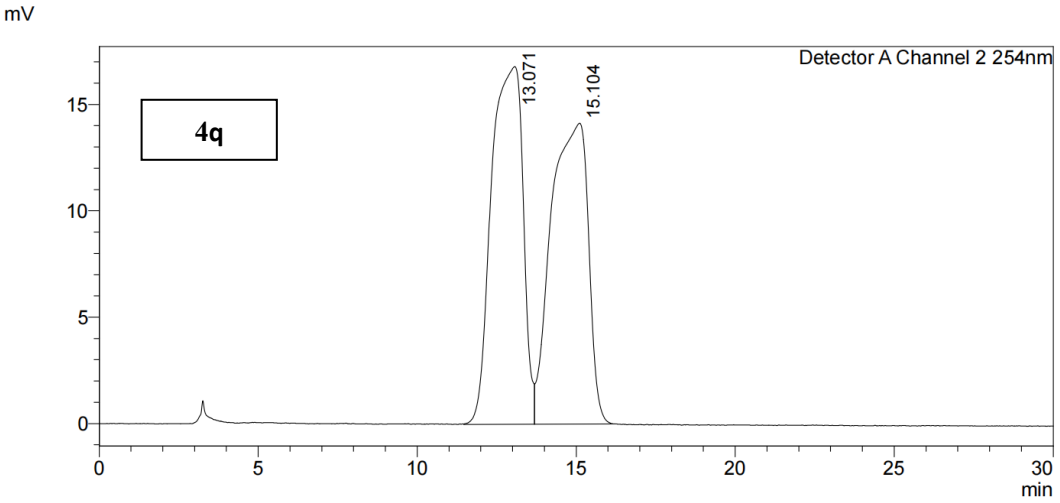
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.885	2456213	164207	49.972
2	8.942	2458951	143778	50.028
Total		4915164	307985	



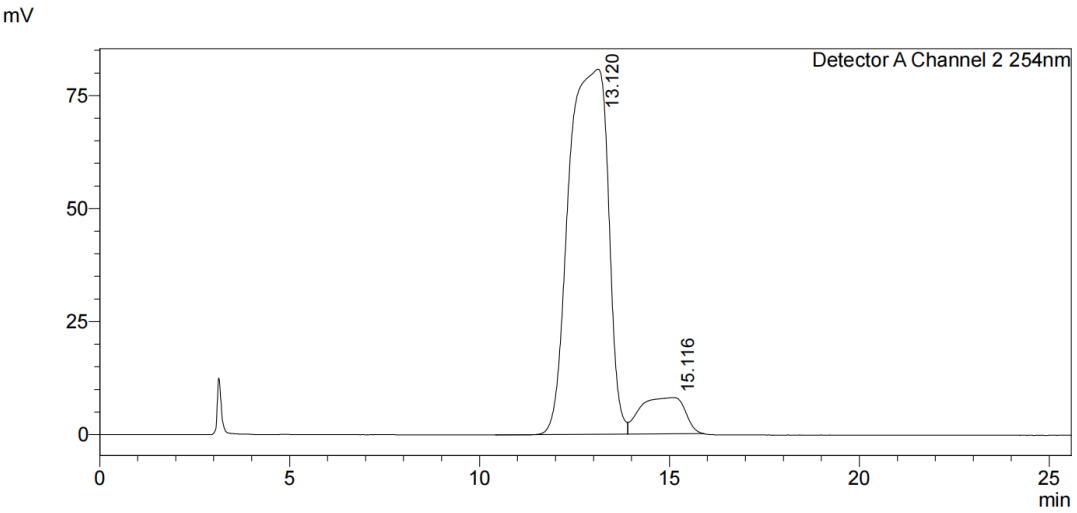
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.867	4050903	264635	90.757
2	8.920	412551	23462	9.243
Total		4463454	288097	



