Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information For:

Copper Catalyzed Asymmetric Dearomative Alkynylation of Isoquinolines

Xun Kou, Qingyang Zhao, and Zheng-Hui Guan*

Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, Department of Chemistry & Materials Science, Northwest University, Xi'an 710127, P. R. China
School of Pharmaceutical Sciences (Shenzhen), Sun Yat-sen University, Shenzhen, 518107, P. R. China

E-mail: guanzhh@nwu.edu.cn

CONTENT

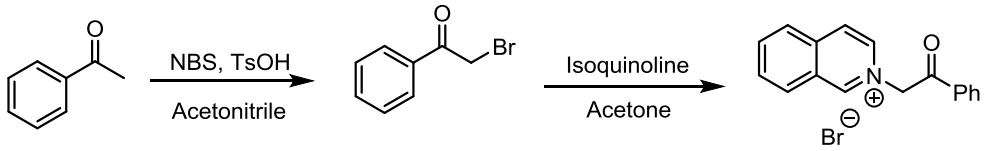
I. General information.

Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and used without further purification. All reactions were carried out under an atmosphere of nitrogen using a glovebox.

Reaction progresses were monitored by analytical thin layer chromatography (TLC) (TLC-Silica gel GF254, coating thickness: 0.20-0.25 mm, particle size: 10-40 μm). The TLC was visualized with a UV lamp (254 or 365 nm). Flash Column chromatography was carried out on silica gel (60 Å, 200-300 mesh) with technical grade solvents as the eluent. ^{1}H and ^{13}C NMR spectra were recorded on Bruker instrument Advance 400 or600 and referenced internally to the residual proton resonance in CDCl3 (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad. Coupling constants *J* were reported in Hertz unit (Hz). Optical rotations were measured with a WZZ-2S automatic polarimeter purchased from Shanghai INESA Physico-Optical instrument company using a sodium lamp (sodium D line, λ = 589 nm) in the indicated solvent at the indicated temperature. The measurements were carried out in a 1.5 mL cell (50 mm length) with concentrations (g/100mL) reported in the corresponding solvent. The optical rotation values ($[\alpha]^{D}$) were reported at a given temperature (°C) in deg. mL g^{-1} dm^{-1}. HRMS were recorded on a liquid chromatography/quadrupole time-of-flight mass spectrometer (MicroTof-Q II mass spectrometer, Bruker Daltonics) using electrospray ionization-time of flight (ESI-TOF). HPLC analysis was performed on an Agilent Technologies 1260 Series using Chiralpak columns IA, IC or IG (Daicel Chiral Reagent Company). The solvents (n-hexane and iso-propanol, HPLC-grade) used as the eluent were purchased from Oceanpak. The column type and the eluent (a mixture of n-hexane and iso-propanol) are indicated for each experiment. X-ray crystallography was performed on a BRUKERSMA RTAPEXIICCD diffractometer.

2. Typical procedure for preparation of substrates.

General Procedure for preparation of *N*-activated isoquinolines.



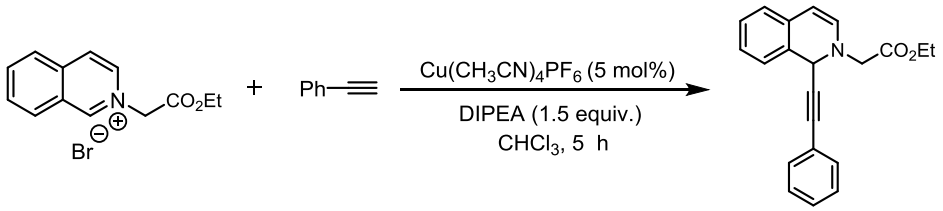
I II

Typical Procedure I: acetophenone (5.0 mmol, 1.0 equiv.), NBS (5.0 mmol, 1.0 equiv.), TsOH (7.5 mmol, 1.5 equiv.) and acetonitrile (20 mL) were added to a flask (50 mL) equipped with a magnetic stirrer. After stirred at 70℃ for 4 hours, acetonitrile was evaporated in vacuo and the aqueous layer was extracted three times with ethyl acetate (3 ×15 mL). The desired 2-bromoacetophenone were obtained by flash chromatography (petroleum ether/ethyl acetate = 50:1) as yellow solid.

