Supporting Information

for

Asymmetric α-amination of β-keto esters using a guanidine–bisurea bifunctional organocatalyst

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Experimental procedures, copies of NMR spectra and HPLC chromatograms

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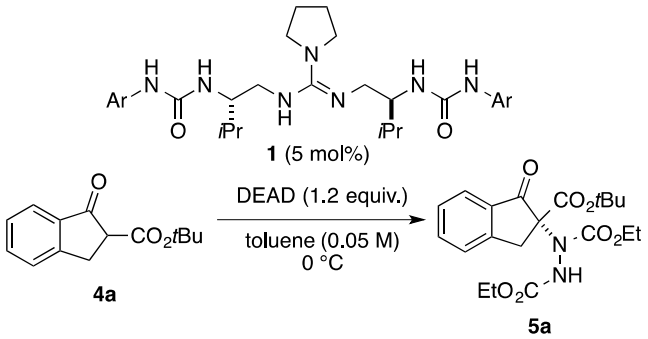
1. Instrumentation

Flash chromatography was performed using silica gel 60 (spherical, particle size 0.040–0.100 mm. Kanto Co., Inc., Tokyo, Japan). Optical rotations were measured on a JASCO P-2200 polarimeter (JASCO, Tokyo, Japan). ^{1}H and ^{13}C NMR spectra were recorded on JNM-AL300 and JNM-ECA500 instruments (JEOL, Tokyo, Japan). Chemical shifts in dimethylsulfoxide-d_6 were reported in the scale relative to residual dimethyl sulfoxide (2.50 ppm) for ^{1}H NMR. For ^{13}C NMR, chemical shift was reported in the scale relative to dimethylsulfoxide-d_6 (39.5 ppm) as an internal reference. Mass spectra were recorded on JEOL JMS-T100LC and JEOL JMA-HX110 spectrometer (JEOL, Tokyo, Japan). HPLC analysis on chiral stationary phase was performed on JASCO 800-series instruments (JASCO, Tokyo, Japan). Daicel Chiralpak AD-H and OD-H columns (Daicel, Osaka, Japan) with hexane/2-propanol and hexane/ethanol as the eluent were used.

2. Details of optimization of reaction conditions for α-amination

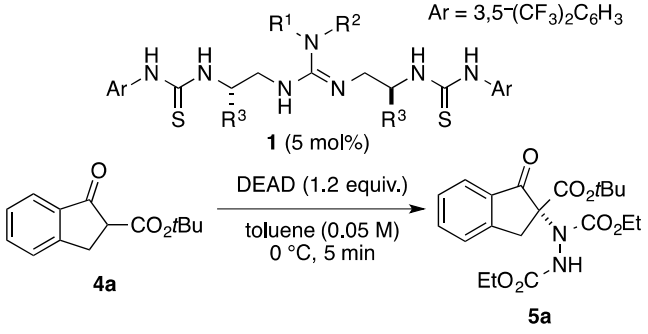
Table S1: Optimization for substituents of urea moiety.[a]



entry	catalyst **1**		time (min)	α-amination product **5a**	
		Ar		yield (%)[b]	ee (%)[c]
1	**1g**	3,5–$(CF_3)_2C_6H_3$	5	99	80
2	**1h**	4–$CF_3C_6H_4$	30	93	74
3	**1i**	3–$CF_3C_6H_4$	60	99	49
4	**1j**	2–$CF_3C_6H_4$	5	96	–24
5	**1k**	3,5–$(F)_2C_6H_3$	5	99	67
6	**1l**	3,5–$(MeO)_2C_6H_3$	60	91	42

[a]Reaction condition: **4a** (0.1 mmol), DEAD (0.12 mmol) and **1** (5 mol %) in toluene at 0 °C. [b]Isolated yield. [c]Determined by HPLC analysis using a chiral stationary phase.

Table S2: Optimization of catalyst structure for guanidine–bisthiourea bifunctional organocatalyst.[a]

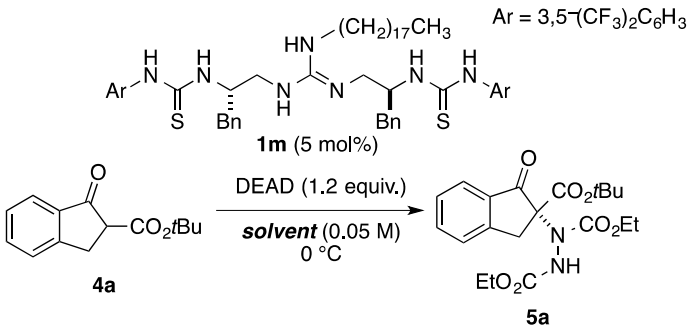


entry	catalyst **1**			α-amination product **5a**	
		R^1, R^2	R^3	yield (%)[b]	ee (%)[c]
1	**1m**	H, $–(CH_2)_{17}CH_3$	Bn	98	71

2	**1n**	H, $-(CH_2)_{17}CH_3$	Ph	96	64
3	**1o**	H, $-(CH_2)_{17}CH_3$	Me	96	65
4	**1p**	H, $-(CH_2)_{17}CH_3$	*i*Pr	99	60
5	**1q**	$-(CH_2)_5-$	Bn	99	14
6	**1r**	$-(CH_2)_4-$	Bn	99	–42

[a]Reaction condition: **4a** (0.1 mmol), DEAD (0.12 mmol) and **1** (5 mol%) in toluene at 0 °C. [b]Isolated yield. [c]Determined by HPLC analysis using a chiral stationary phase.

Table S3: Investigation of solvent effect.[a]

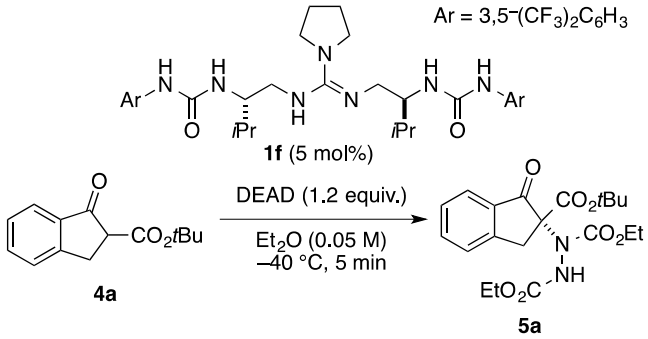


entry	solvent	time (min)	α-amination product **5a**	
			yield (%)[b]	ee (%)[c]
1	toluene	5	98	71
2	EtOAc	5	99	37
3	DCM	5	99	26
4	MeCN	30	99	7
5	Et_2O	5	99	64

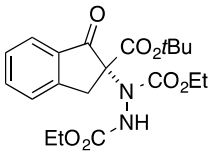
[a]Reaction condition: **4a** (0.1 mmol), DEAD (0.12 mmol) and **1m** (5 mol%) in toluene at 0 °C. [b]Isolated yield. [c]Determined by HPLC analysis using a chiral stationary phase.

3. General procedure for α-amination

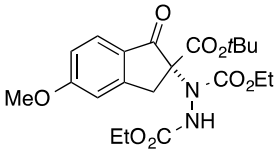
*Asymmetric α-amination of **4a** in the presence of **1f***



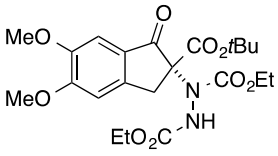
To a solution of β-keto ester **4a** (23.2 mg, 0.100 mmol) and guanidine–bisurea bifunctional organocatalyst **1f** (1.0 mg, 0.005 mmol) in diethyl ether (2 mL) was added dropwise diethyl azodicarboxylate (2.2 M in toluene, 55 μL, 0.120 mmol) at –40 °C. After being stirred for 5 min, the reaction mixture was quenched with saturated NH_4Cl solution. The organic phase was separated. Then, the aqueous phase was extracted with ethyl acetate three times. The combined organic solution was dried over $MgSO_4$, and concentrated in vacuo. The residue was purified by column chromatography on SiO_2 (ethyl acetate/hexane 1:10 to 1:1) to give α-amination product **5a** (40.5 mg, 99%) as a colorless amorphous. Enantiomeric excess was determined by HPLC analysis.



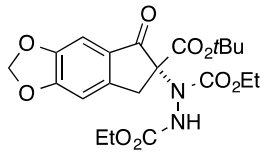
5a: $[\alpha]^{25}_D$ = −72.4 (*c* 3.95, $CHCl_3$, 90% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 95:5, flow rate = 1.0 mL/min, τ_1 (minor) = 11.1, τ_2 (major) = 15.5.



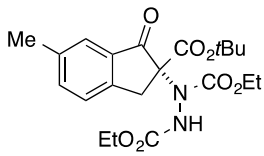
5b: $[\alpha]^{25}_D$ = −90.9 (*c* 3.60, $CHCl_3$, 80% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (minor) = 21.7, τ_2 (major) = 28.5.



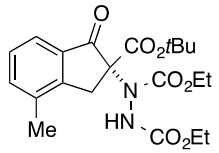
5c: $[\alpha]^{25}_D$ = −51.5 (*c* 3.98, $CHCl_3$, 77% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (minor) = 27.3, τ_2 (major) = 37.8.



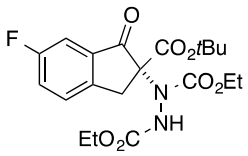
5d: $[\alpha]^{25}_{D}$ = −112.3 (*c* 3.45, $CHCl_3$, 80% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (minor) = 13.2, τ_2 (major) = 18.4; ^{1}H NMR (300 MHz, DMSO-*d6*, 100 °C) δ 7.03 (s, 1H), 7.01 (s, 1H), 6.13 (s, 2H), 4.17-3.91 (m, 4H), 3.86 (d, *J* = 17.2 Hz, 1H), 3.5 (d, *J* = 17.2 Hz, 1H), 1.36 (s, 9H), 1.18 (t, *J* = 6.9 Hz, 3H), 1.09 (br, 3H), 7.51 (d, *J* = 7.3 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-*d6*, 100 °C) δ 191.02, 155.61, 154.62, 154.32, 147.81, 127.31, 104.88, 102.08, 101.6, 81.57, 78.54, 61.54, 60.36, 26.86, 13.58; HRMS (ESI, M+Na) calcd for 473.1536, found 473.1556.



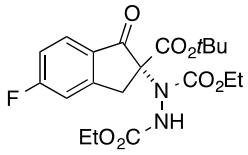
5e: $[\alpha]^{25}_{D}$ = −70.8 (*c* 4.74, $CHCl_3$, 94% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 98:2, flow rate = 1.0 mL/min, τ_1 (minor) = 30.8, τ_2 (major) = 35.5; ^{1}H NMR (500 MHz, DMSO-*d6*, 100 °C) δ 7.5 (d, *J* = 8.0 Hz, 1H), 7.46 (s, 1H), 7.46 (s, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 4.15-3.86 (m, 5H), 3.57 (d, *J* = 16.0 Hz, 1H), 2.36 (s, 3H), 1.35 (s, 9H), 1.21-0.99 (m, 6H); ^{13}C NMR (125 MHz, DMSO-*d6*, 100 °C) δ 193.19, 155.60, 154.59, 136.82, 136.20, 133.26, 125.40, 123.39, 81.69, 78.56, 61.56, 60.34, 26.83, 19.84, 13.55; HRMS (ESI, M+Na) calcd for 443.1794, found 443.1759.



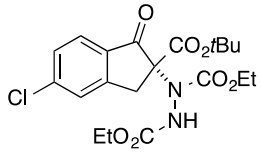
5f: $[\alpha]^{25}_{D}$ = −98.5 (*c* 4.16, $CHCl_3$, 86% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 98:2, flow rate = 1.0 mL/min, τ_1 (minor) = 19.1, τ_2 (major) = 21.6; ^{1}H NMR (300 MHz, DMSO-*d6*, 100 °C) δ 7.51 (d, *J* = 7.3 Hz, 1H), 7.5 (d, *J* = 7.3 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 1H), 4.15-3.83 (m, 5H), 3.5 (d, *J* = 17.3 Hz, 1H), 2.34 (s, 9H), 1.18 (t, *J* = 6.9 Hz, 3H), 1.07 (br, 3H); ^{13}C NMR (75 MHz, DMSO-*d6*, 100 °C) δ 193.44, 155.59, 154.61, 135.34, 134.67, 132.89, 127.23, 121, 91.74, 78.54, 61.59, 60.34, 59.89, 26.81, 16.51, 13.55; HRMS (ESI, M+Na) calcd for 443.1794, found 443.1809.



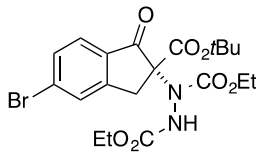
5g: $[\alpha]^{25}_{D}$ = −44.2 (*c* 3.29, $CHCl_3$, 73% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 95:5, flow rate = 1.0 mL/min, τ_1 (minor) = 9.8, τ_2 (major) = 12.2; ^{1}H NMR (500 MHz, DMSO-*d6*, 100 °C) δ7.62 (dd, *J* = 8.02, 4.58 Hz, 1H), 7.51 (td, *J* = 8.59, 2.29 Hz, 1H), 7.51 (td, *J* = 8.59, 2.29 Hz, 1H), 7.39 (dd, *J* = 7.45, 2.29 Hz, 1H), 4.15-3.89 (m, 5H), 3.59 (d, *J* = 16 Hz, 1H), 1.35 (s, 9H), 1.19-1.03 (m, 6H); ^{13}C NMR (125 MHz, DMSO-*d6*, 100 °C) δ192.54, 161.38 (d, *J* = 245.7 Hz, H), 155.66, 154.55, 134.7 (d, *J* = 7.3 Hz, H), 127.76 (d, *J* = 7.3 Hz, H), 122.59 (d, *J* = 23.2 Hz, H), 109.1 (d, *J* = 22.0 Hz, H), 82.11, 61.73, 60.45, 26.79, 13.59, 13.53; HRMS (ESI, M+Na) calcd for 447.1543, found 447.1520.



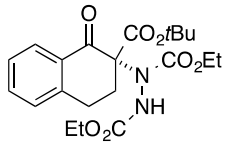
5h: $[\alpha]^{25}_{D}$ = −77.1 (*c* 4.34, $CHCl_3$, 86% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (major) = 12.5, τ_2 (minor) = 14.4 ^{1}H NMR (500 MHz, DMSO-*d6*, 100 °C) δ7.74 (dd, *J* = 8.26, 5.16 Hz, 1H), 7.39 (d, *J* = 8.59 Hz, 1H), 7.39 (d, *J* = 8.59 Hz, 1H), 7.23 (t, *J* = 8.59 Hz, 1H), 4.16-3.90 (m, 5H), 3.65 (d, *J* = 17.5 Hz, 1H), 1.36 (s, 9H), 1.17 (br, 3H), 1.09 (br, 3H); ^{13}C NMR (125 MHz, DMSO-*d6*, 100 °C) δ191.53, 166.52 (d, *J* = 255.5 Hz, H), 155.65, 154.58, 126.69 (d, *J* = 11 Hz, H), 115.37 (d, *J* = 24.4 Hz, H), 112.42 (d, *J* = 22 Hz, H), 81.98, 78.56, 61.69, 60.43, 26.8, 13.54; HRMS (ESI, M+Na) calcd for 447.1543, found 447.1586.



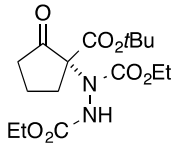
5i: $[\alpha]^{25}_{D}$ = −102.4 (*c* 4.28, $CHCl_3$, 80% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/ethanol = 99:1, flow rate = 1.0 mL/min, τ_1 (minor) = 24.5, τ_2 (major) = 27.2.



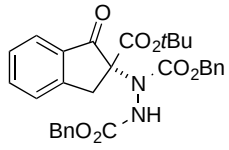
5j: $[\alpha]^{25}_{D}$ = −34.8 (*c* 4.32, $CHCl_3$, 80% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (major) = 10.8, τ_2 (minor) = 13.0; ^{1}H NMR (500 MHz, DMSO-*d6*, 100 °C) δ 7.83 (d, *J* = 9.7 Hz, 1H), 7.62-7.57 (m, 2H), 7.62-7.57 (m, 2H), 4.17-3.86 (m, 5H), 3.65 (br, 1H), 1.36 (s, 9H), 1.22-0.99 (m, 6H); ^{13}C NMR (125 MHz, DMSO-*d6*, 100 °C) δ 192.20, 155.62, 154.53, 132.10, 130.59, 129.50, 128.90, 125.24, 82.05, 61.72, 60.45, 26.80, 13.55; HRMS (ESI, M+Na) calcd for 507.0742, found 507.0786.



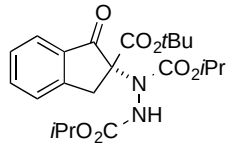
5k: $[\alpha]^{25}_{D}$ = +0.42 (*c* 3.27, $CHCl_3$, 61% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 90:10, flow rate = 1.0 mL/min, τ_1 (minor) = 7.3, τ_2 (major) = 11.1.