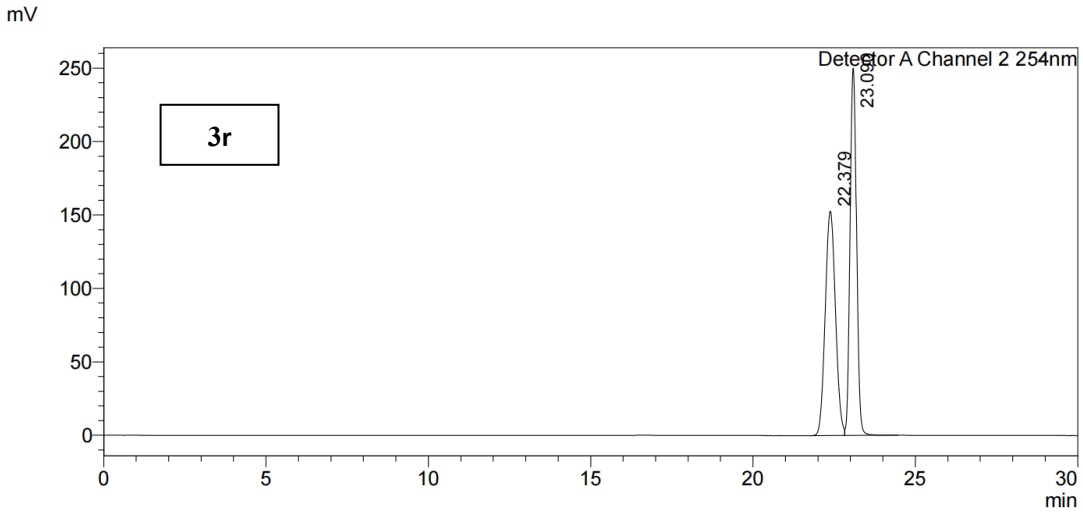
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.071	1162348	16807	50.273
2	15.104	1149716	14142	49.727
Total		2312064	30949	



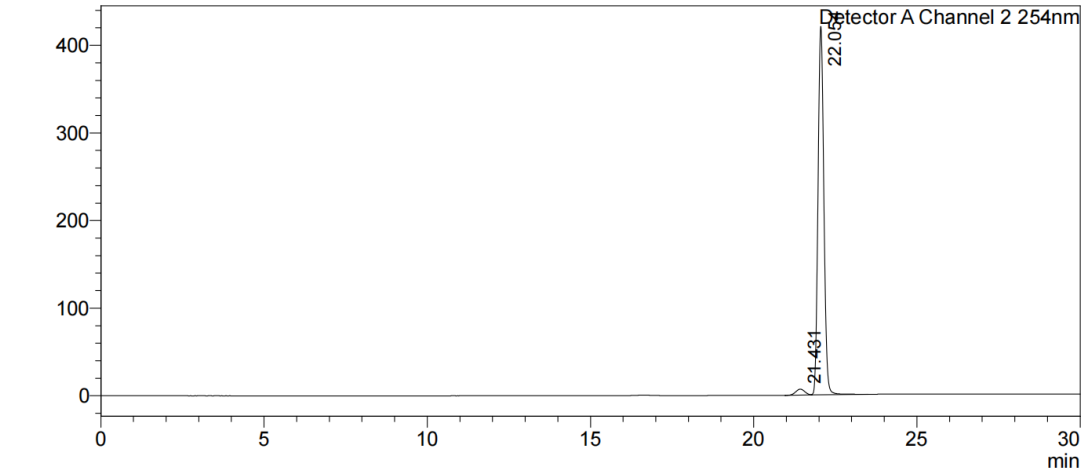
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.120	5820715	80766	89.919
2	15.116	652570	8036	10.081
Total		6473285	88802	



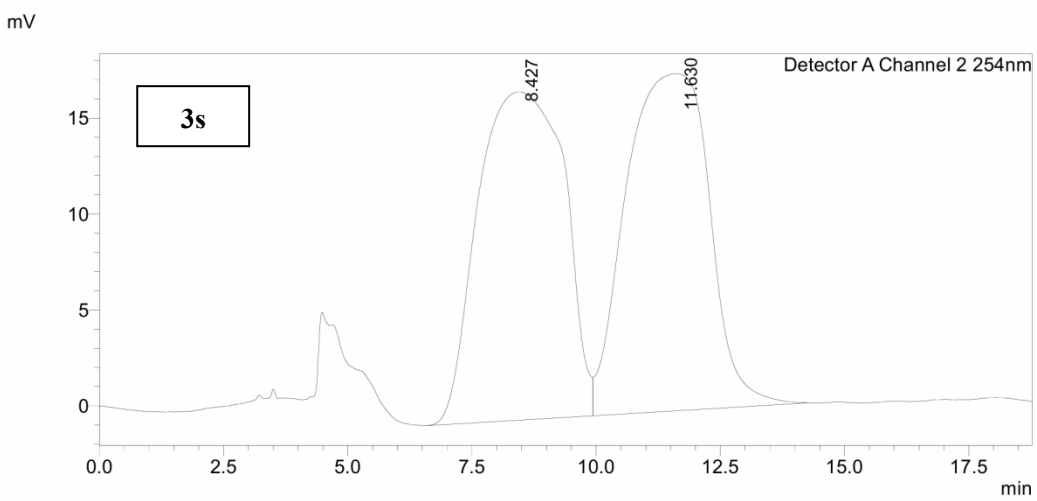
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	22.379	3374060	152854	49.560
2	23.090	3434029	250004	50.440
Total		6808090	402859	