Typical Procedure II: 2-bromoacetophenone (5 mmol, 1.0 equiv.), isoquinoline (5 mmol, 1.0 equiv.) and acetone (20 mL) was added to a flask (50 mL) equipped with a magnetic stirrer. Then, the mixture was stirred at 70 °C for 5 hours. The desired *N*-activated isoquinolines were obtained by suction filtration as white solid.

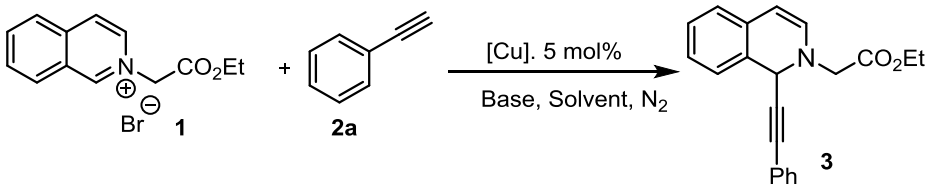
3. Racemic synthesis

General Procedure for racemic synthesis.



In a nitrogen-filled glove box, $Cu(CH_3CN)_4PF_6$ (0.005 mmol, 5 mol%) and $CHCl_3$ (1.0 mL) was added to a 10 mL tube (tube A) which was charged with phenylacetylene (0.2 mmol, 2.0 equiv.). Then the mixture was stirred for 5 min. In another 10 mL tube (tube B) charged with *N*-activated isoquinolines (0.1 mmol, 1.0 equiv.), *N,N*-diisopropylethylamine (0.15 mmol, 1.5 equiv.) and $CHCl_3$ (2.0 mL). After that, the mixture in tube A was transferred into the tube B under room temperature, and then, the resulting reaction mixture was stirred for 5 h at room temperature before direct separation by column chromatography (Hexanes /ethyl acetate = 10:1 as the eluent) to afford the corresponding pure products.

Supplementary Table 1 Conditions for racemic synthesis[a]

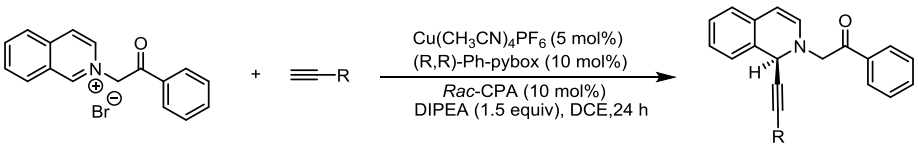


entry	[Cu]	Base	Solvent	Yield (%)
1	$Cu(OAc)_2$	Et_3N	DCM	42
2	$Cu(OTf)_2$	Et_3N	DCM	0
3	$Cu(CH_3CN)_4BF_4$	Et_3N	DCM	38
4	$Cu(CH_3CN)_4PF6$	Et_3N	DCM	47
5	$Cu(CH_3CN)_4PF6$	^tBuOK	DCM	0
6	$Cu(CH_3CN)_4PF6$	NaOH	DCM	38
7	$Cu(CH_3CN)_4PF6$	K_2CO_3	DCM	29
8	$Cu(CH_3CN)_4PF6$	DIPEA (i-Pr_2NEt)	DCM	52
9	$Cu(CH_3CN)_4PF6$	DIPA(i-Pr_2NH)	DCM	42
10	$Cu(CH_3CN)_4PF6$	DIPEA	DCE	56
11	$Cu(CH_3CN)_4PF6$	DIPEA	1,4-dioxane	60
12	$Cu(CH_3CN)_4PF6$	DIPEA	$CHCl_3$	86

[a] Reaction conditions: **1** (0.10 mmol), **2a** (0.2 mmol), [Cu] (5 mol%) and bases (1.5 equiv.) in solvent (3 mL) at room temperature for 5 h, [b] isolated yield.