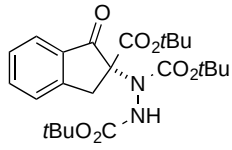
5l: $[\alpha]^{25}_{D}$ = +1.1 (*c* 2.14, $CHCl_3$, 38% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/2-propanol = 95:5, flow rate = 1.0 mL/min, τ_1 (minor) = 7.9, τ_2 (major) = 11.6.



6a: $[\alpha]^{25}_{D}$ = −52.3 (*c* 4.62, $CHCl_3$, 64% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 95:5, flow rate = 1.0 mL/min, τ_1 (minor) = 20.1, τ_2 (major) = 23.2.

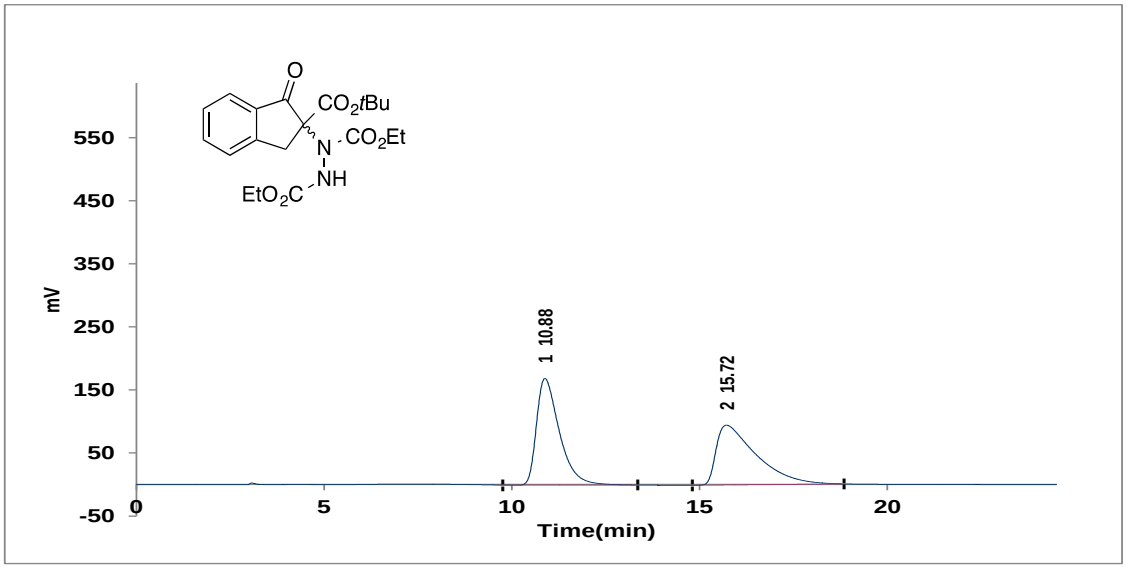


7a: $[\alpha]^{25}_{D}$ = −88.4 (*c* 4.17, $CHCl_3$, 79% ee); HPLC analysis: Daicel Chiralpak OD-H, hexane/2-propanol = 98:2, flow rate = 1.0 mL/min, τ_1 (minor) = 8.4, τ□ (major) = 9.4.



8a: $[\alpha]^{25}_{D}$ = −45.3 (*c* 2.05, $CHCl_3$, 44% ee); HPLC analysis: Daicel Chiralpak AD-H, hexane/ethanol = 95:5, flow rate = 1.0 mL/min, τ_1 (minor) = 8.7, τ_2 (major) = 13.7.

4. Chiral HPLC analysis



No.	Rt	Area	Area(%)	Height
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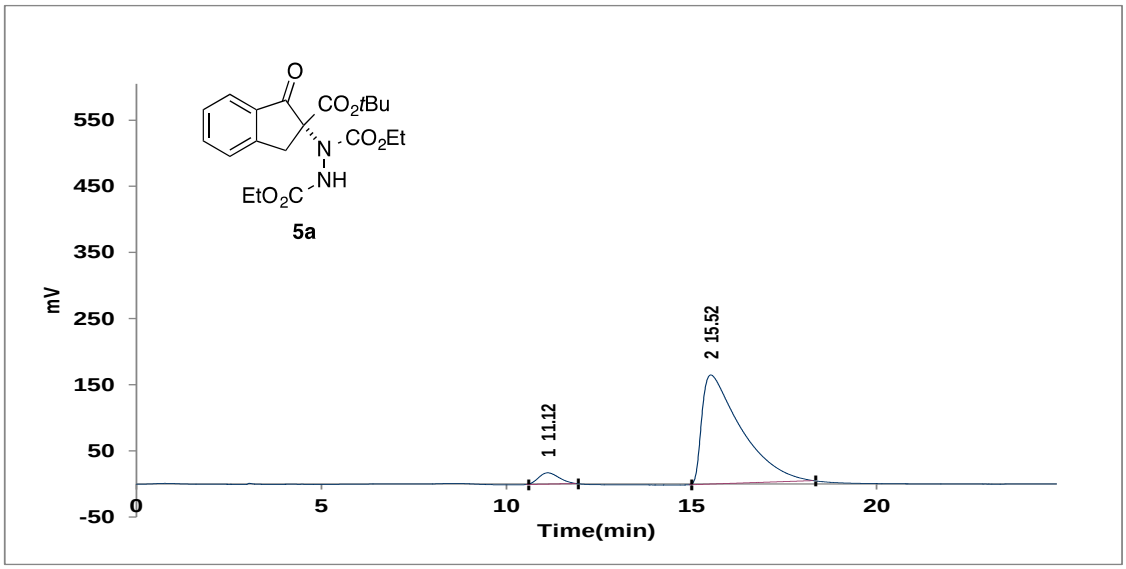
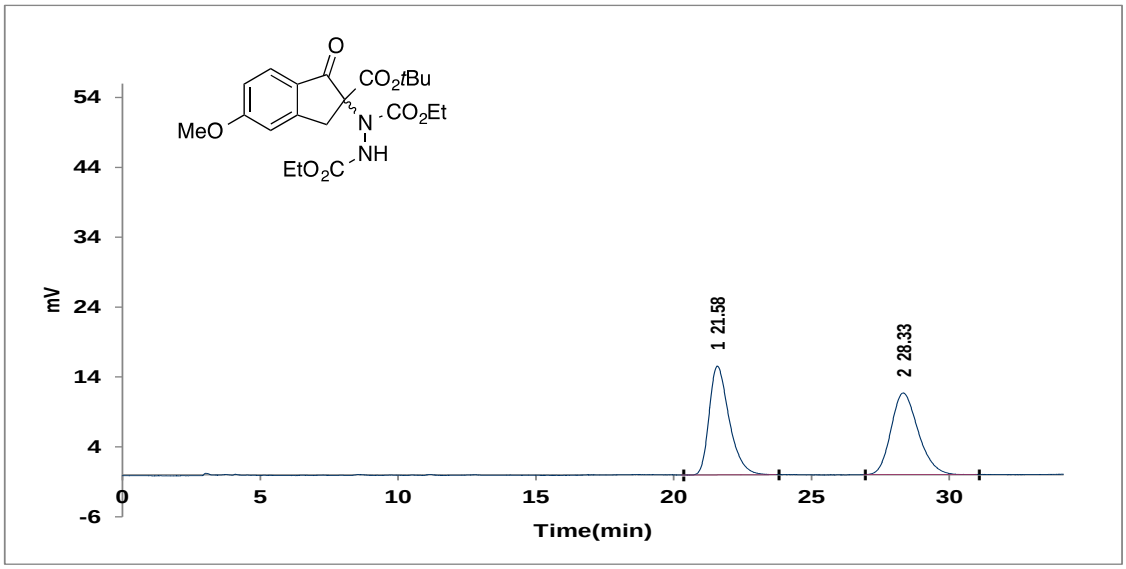
2	15.72	6999750	49.4544	94857
		14153942	100	264049



No.	Rt	Area	Area(%)	Height
1	11.12	649968.4	5.0856	17075
2	15.52	12130522	94.9144	164947
		12780490	100	182022



No.	Rt	Area	Area(%)	Height
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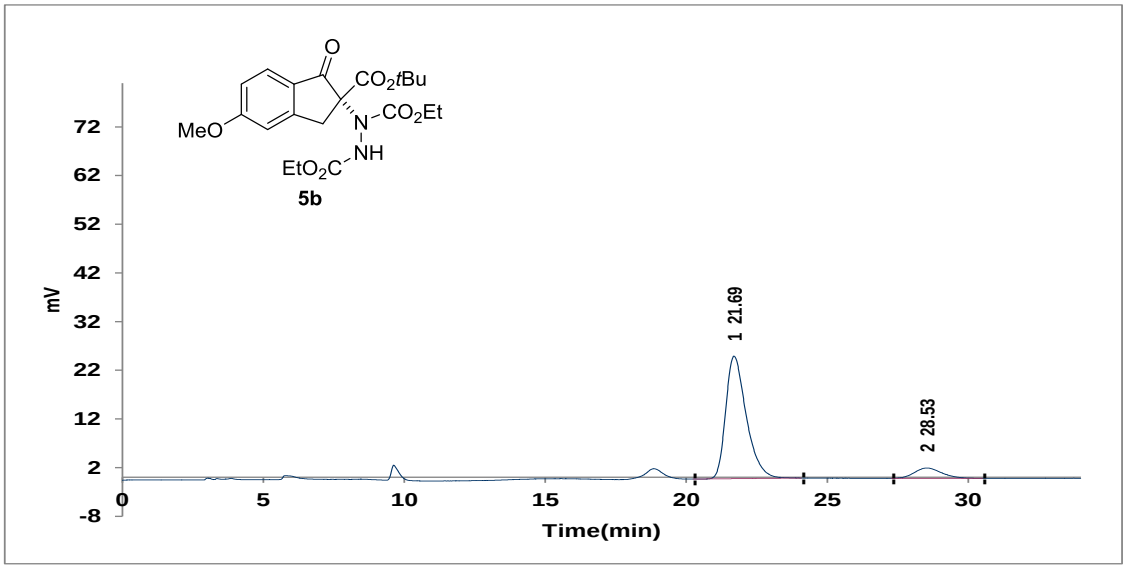
		1588611	100	27287



No.	Rt	Area	Area(%)	Height
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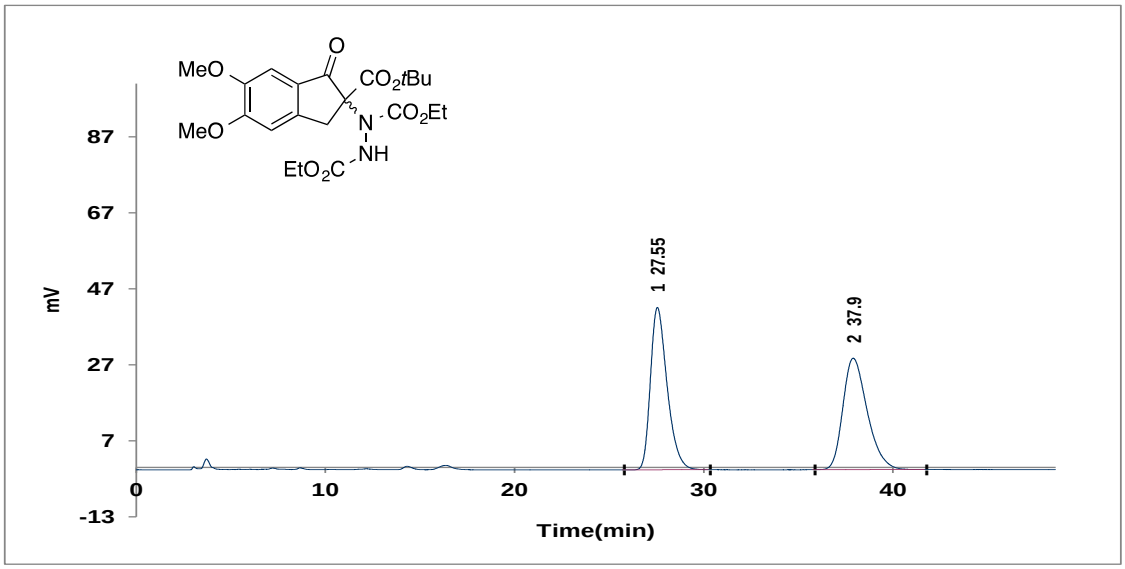
		1419675	100	27320



No.	Rt	Area	Area(%)	Height
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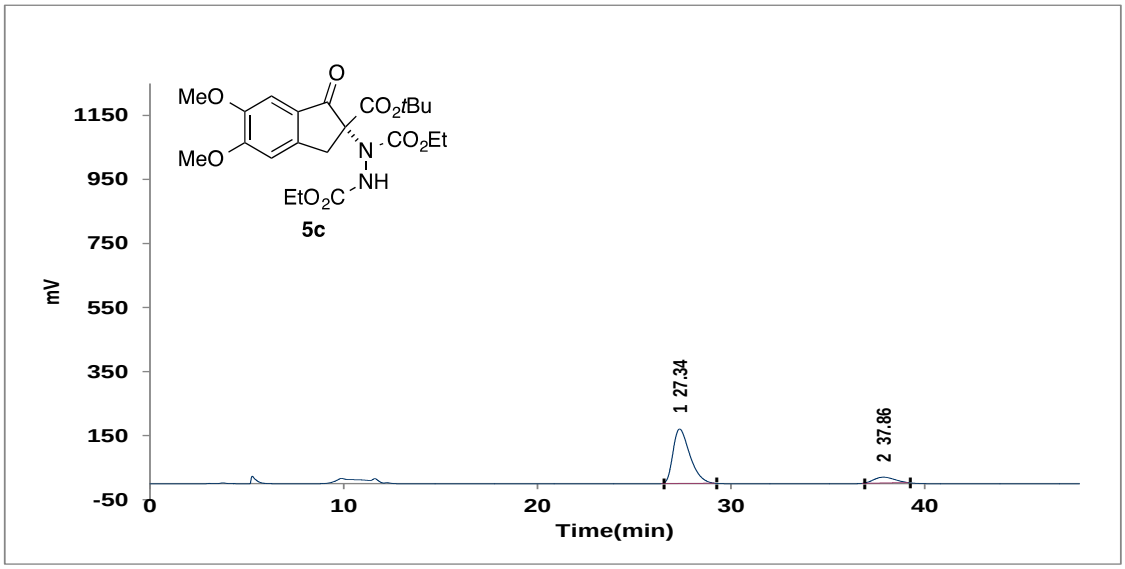
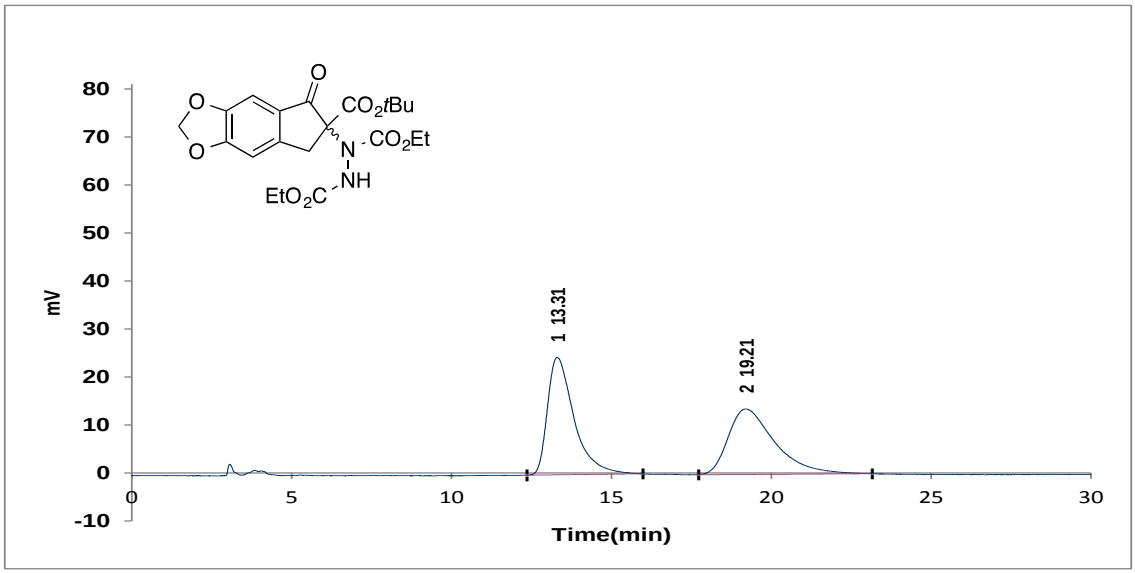
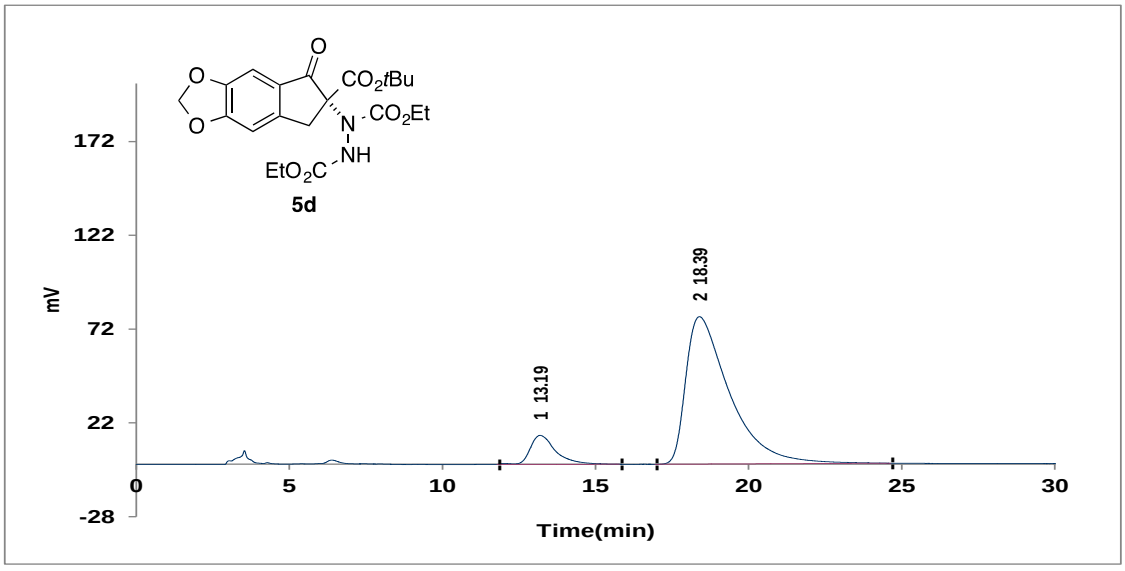
		5240465	100	72050