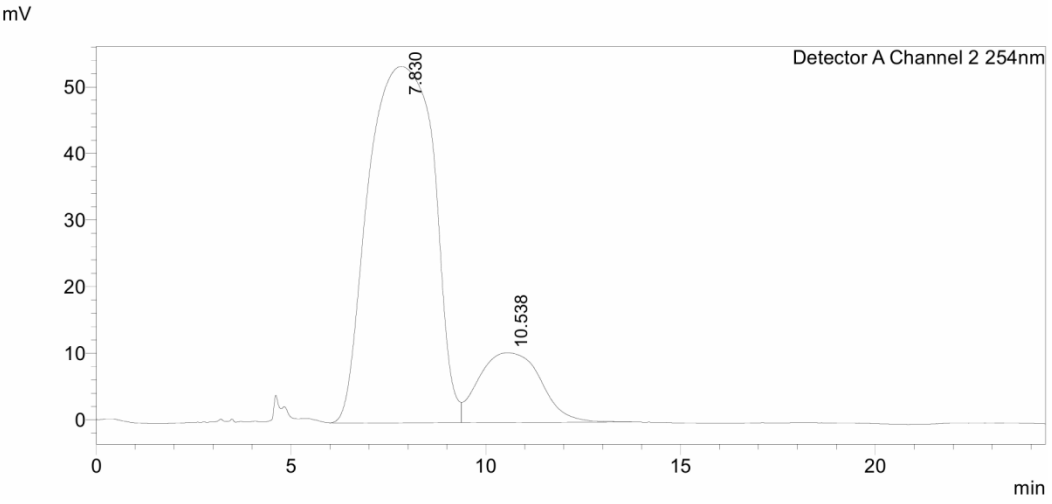
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	21.431	134391	6878	2.488
2	22.054	5267330	420544	97.512
Total		5401722	427421	



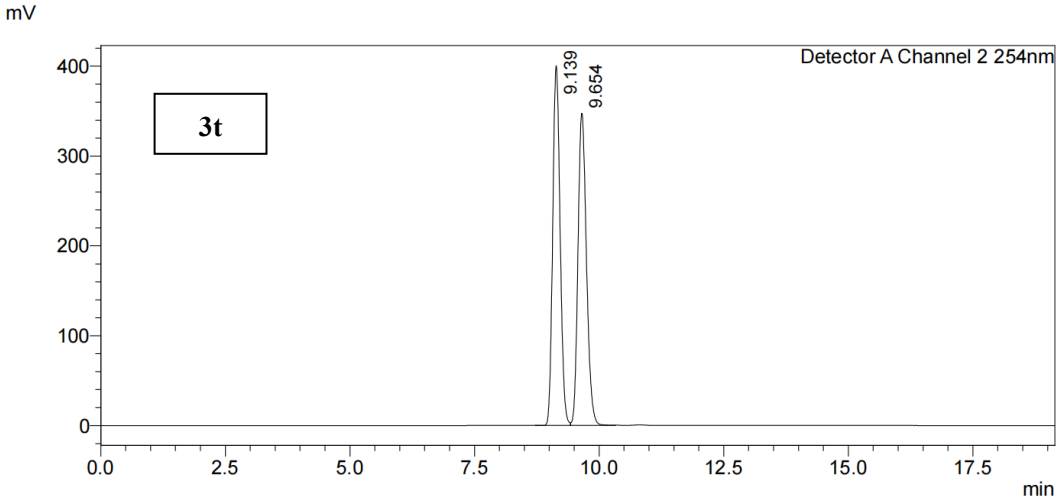
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	8.427	2075810	17121	50.114	
2	11.630	2066352	17584	49.886	
Total		4142163	34705		