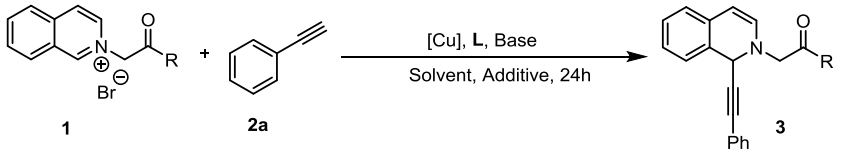
4. Asymmetric synthesis.

General procedure for asymmetric synthesis.



In a nitrogen-filled glove box, (*R*,*R*)-Ph-pybox (0.01 mmol, 10 mol%), *Rac*-CPA (0.01 mmol, 10 mol%) and dry DCE (1.0 mL) was added to a 10 mL tube (tube A) charged with $Cu(CH_3CN)_4PF_6$ (0.005 mmol, 5 mol%) and then the mixture was stirred for 1 h. In another 10 mL tube (tube B) charged with *N*-activated isoquinolines (0.1 mmol, 1.0 equiv.), aryl acetylene (0.2 mmol, 2 equiv.), *N,N*-diisopropylethylamine (0.15 mmol, 1.5 equiv.) and dry DCE (2.0 mL). After that, the solution in tube A was transferred into the tube B, and the resulting reaction mixture was stirred for 24 h at -30 ^oC. Then, the reaction was warmed to room temperature before direct separation by column chromatography (Hexanes /ethyl acetate = 10:1 as the eluent) to afford the corresponding pure products.

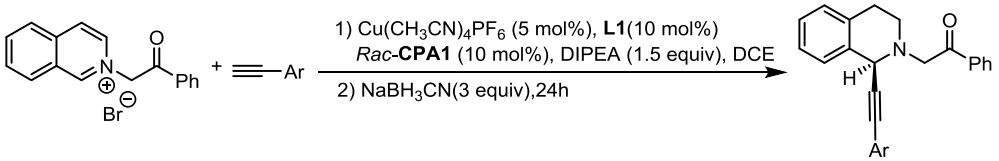
Supplementary Table 2 Conditions for asymmetric synthesis: solvents, temperature and bases. [a]



1 2a 3

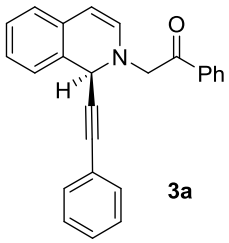
entry	Ligand	[Cu]	R	Base	Temp.	Solvent	Yield(%)	ee(%)
1	L1(6%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	RT	$CHCl_3$	85	20
2	L1(6%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	RT	DCM	52	37
3	L1(6%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	RT	DCE	56	42
4	L1(8%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	RT	DCE	56	46
5	L1(10%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	RT	DCE	56	50
6	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	DIPEA	RT	DCE	75	76
7	L1(10%)	$Cu(CH_3CN)_4BF_4$	Ph	DIPEA	RT	DCE	60	36
8	L1(10%)	$Cu(OAc)_2$	Ph	DIPEA	RT	DCE	52	58
9	L1(10%)	$Cu(OTf)_2$	Ph	DIPEA	RT	DCE	30	56
10	L1(10%)	CuI	Ph	DIPEA	RT	DCE	28	61
11	L1(10%)	$Cu(TFA)_2$	Ph	DIPEA	RT	DCE	41	64
12	L1(10%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	0℃	DCE	60	62
13	L1(10%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	-10℃	DCE	76	66
14	L1(10%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	-20℃	DCE	80	73
15	L1(10%)	$Cu(CH_3CN)_4PF_6$	OEt	DIPEA	-30℃	DCE	81	75
16	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	DIPEA	-30℃	DCE	65	92
17	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	Et_3N	-30℃	DCE	33	94
18	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	NaOH	-30℃	DCE	40	92
19	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	DIPA	-30℃	DCE	37	93
20	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	CsOH	-30℃	DCE	35	91
21	L1(10%)	$Cu(CH_3CN)_4PF_6$	Ph	KOH	-30℃	DCE	20	90

General Procedure for one-pot stepwise asymmetric alkynylation/reduction reaction.