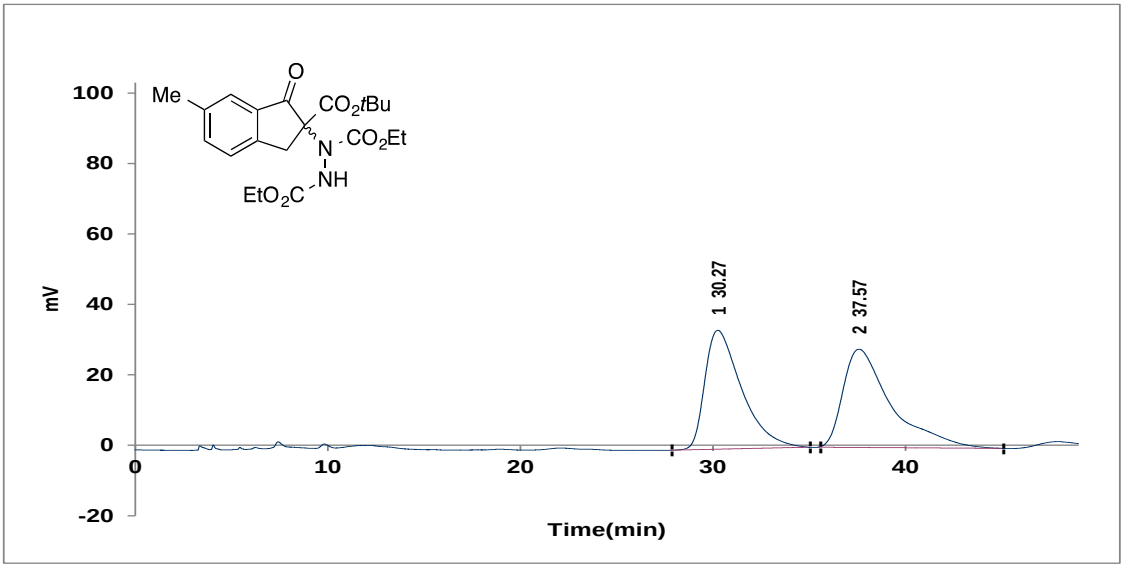
No.	Rt	Area	Area(%)	Height
1	27.34	10247155	88.5274	170219
2	37.86	1327962	11.4726	18196
		11575117	100	188415



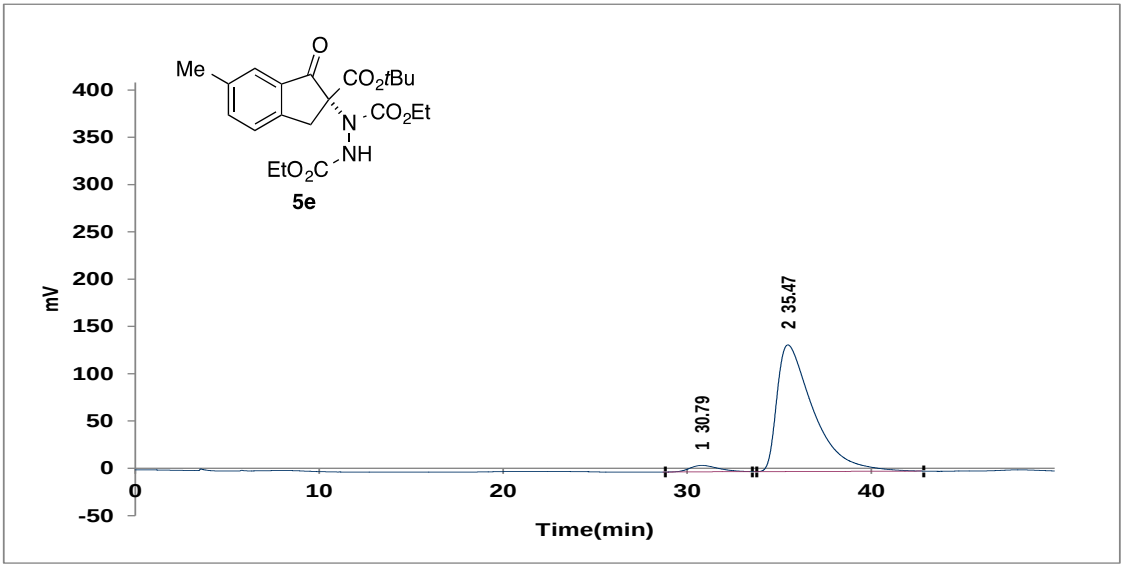
No.	Rt	Area	Area(%)	Height
1	13.31	1413088	50.6118	24469
2	19.21	1378923	49.3882	13653
		2792011	100	38122



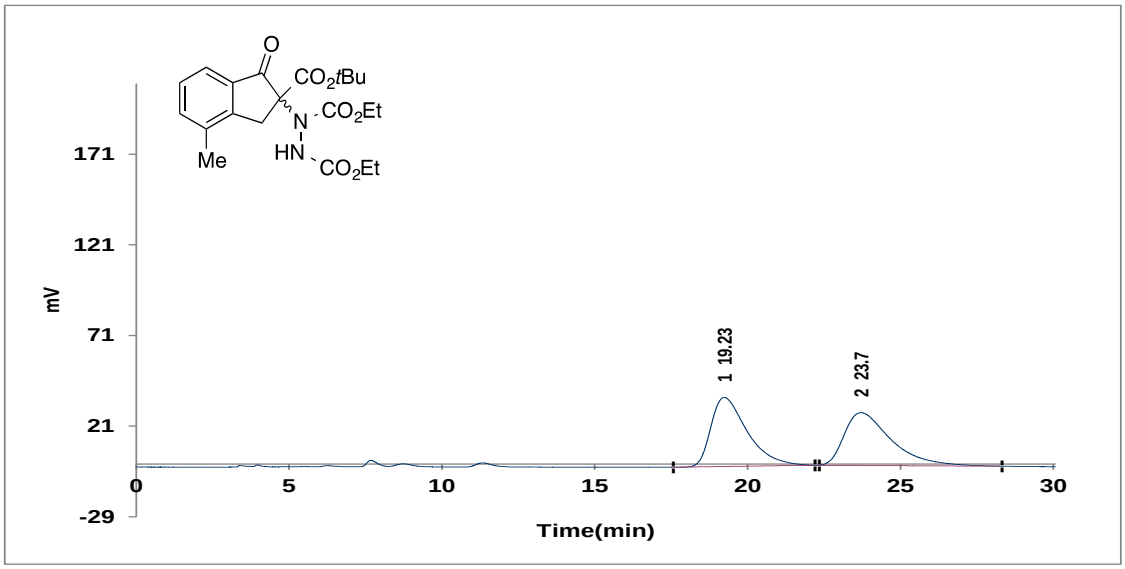
No.	Rt	Area	Area(%)	Height
1	13.19	889911.4	10.2251	15423
2	18.39	7813291	89.7749	78610
		8703203	100	94033



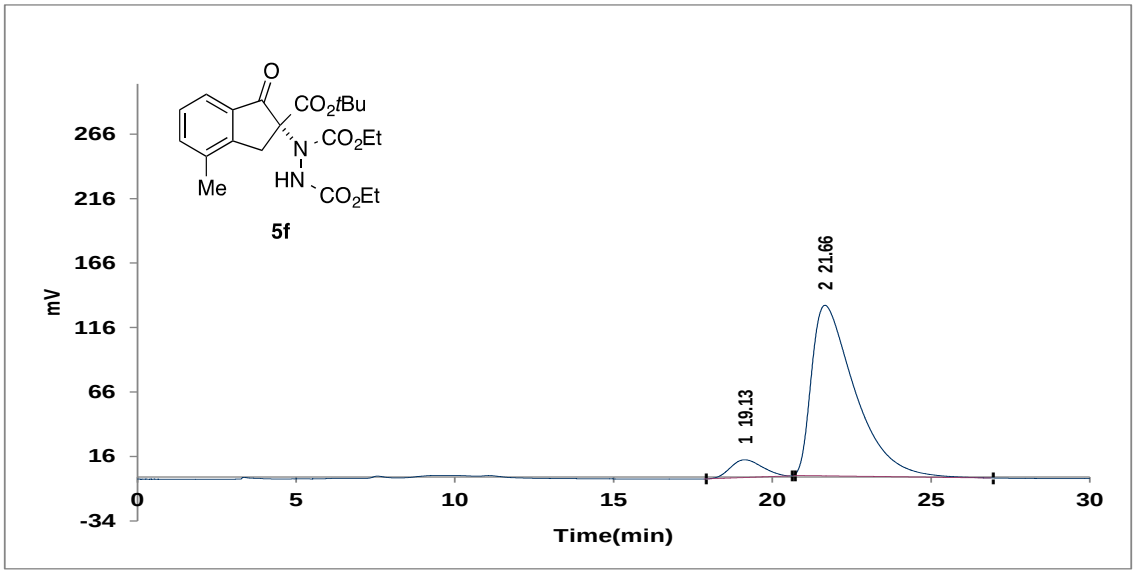
No.	Rt	Area	Area(%)	Height
1	30.27	4478031	48.0885	33749
2	37.57	4834029	51.9115	27904
		9312060	100	61653



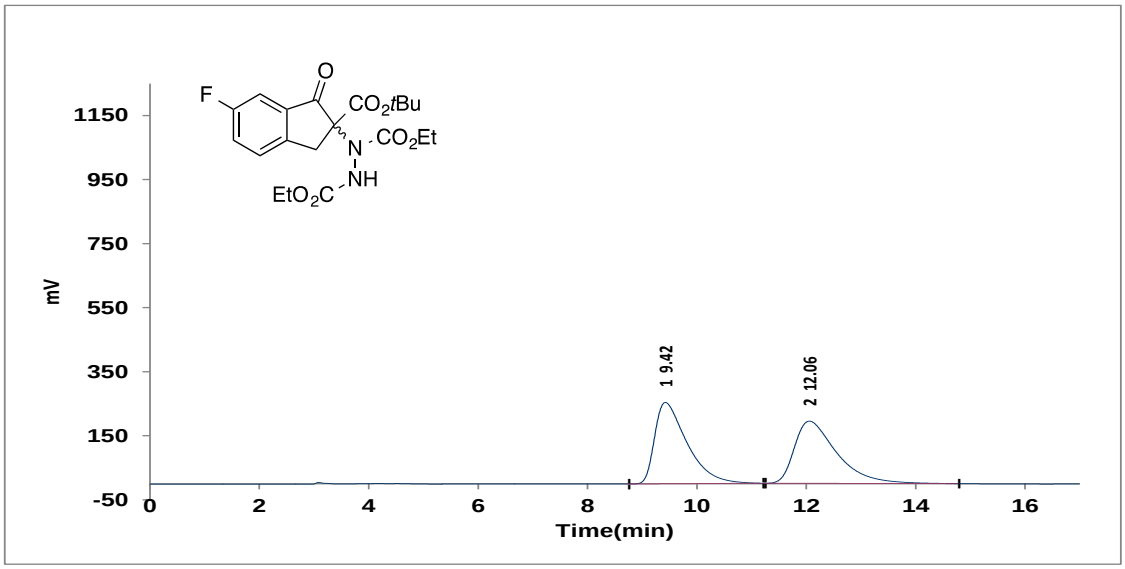
No.	Rt	Area	Area(%)	Height
1	30.79	725378.2	3.7986	6767
2	35.47	18370579	96.2014	133922
		19095957	100	140689



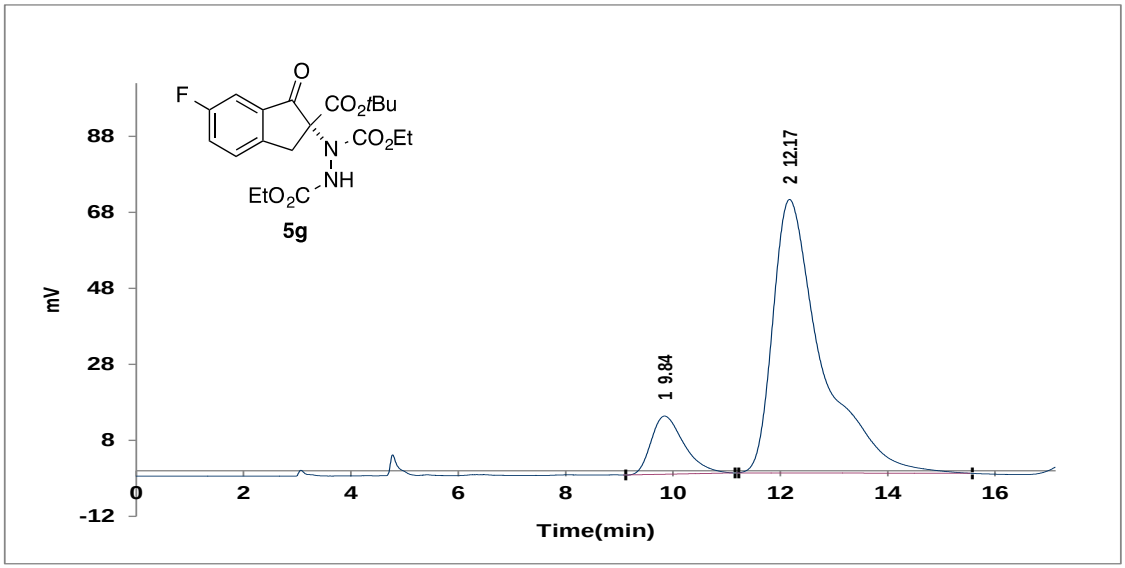
No.	Rt	Area	Area(%)	Height
1	19.23	3139235	50.2216	38152
2	23.7	3111526	49.7784	29153
		6250761	100	67305



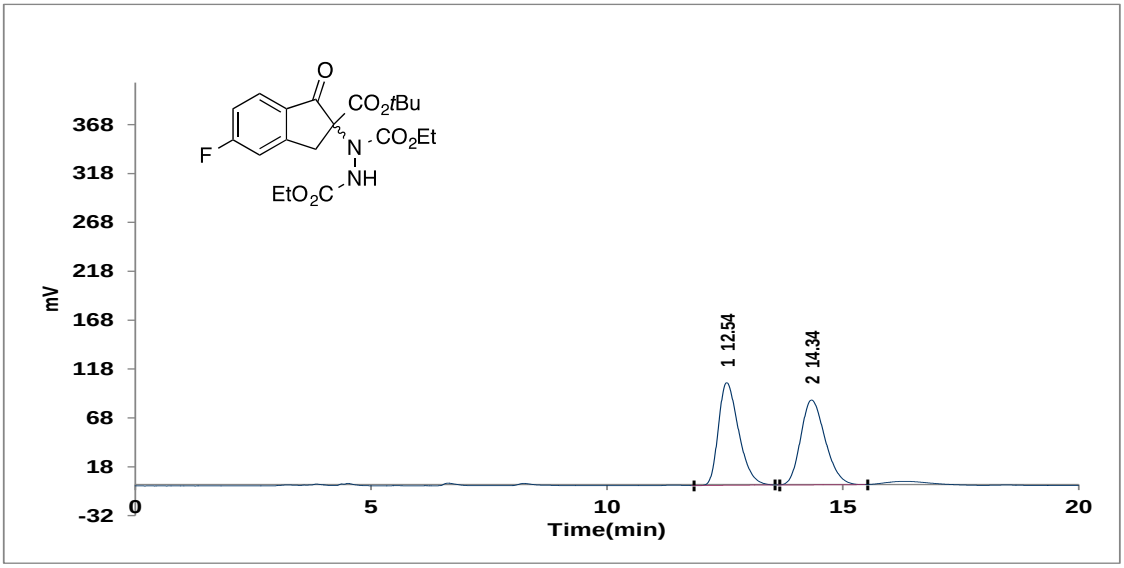
No.	Rt	Area	Area(%)	Height
1	19.13	955852.7	7.056	13747
2	21.66	12590880	92.944	132302
		13546733	100	146049