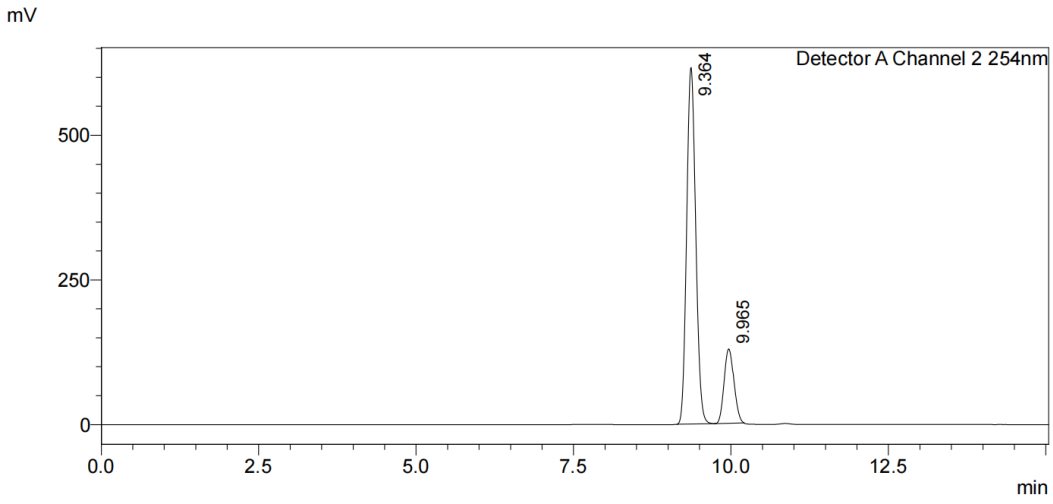
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	7.830	6280871	53548	84.430	
2	10.538	1158278	10471	15.570	
Total		7439149	64019		



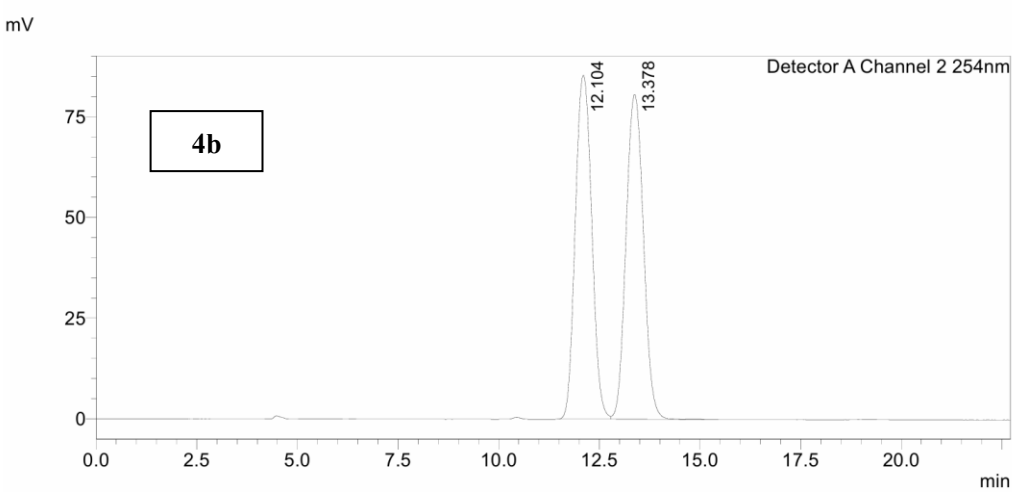
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.139	4144913	400513	50.131
2	9.654	4123223	347480	49.869
Total		8268136	747993	



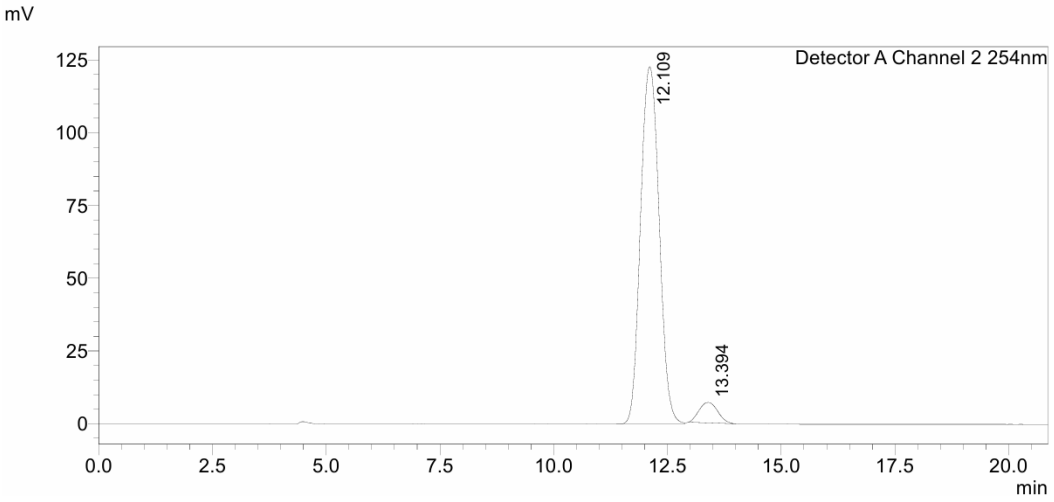
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.364	6197093	616106	81.790
2	9.965	1379741	128432	18.210
Total		7576834	744538	