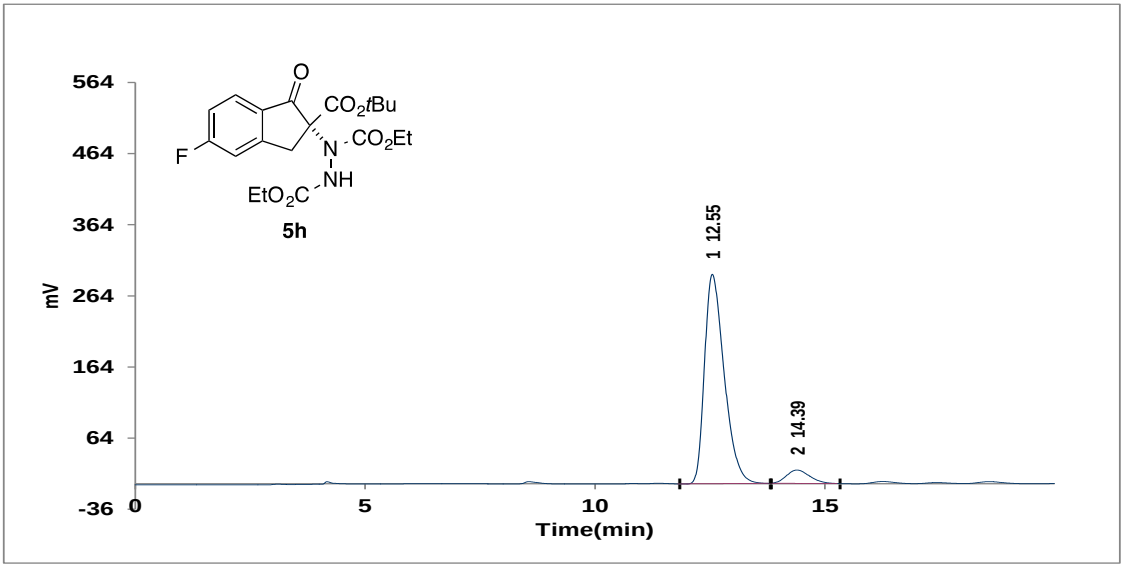
No.	Rt	Area	Area(%)	Height
1	9.84	650706.8	12.5099	15318
2	12.17	4550817	87.4901	71997
		5201524	100	87315



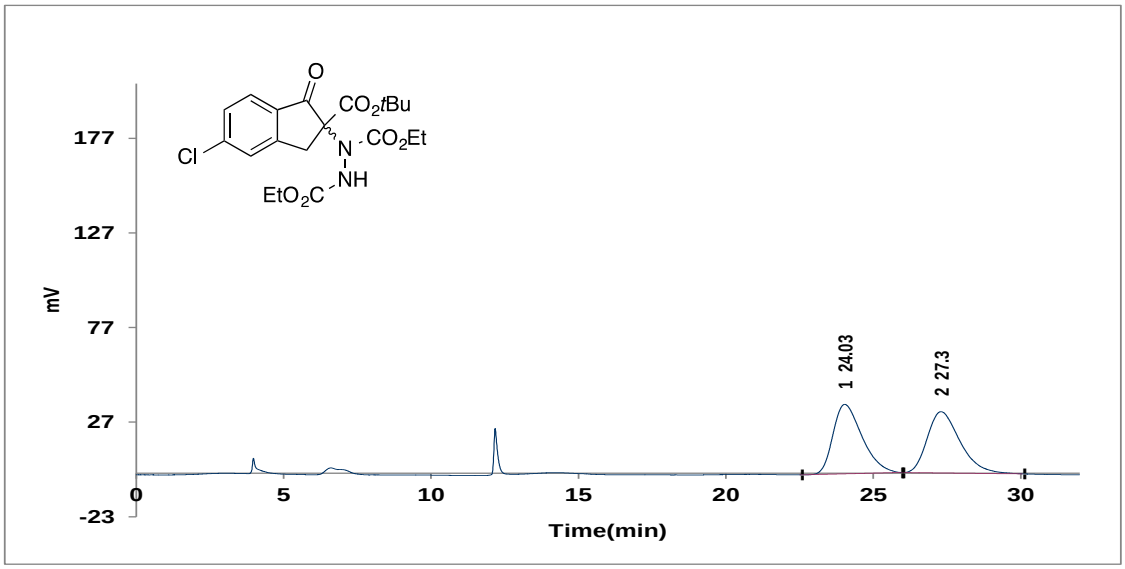
No.	Rt	Area	Area(%)	Height
1	9.42	10418790	49.969	254206
2	12.06	10431716	50.031	194350
		20850506	100	448556



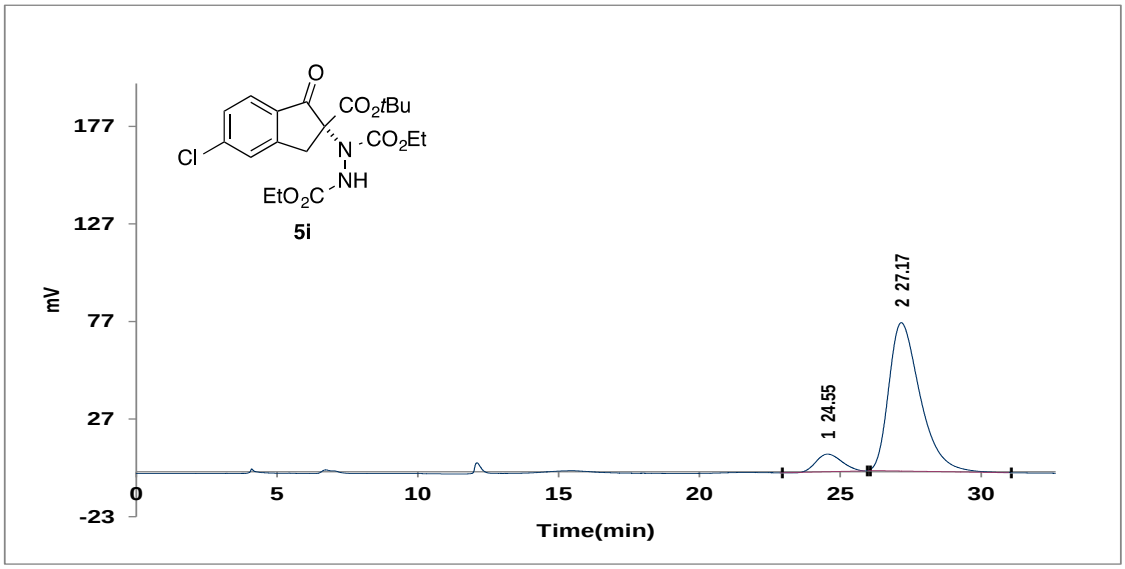
No.	Rt	Area	Area(%)	Height
1	12.54	3128289	50.0666	104900
2	14.34	3119969	49.9334	86807
		6248258	100	191707



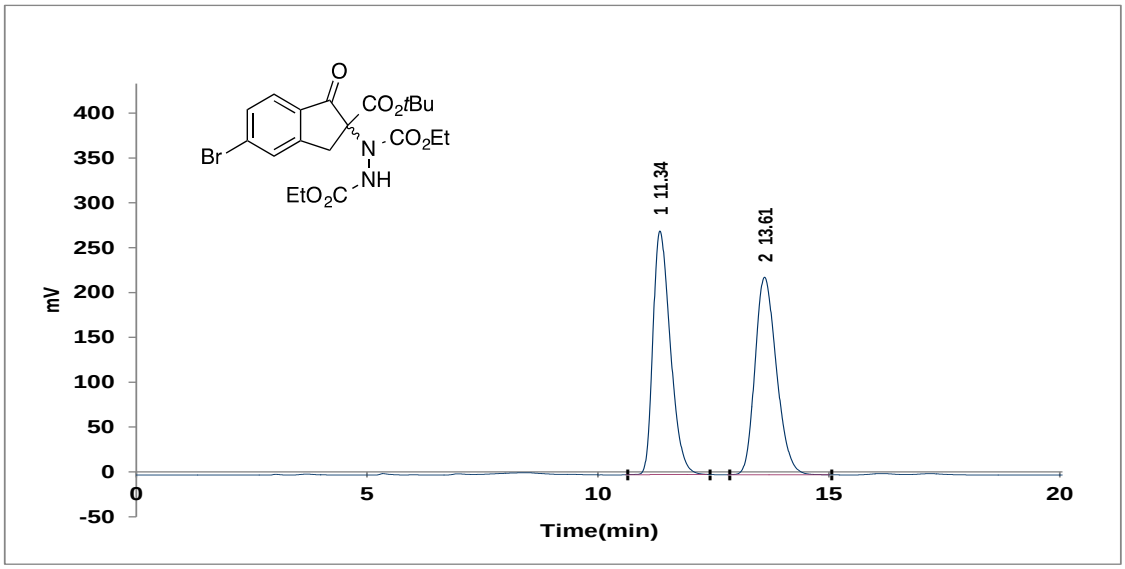
No.	Rt	Area	Area(%)	Height
1	12.55	8748736	92.9766	294359
2	14.39	660879.2	7.0234	18766
		9409615	100	313125



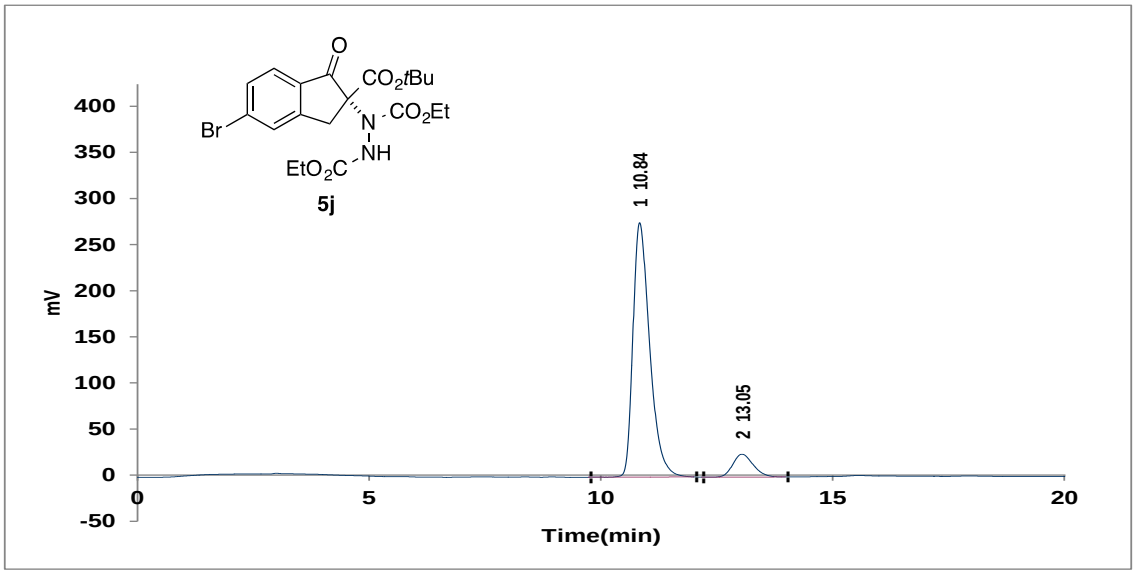
No.	Rt	Area	Area(%)	Height
1	24.03	2508261	50.0499	36714
2	27.3	2503260	49.9501	32395
		5011521	100	69109



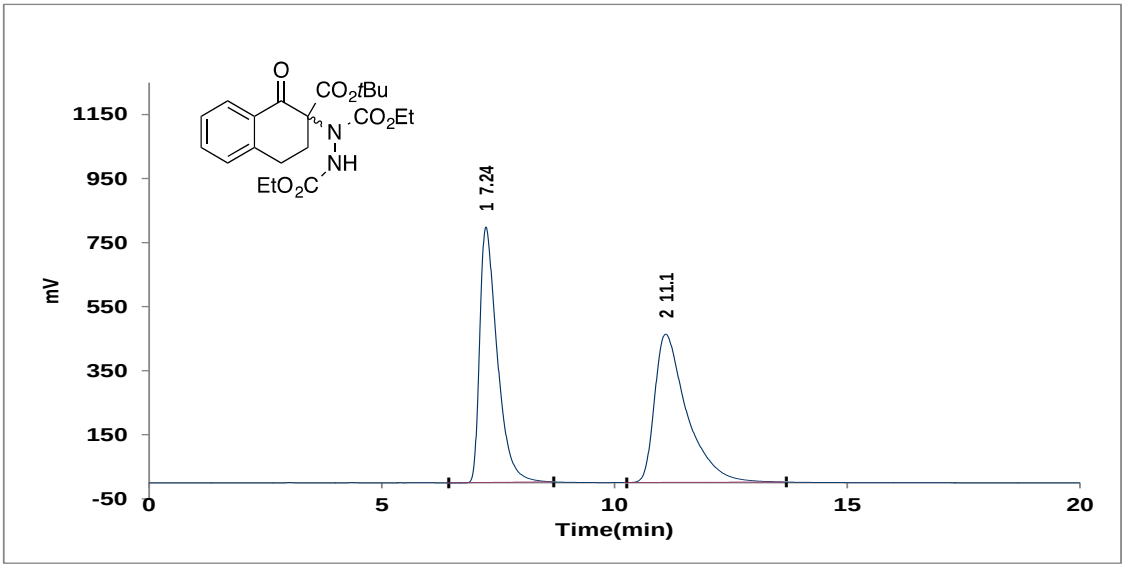
No.	Rt	Area	Area(%)	Height
1	24.55	566194.9	8.7922	9046
2	27.17	5873580	91.2078	76047
		6439775	100	85093



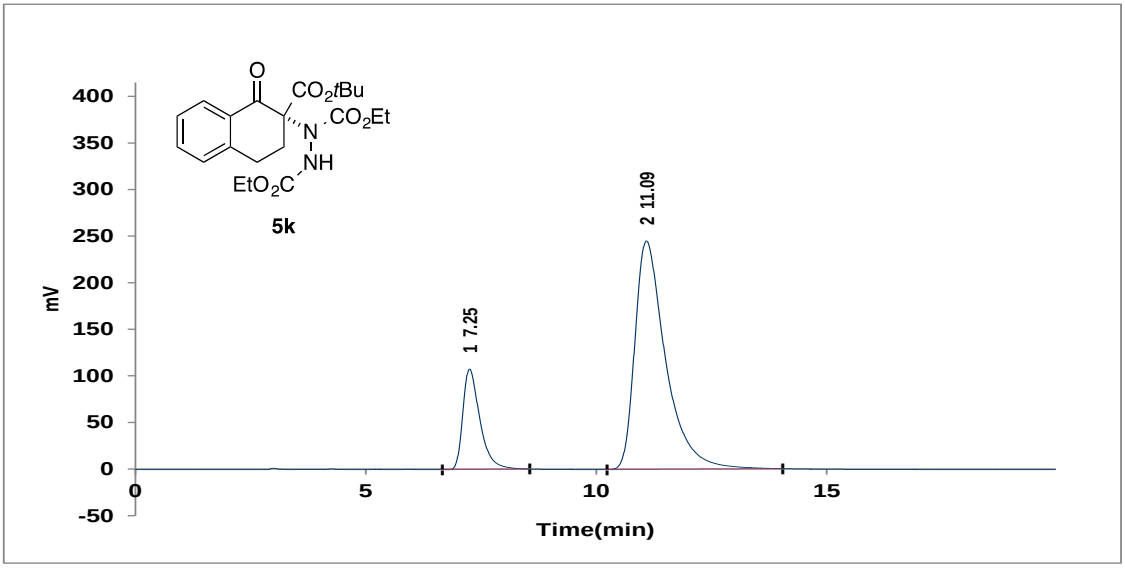
No.	Rt	Area	Area(%)	Height
1	11.34	7124806	50.0097	271745
2	13.61	7122039	49.9903	220337
		14246845	100	492082



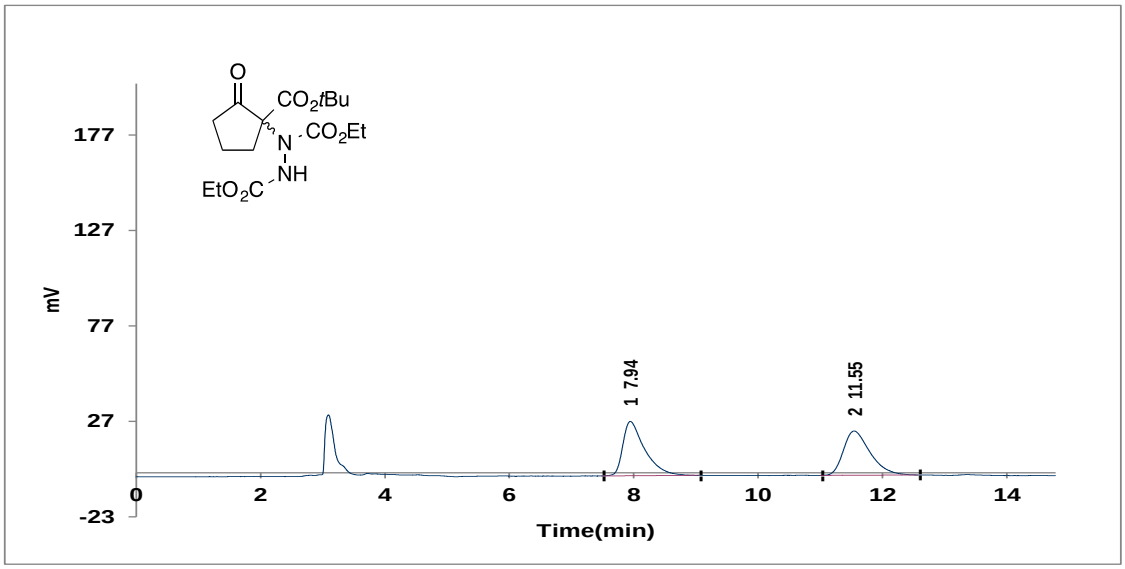
No.	Rt	Area	Area(%)	Height
1	10.84	6933706	90.1684	275952
2	13.05	756021.4	9.8316	24754
		7689728	100	300706



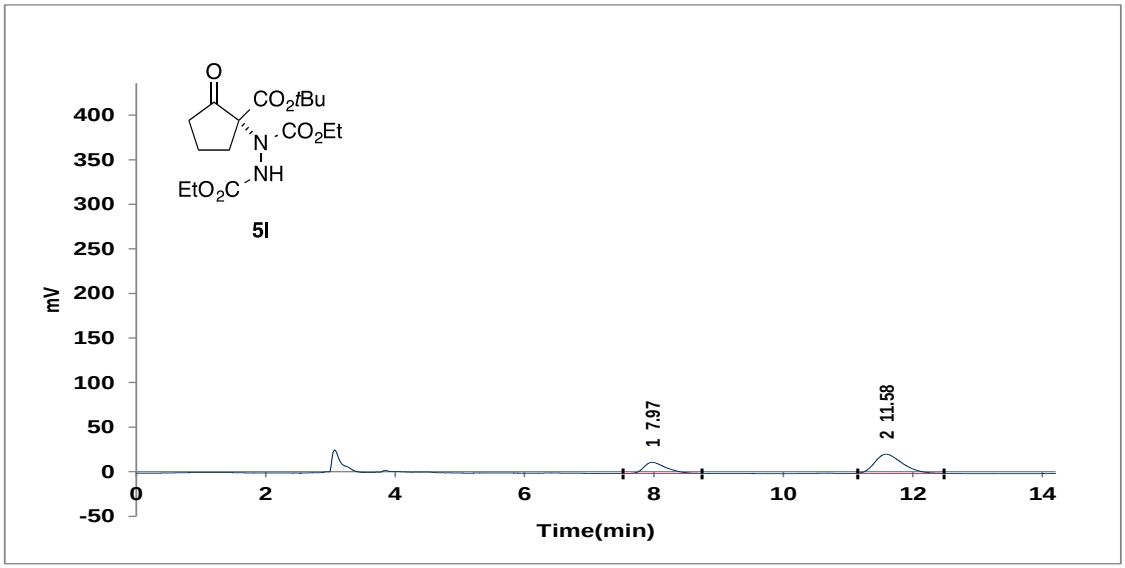
No.	Rt	Area	Area(%)	Height
1	7.24	20813954	48.347	798060
2	11.1	22237189	51.653	463385
		43051143	100	1261445



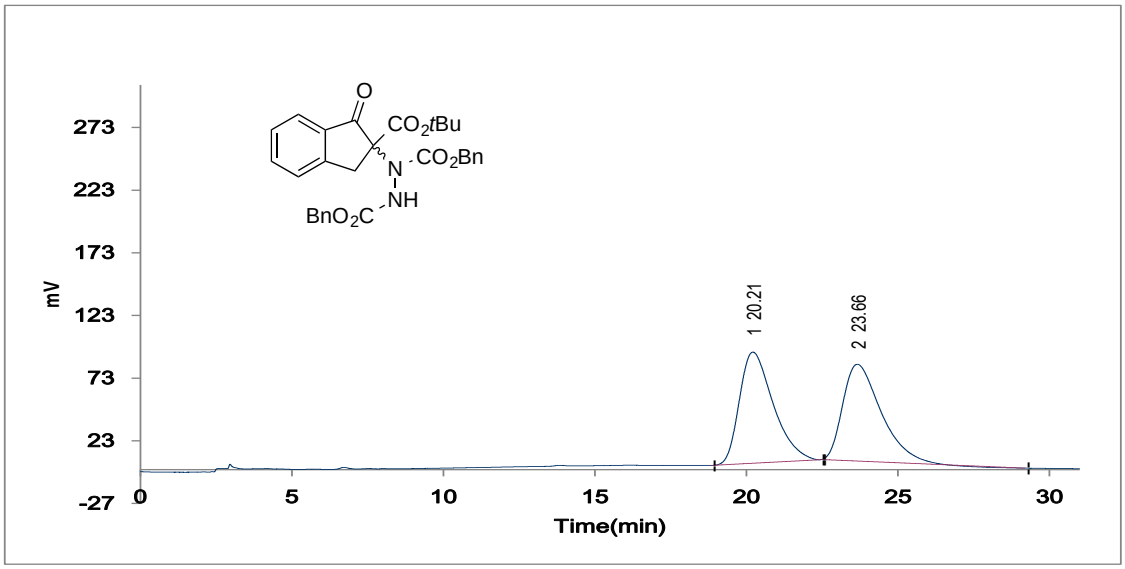
No.	Rt	Area	Area(%)	Height
1	7.25	2769507	19.5392	107824
2	11.09	11404599	80.4608	245252
		14174106	100	353076



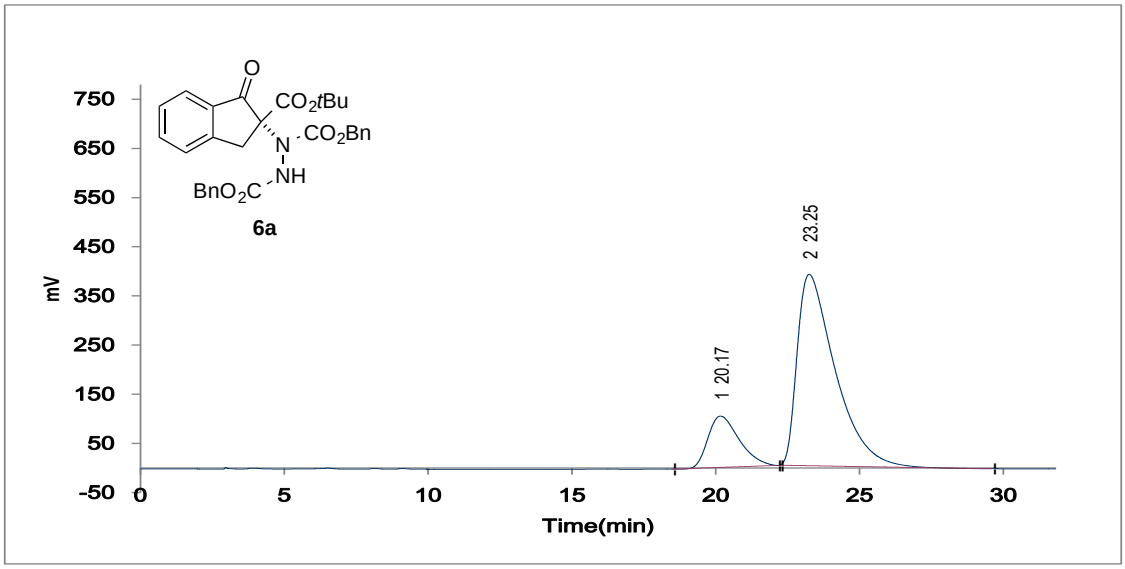
No.	Rt	Area	Area(%)	Height
1	7.94	694449.2	50.1708	28500
2	11.55	689720.6	49.8292	23174
		1384170	100	51674



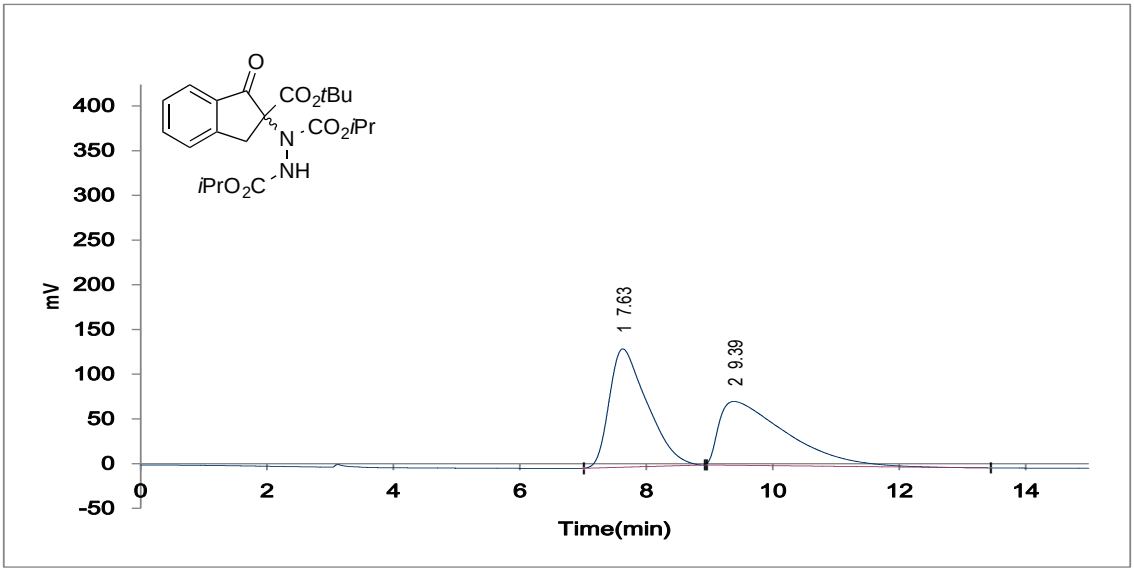
No.	Rt	Area	Area(%)	Height
1	7.97	295183.2	31.6648	12419
2	11.58	637029.3	68.3352	21472
		932212.5	100	33891



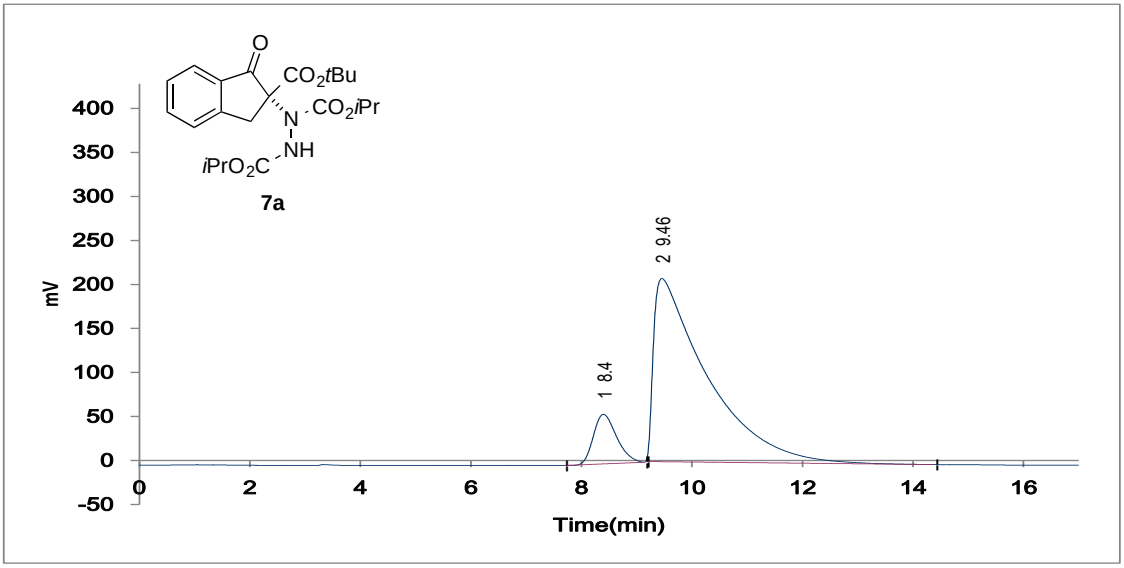
No.	Rt	Area	Area(%)	Height
1	20.21	6874927	50.3844	88722
2	23.66	6770026	49.6156	77207
		13644953	100	165929



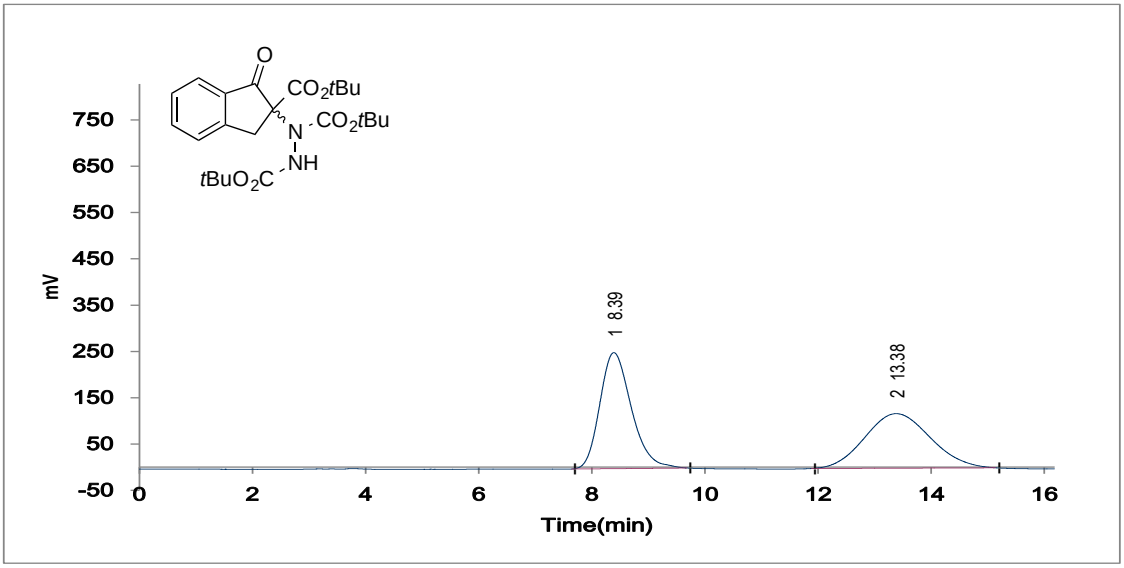
No.	Rt	Area	Area(%)	Height
1	20.17	7820545	17.9652	104472
2	23.25	35711101	82.0348	389152
		43531646	100	493624



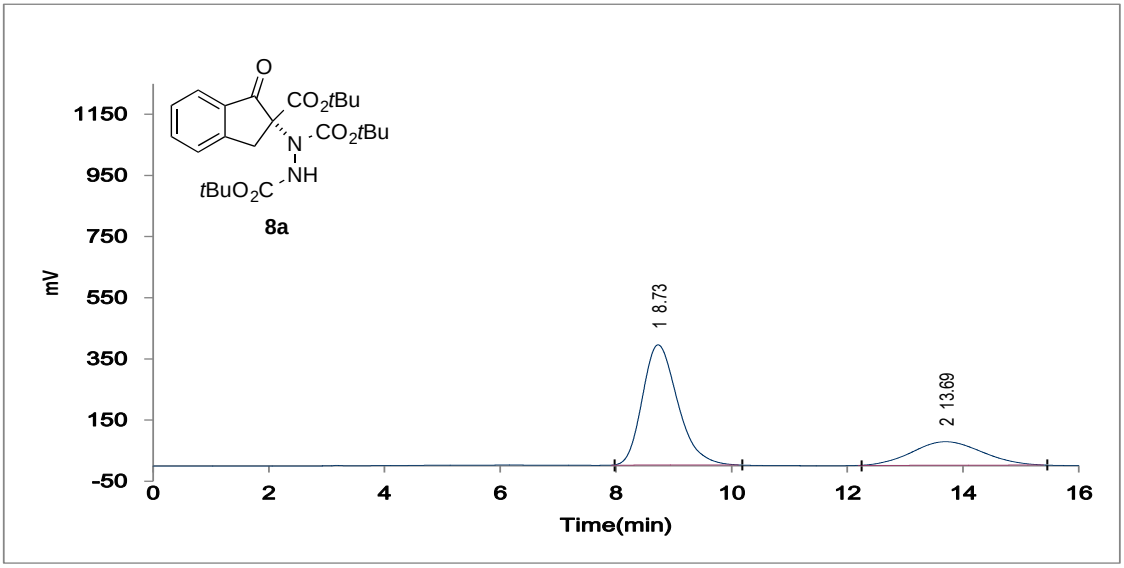
No.	Rt	Area	Area(%)	Height
1	7.63	5506573	51.0023	132396
2	9.39	5290147	48.9977	71312
		10796721	100	203708