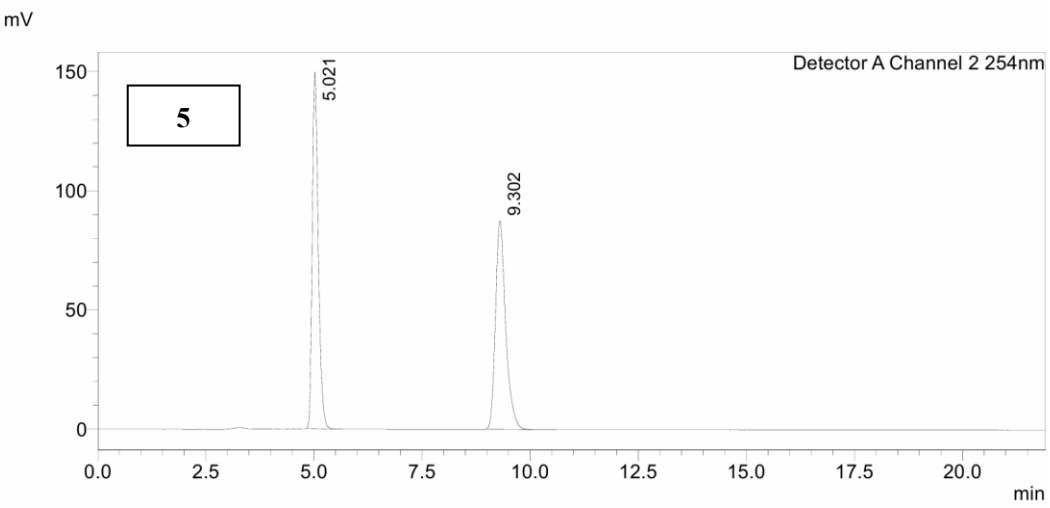
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	12.104	2430515	85389	49.991	
2	13.378	2431434	80664	50.009	
Total		4861949	166053		



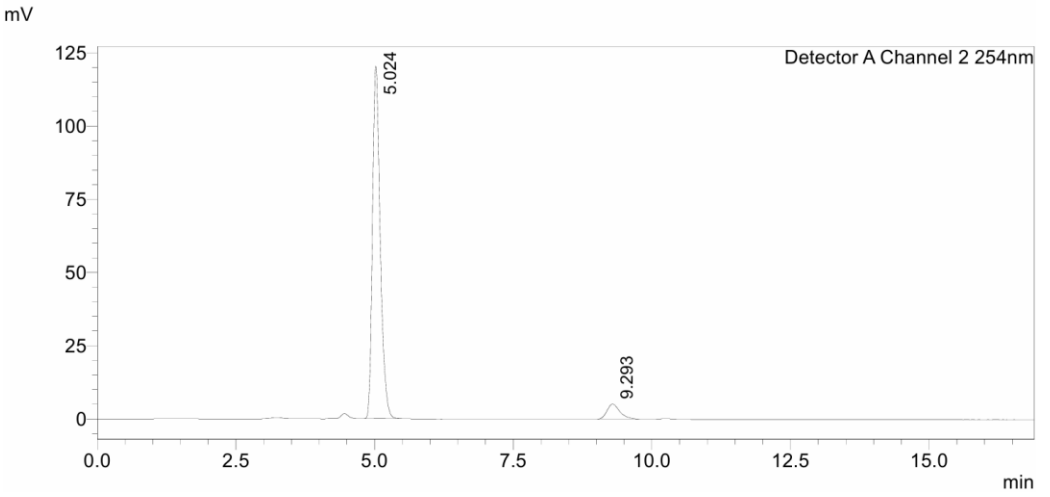
Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	12.109	3504073	122850	94.577	
2	13.394	200935	7043	5.423	
Total		3705008	129893		



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	5.021	1444887	149475	50.224	
2	9.302	1432002	87461	49.776	
Total		2876889	236936		



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	
1	5.024	1167197	120320	93.337	
2	9.293	83315	5164	6.663	
Total		1250513	125484		