No.	Rt	Area	Area(%)	Height
1	8.4	1640928	10.509	56356
2	9.46	13973642	89.491	208102
		15614570	100	264458

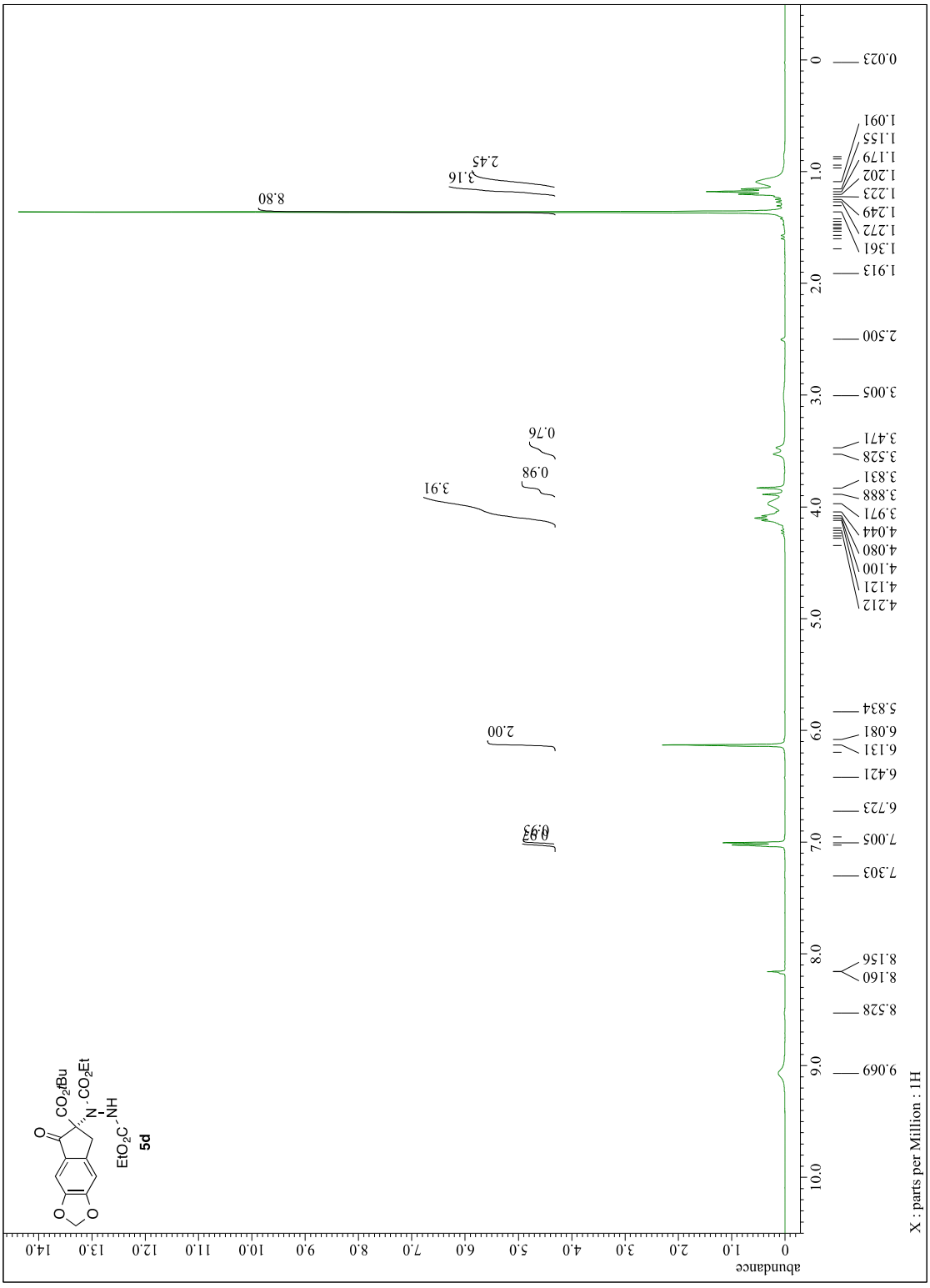


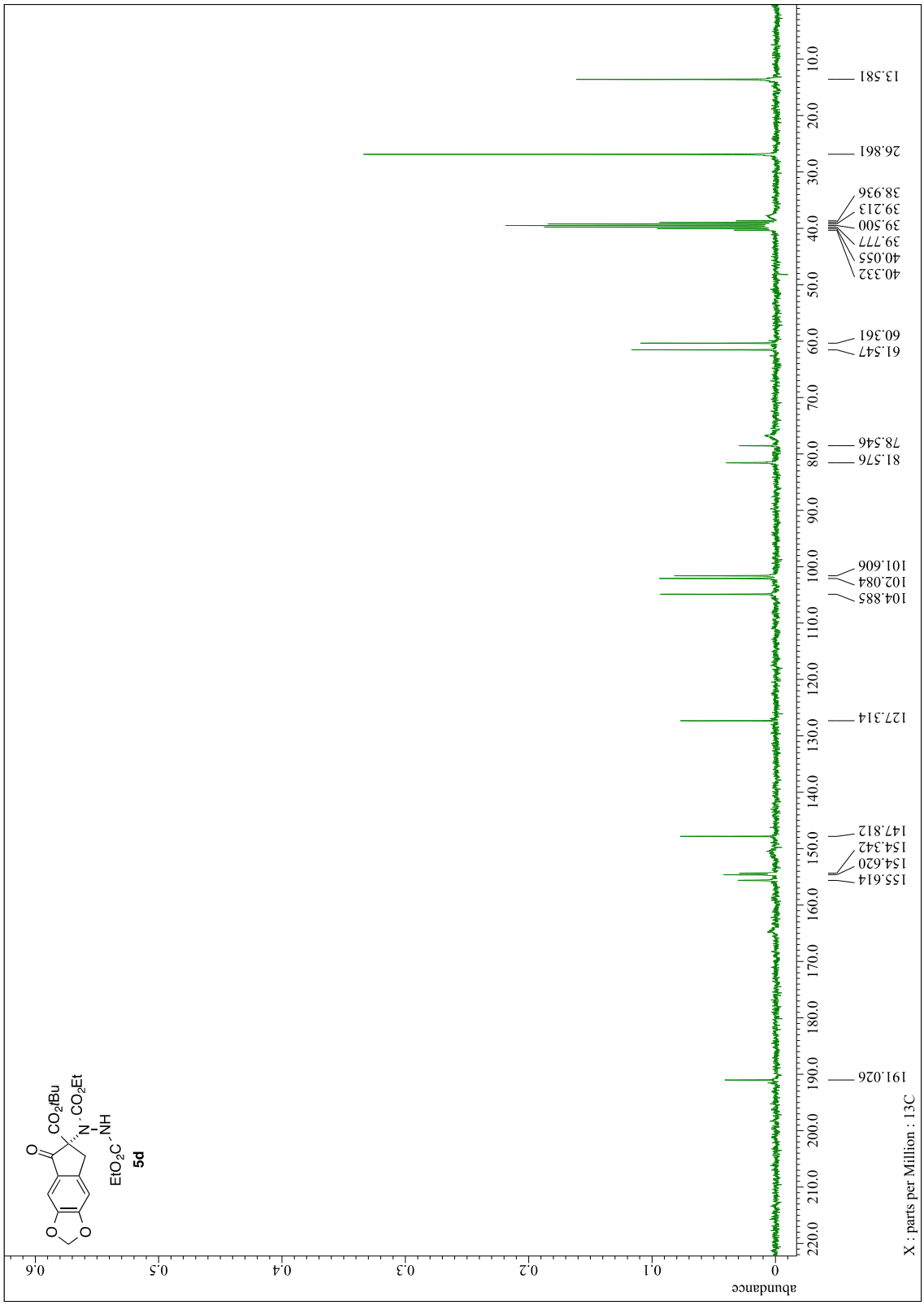
No.	Rt	Area	Area(%)	Height
1	8.39	9699897	50.5589	250744
2	13.38	9485447	49.4411	117814
		19185345	100	368558

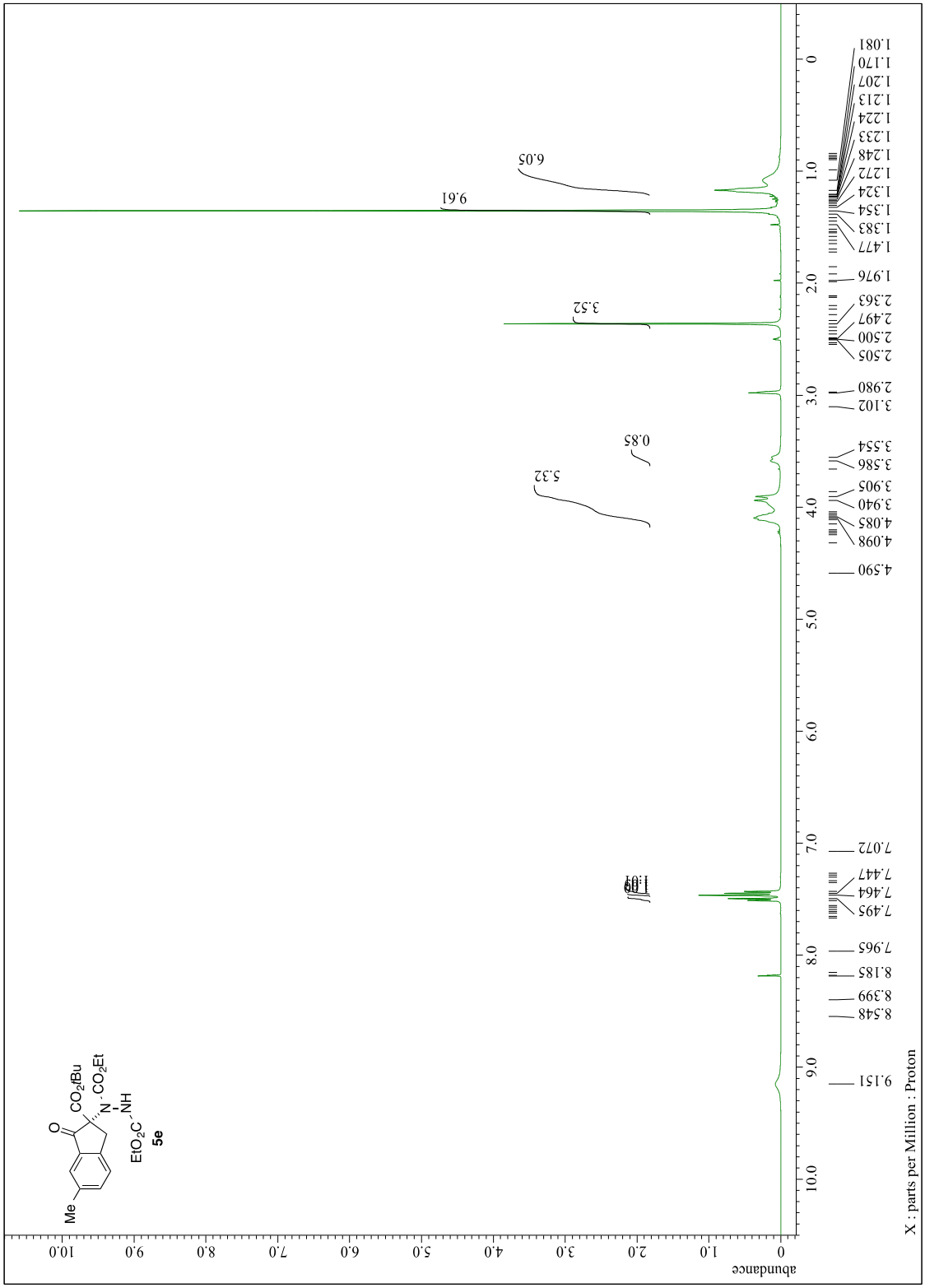


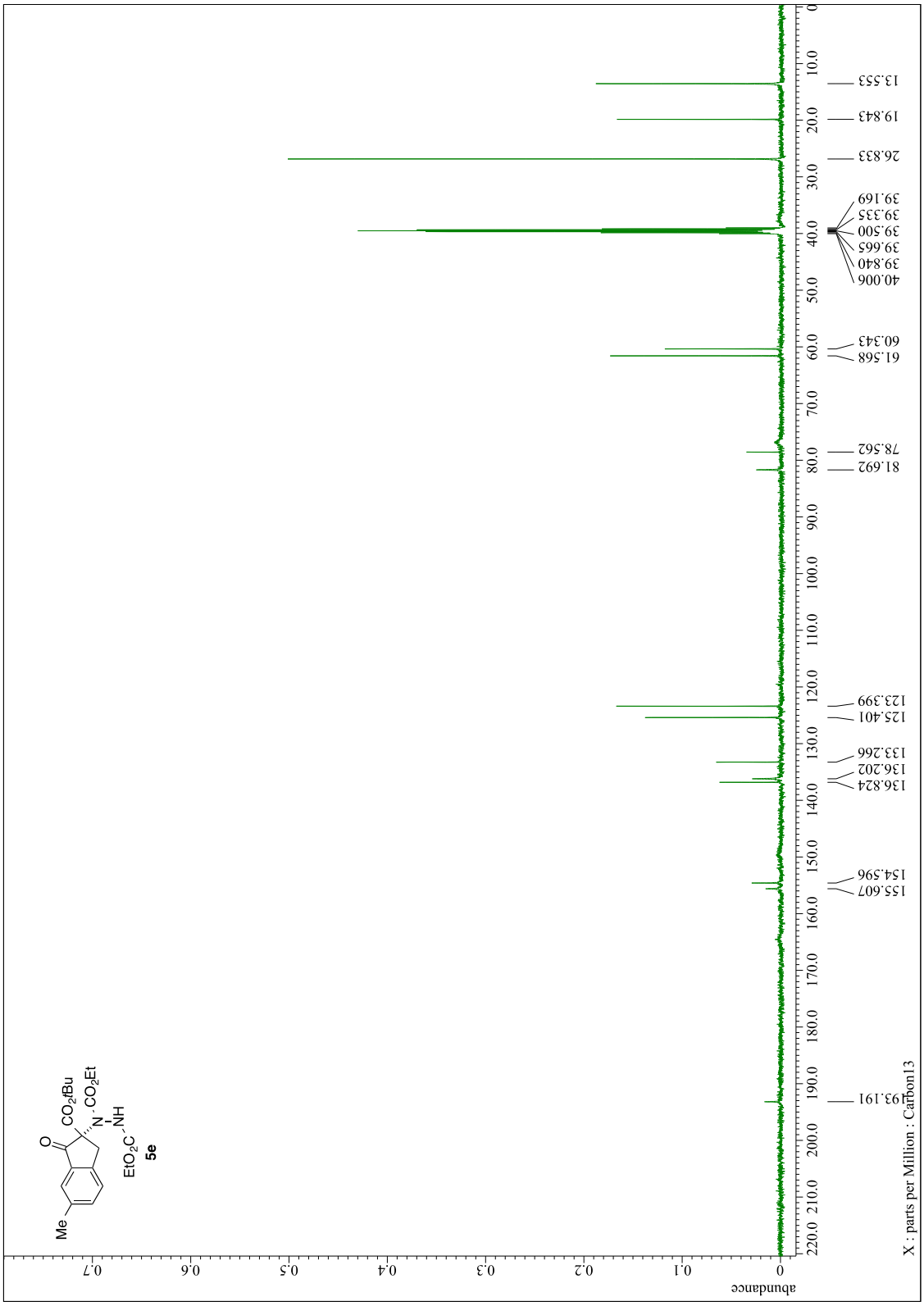
No.	Rt	Area	Area(%)	Height
1	8.73	16624336	72.0583	393342
2	13.69	6446350	27.9417	76819
		23070685	100	470161

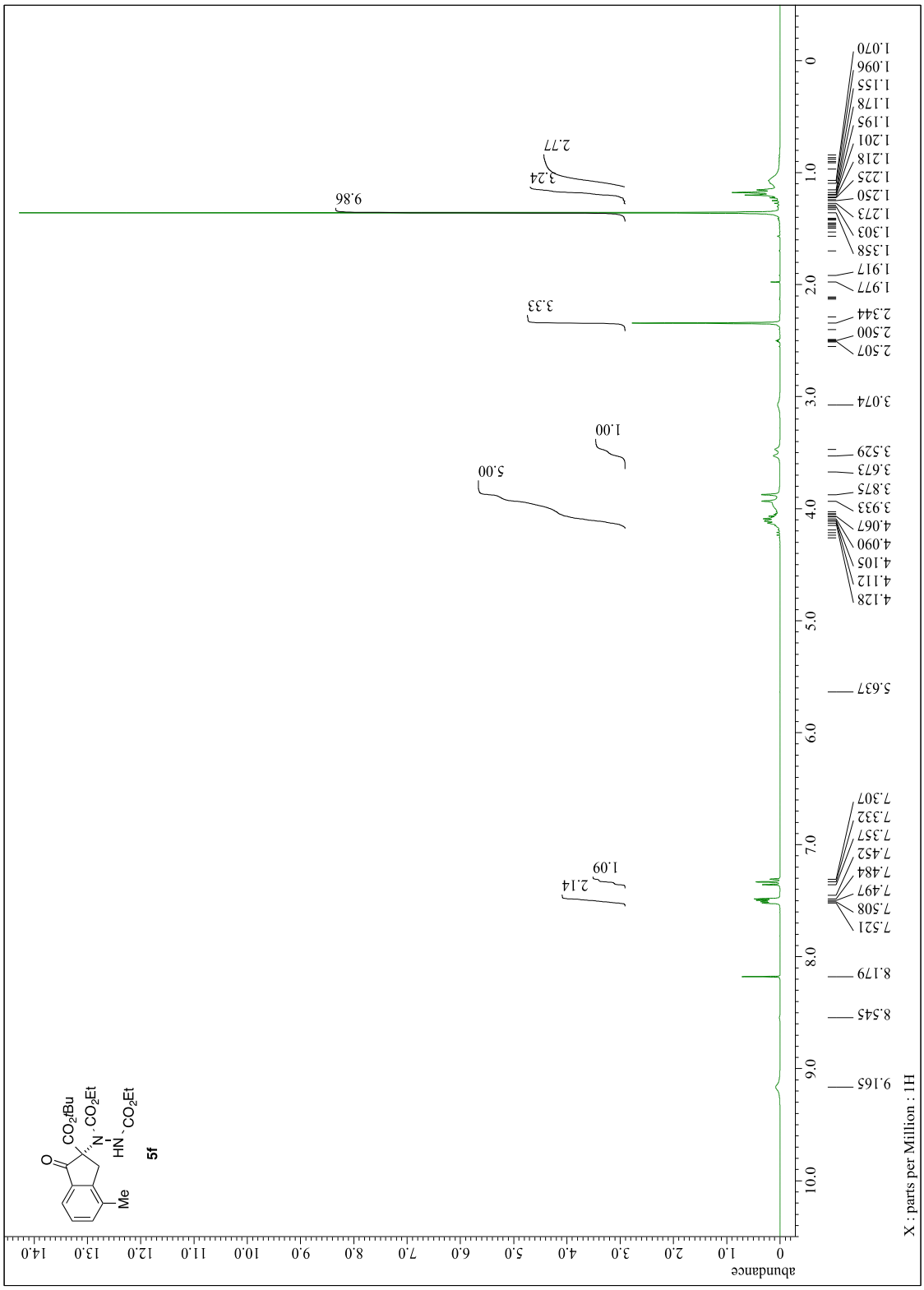
5. ^{1}H and ^{13}C NMR spectra of new compounds 5d–h, 5j

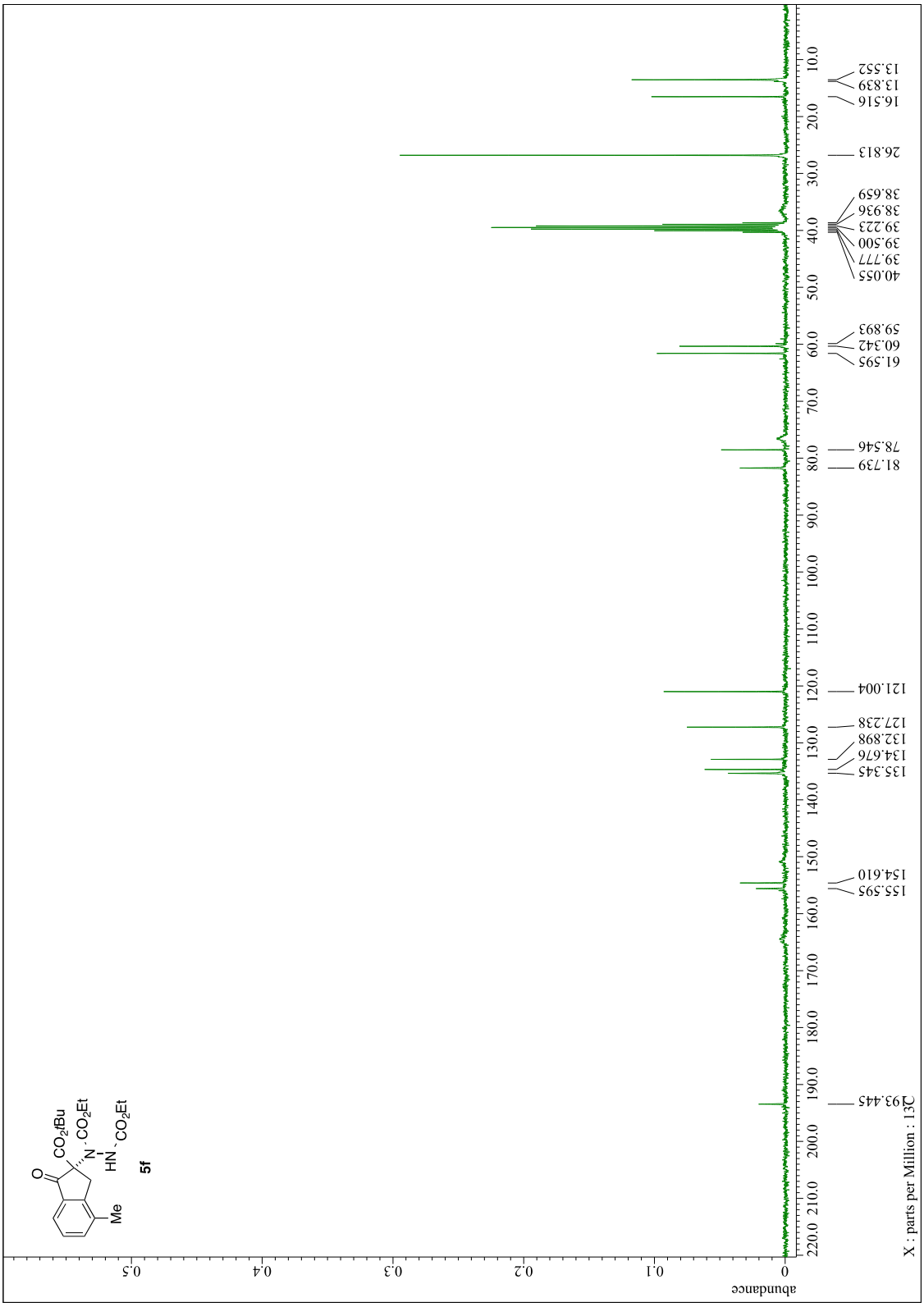


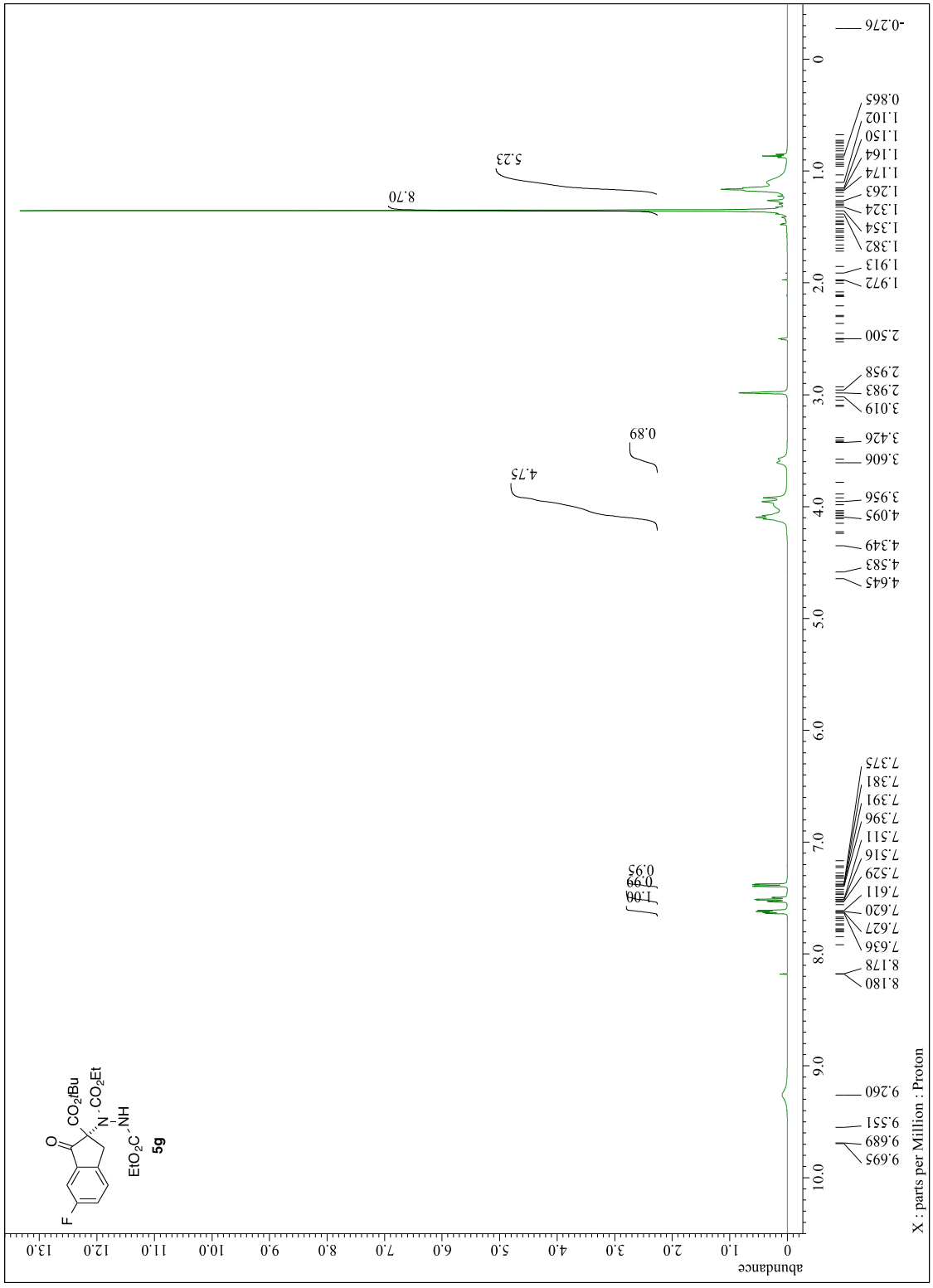

abundance
X : parts per Million : 13C
191.026
155.614
154.620
154.342
147.812
127.314
104.885
102.084
101.606
81.576
78.546
61.547
60.361
40.332
40.055
39.777
39.500
39.213
38.936
26.861
13.581
5d

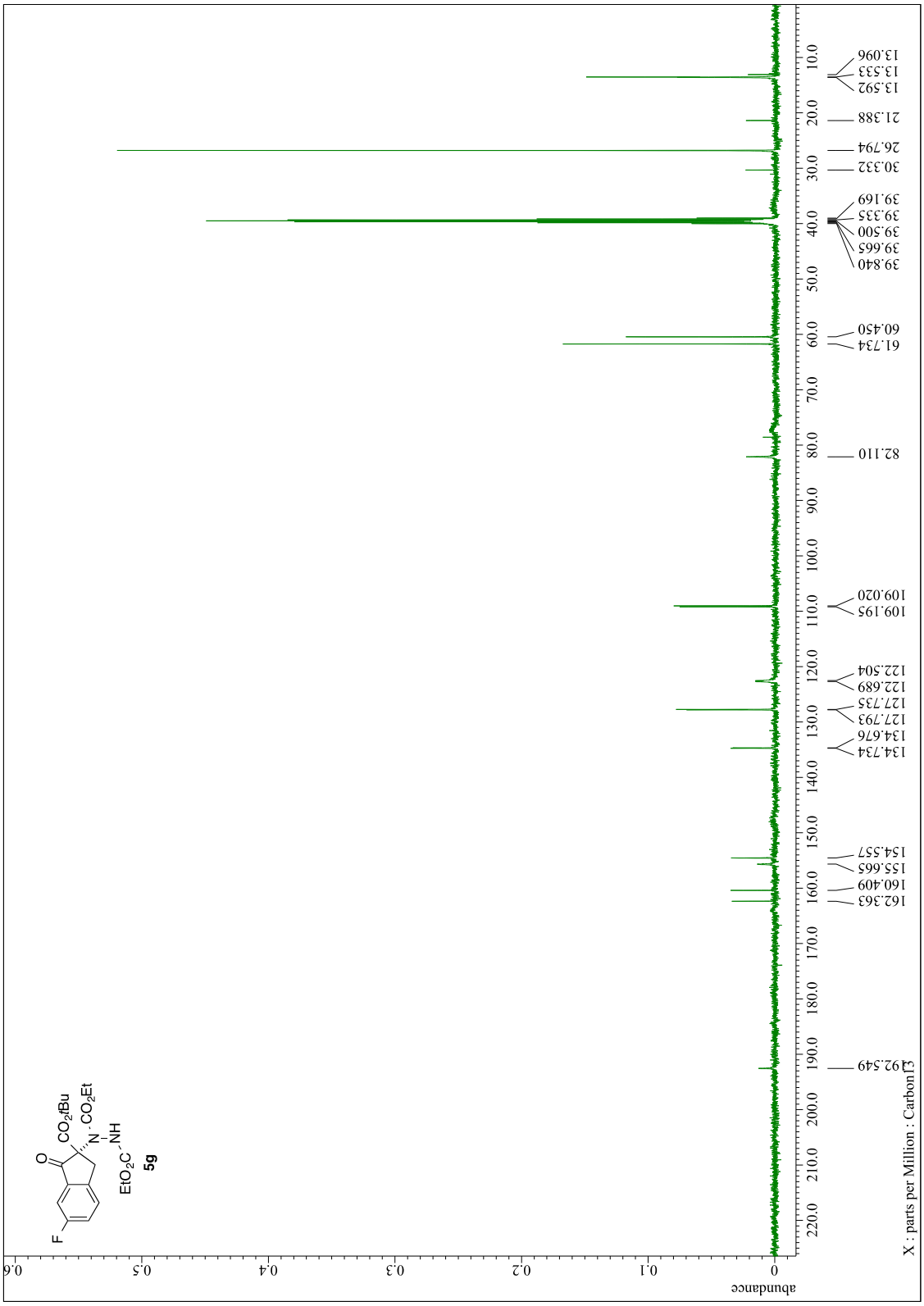

Me
O
CO2tBu
N
CO2Et
NH
EtO2C
5e
abundance
X : parts per Million : Proton
9.151
8.548
8.399
8.185
7.965
7.495
7.464
7.447
7.072
4.590
4.098
4.085
3.940
3.905
3.586
3.554
3.102
2.980
2.505
2.500
2.497
2.363
1.976
1.477
1.383
1.354
1.324
1.272
1.248
1.233
1.224
1.213
1.207
1.170
1.081
6.05
9.61
3.52
0.85
5.32

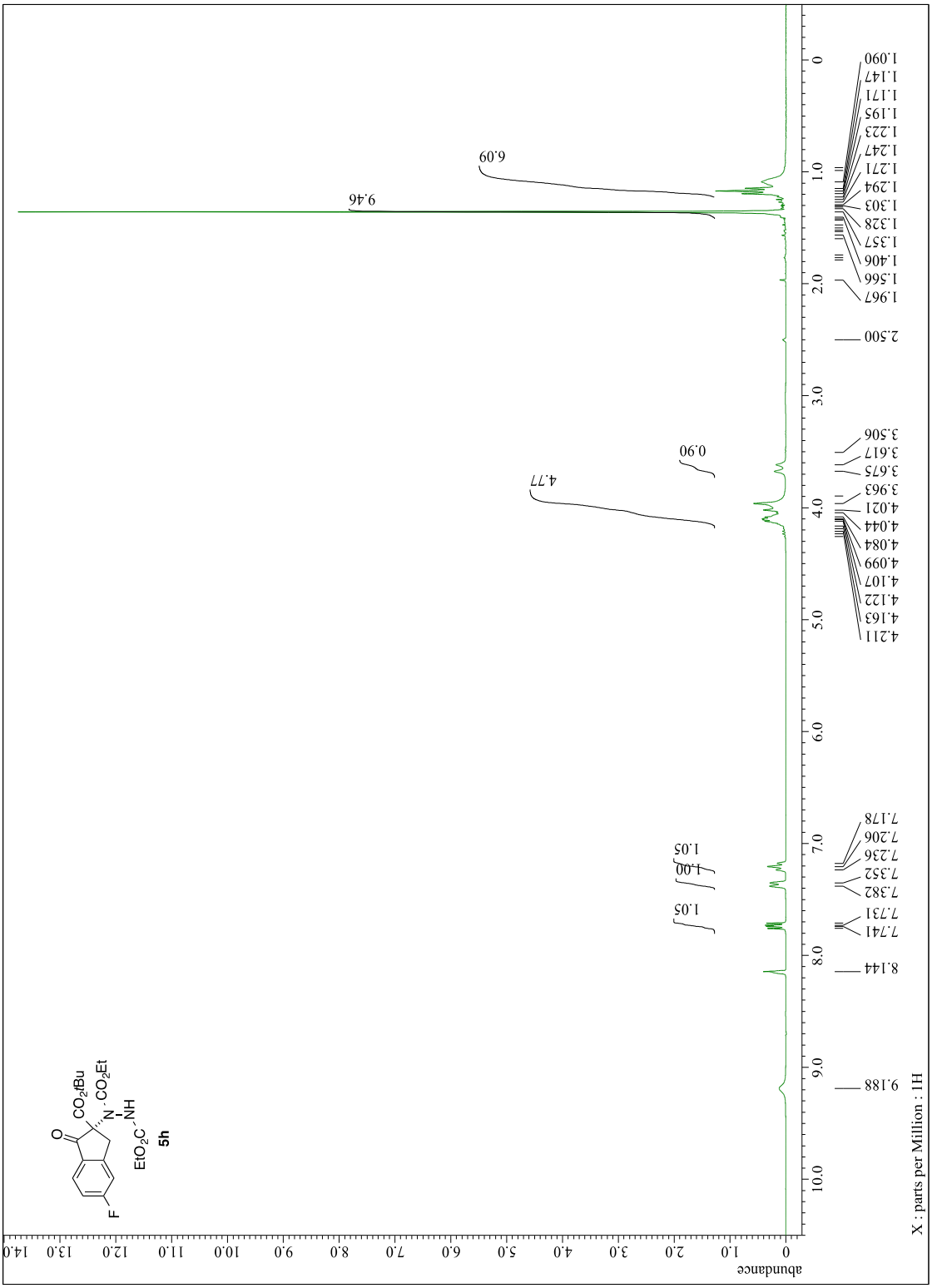

abundance
X : parts per Million : Carbon13
13.553
19.843
26.833
39.169
39.335
39.500
39.665
39.840
40.006
60.343
61.568
78.562
81.692
123.399
125.401
133.266
136.202
136.824
154.596
155.607
193.191
Me
CO2tBu
CO2Et
N
NH
EtO2C
5e

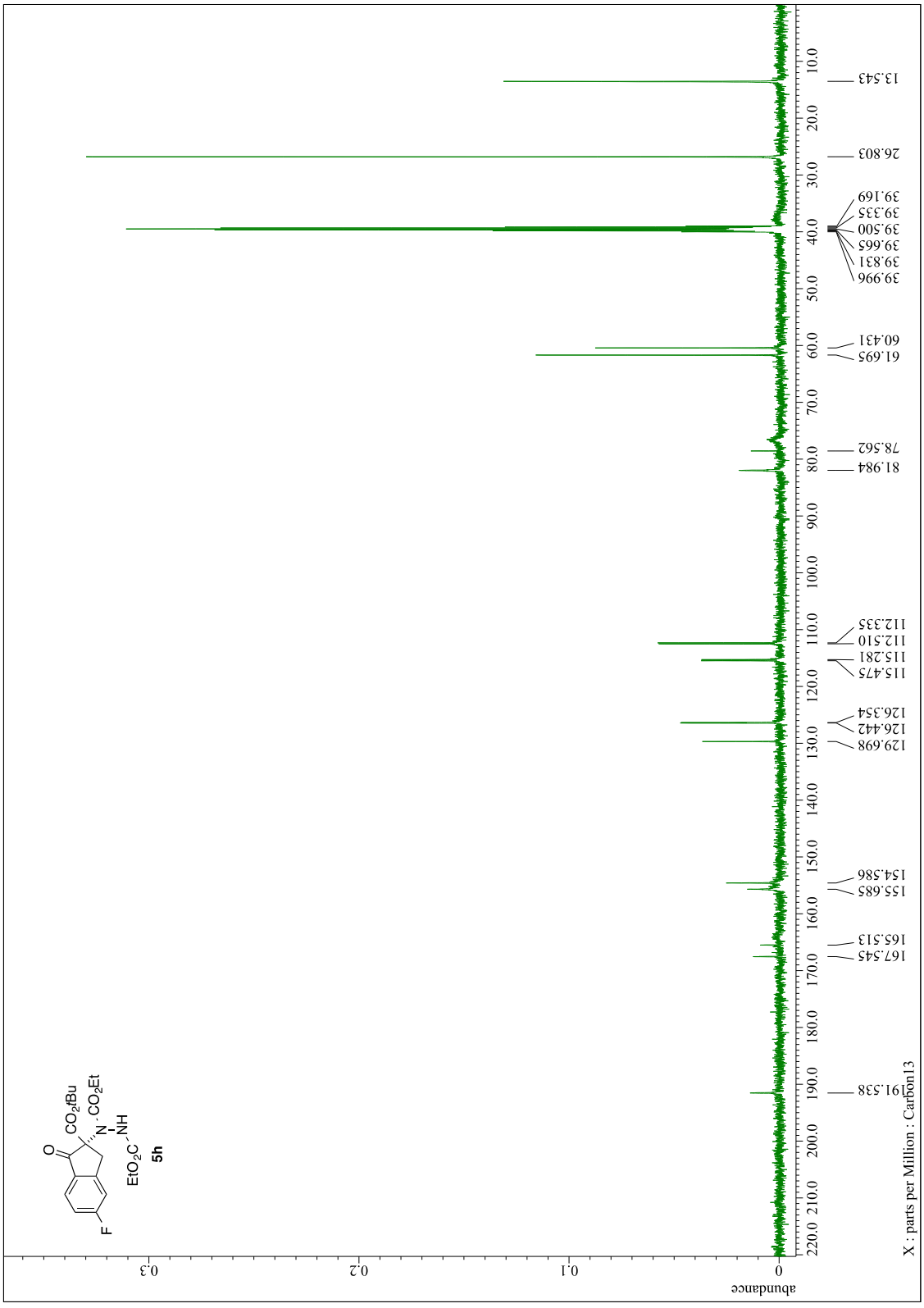

abundance
X : parts per Million : 1H
5f
Me
CO2tBu
CO2Et
CO2Et
HN
N
O
9.165
8.545
8.179
7.521
7.508
7.497
7.484
7.452
7.357
7.332
7.307
5.637
4.128
4.112
4.105
4.090
4.067
3.933
3.875
3.673
3.529
3.074
2.507
2.500
2.344
1.977
1.917
1.358
1.303
1.273
1.250
1.225
1.218
1.201
1.195
1.178
1.155
1.096
1.070
9.86
3.24
2.77
3.33
1.00
5.00
1.09
2.14

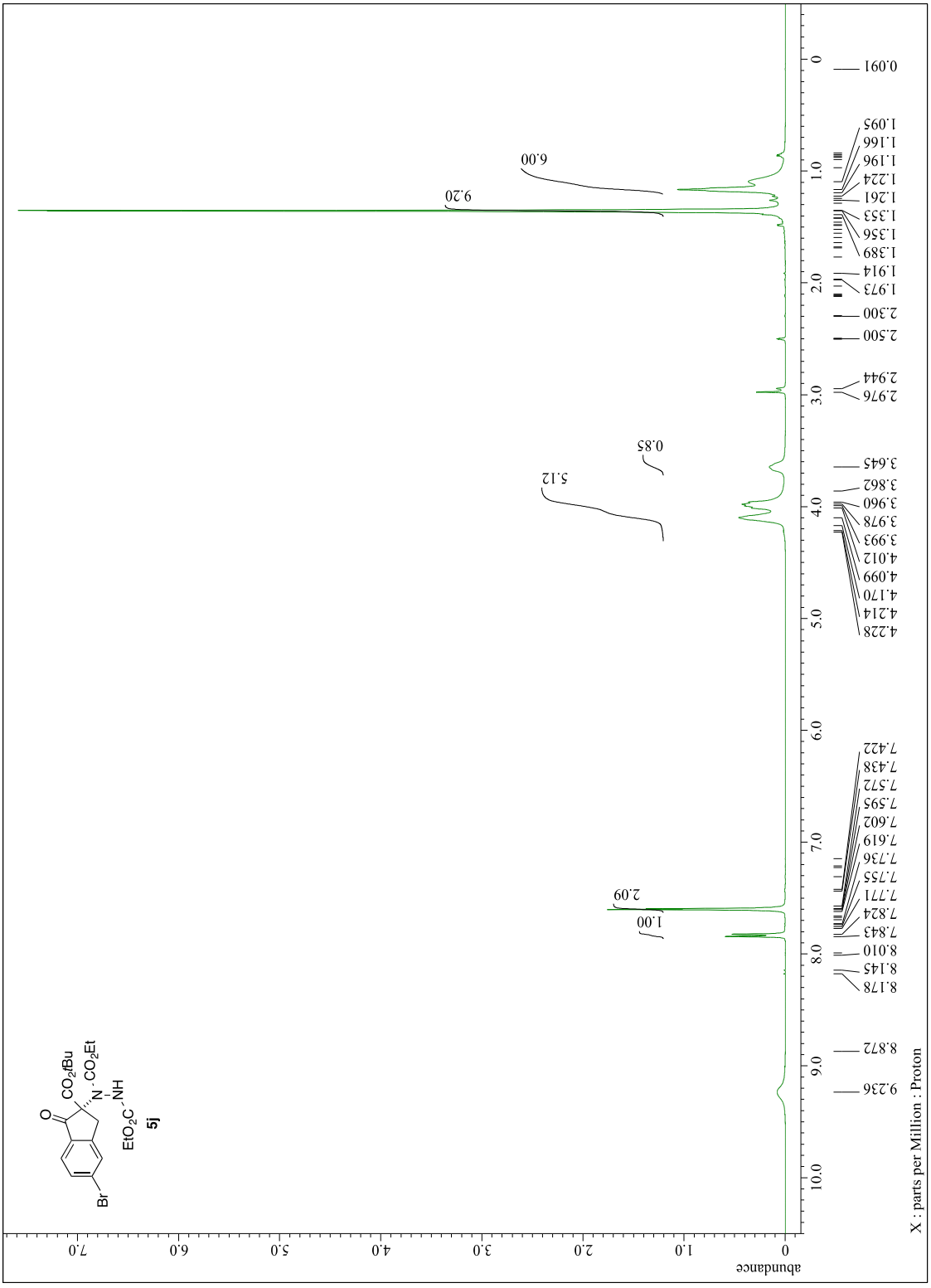

abundance
X : parts per Million : 13C
5f
Me
HN
CO2Et
N
CO2Et
O
CO2tBu
193.445
155.595
154.610
135.345
134.676
132.898
127.238
121.004
81.739
78.546
61.595
60.342
59.893
40.055
39.777
39.500
39.223
38.936
38.659
26.813
16.516
13.839
13.552

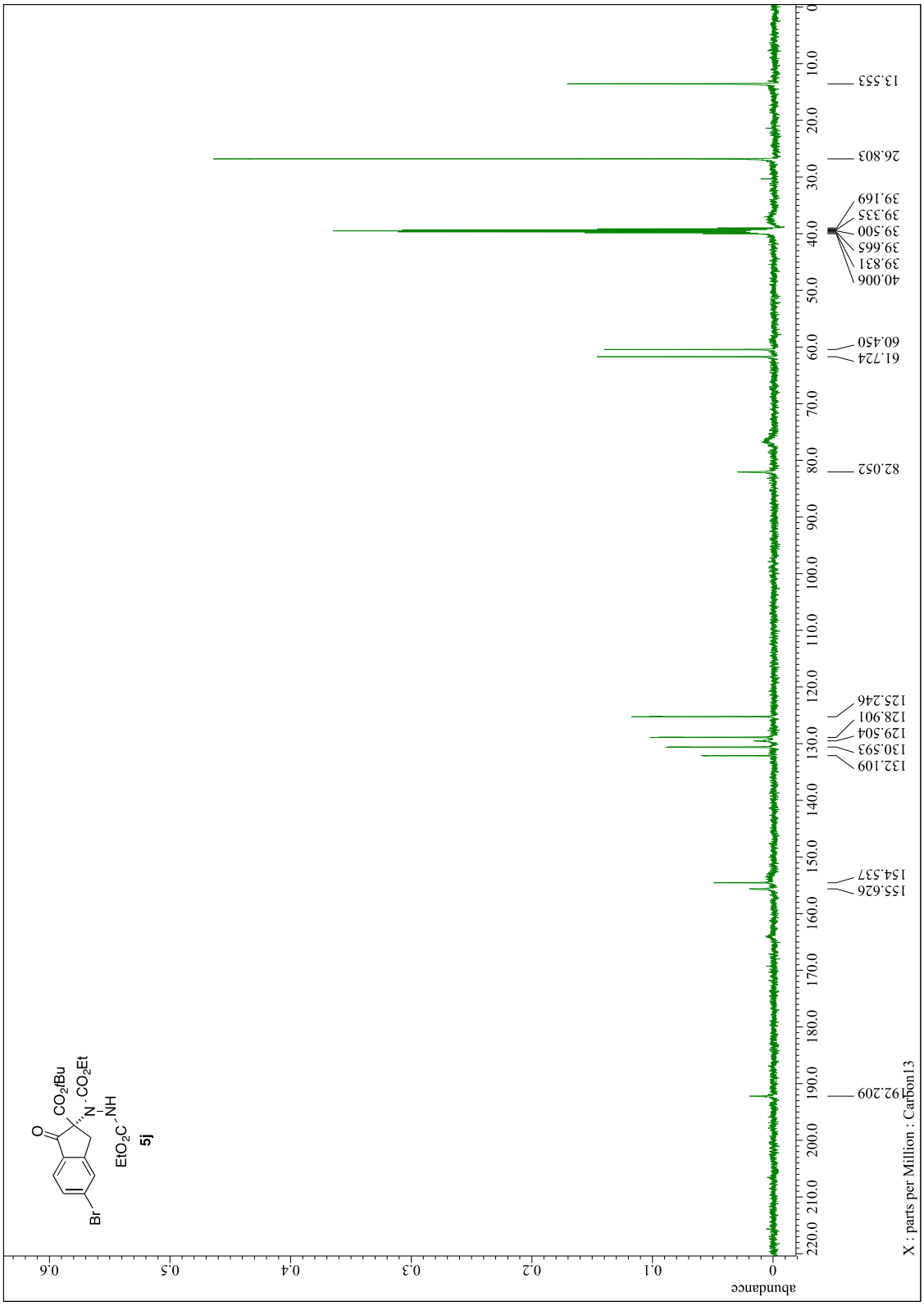

abundance
X : parts per Million : Proton
5g
9.695
9.689
9.551
9.260
8.180
8.178
7.636
7.627
7.620
7.611
7.529
7.516
7.511
7.396
7.391
7.381
7.375
4.645
4.583
4.349
4.095
3.956
3.606
3.426
3.019
2.983
2.958
2.500
1.972
1.913
1.382
1.354
1.324
1.263
1.174
1.164
1.150
1.102
0.865
-0.276
8.70
5.23
4.75
0.89
1.06
0.99
0.95


5g
X : parts per Million : Carbon13
abundance
192.549
162.363
160.409
155.665
154.557
134.734
134.676
127.793
127.735
122.689
122.504
109.195
109.020
82.110
61.734
60.450
39.840
39.665
39.500
39.335
39.169
30.332
26.794
21.388
13.592
13.533
13.096


O
CO2tBu
N
CO2Et
EtO2C
NH
F
5h
X : parts per Million : 1H
abundance
9.188
8.144
7.741
7.731
7.382
7.352
7.236
7.206
7.178
4.211
4.163
4.122
4.107
4.099
4.084
4.044
4.021
3.963
3.675
3.617
3.506
2.500
1.967
1.566
1.406
1.357
1.328
1.303
1.294
1.271
1.247
1.223
1.195
1.171
1.147
1.090
9.46
6.09
4.77
0.90
1.05
1.00
1.05


O
CO2tBu
N
CO2Et
NH
EtO2C
F
5h
abundance
0
0.1
0.2
0.3
X : parts per Million : Carbon13
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
191.538
167.545
165.513
155.685
154.586
129.698
126.442
126.354
115.475
115.281
112.510
112.335
81.984
78.562
61.695
60.431
39.996
39.831
39.665
39.500
39.335
39.169
26.803
13.543


abundance
X : parts per Million : Proton
5j
9.236
8.872
8.178
8.145
8.010
7.843
7.824
7.771
7.755
7.736
7.619
7.602
7.595
7.572
7.438
7.422
4.228
4.214
4.170
4.099
4.012
3.993
3.978
3.960
3.862
3.645
2.976
2.944
2.500
2.300
1.973
1.914
1.389
1.356
1.353
1.261
1.224
1.196
1.166
1.095
0.091
1.00
2.09
5.12
0.85
9.20
6.00


O
CO2tBu
N
CO2Et
NH
EtO2C
Br
5j
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : Carbon13
0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
180.0
190.0
200.0
210.0
220.0
13.553
26.803
39.169
39.335
39.500
39.665
39.831
40.006
61.724
60.450
82.052
125.246
128.901
129.504
130.593
132.109
154.537
155.626
192.209