In a 10 mL tube (tube A) was charged with $Cu(CH_3CN)_4PF_6$ (0.005 mmol, 5 mol%), **L1** (0.01 mmol, 10 mol%), *Rac*-CPA (0.01 mmol, 10 mol%) and DCE (1.0 mL). In another 10 mL tube (tube B) charged with *N*-activated isoquinolines (0.1 mmol, 1.0 equiv.), aryl acetylene (0.2 mmol, 2.0 equiv.), *N,N*-diisopropylethylamine (0.15 mmol, 1.5 equiv.) and dry DCE (2.0 mL). The mixture in tube A was stirred for 1 h and then transferred into the tube B. The reaction mixture in tube B was stirred for 24 h at -30 ^oC. After that, the reaction was warmed to room temperature and the $NaBH_3CN$ (0.3 mmol, 3 equiv.) was added. The reaction mixture was stirred for additional 24 h at room temperature before direct separation by column chromatography (hexanes /ethyl acetate = 10:1 as the eluent) to afford the corresponding pure products.

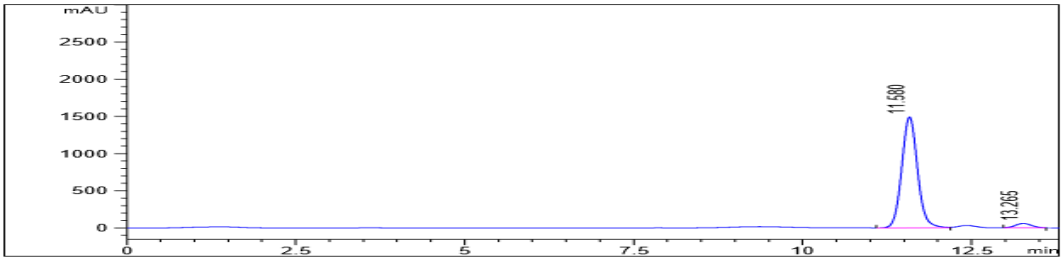
5. Spectroscopic Data for Products



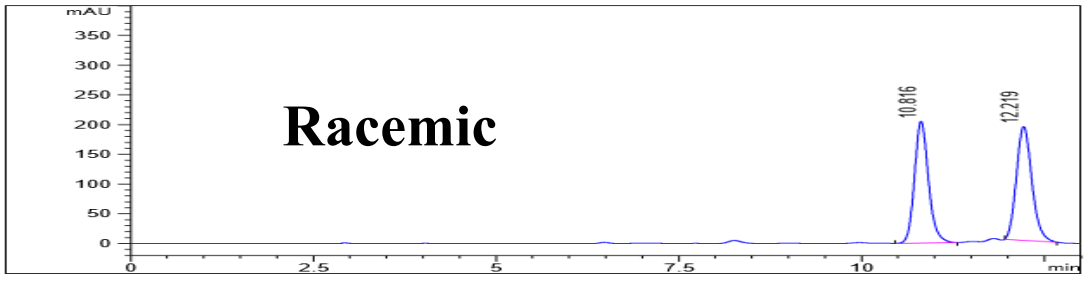
3a

(*S*)-1-phenyl-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

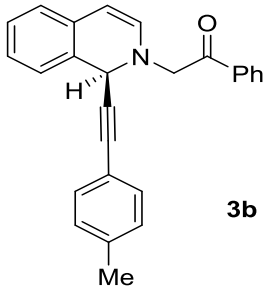
Yellow oil. Yield = 83%. $[\alpha]^{15}_{D}$ = -94.55 (c = 0.985, $CHCl_3$, 92% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.36 – 7.34 (m, 2H), 7.29 – 7.22 (m, 4H), 7.17 (t, *J* = 7.2 Hz, 1H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.14 (d, *J* = 7.6 Hz, 1H), 5.71 (s, 1H), 5.55 (d, *J* = 7.6 Hz, 1H), 4.97 (d, *J* = 17.6 Hz, 1H), 4.48 (d, *J* = 17.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.46, 136.83, 135.32, 133.59, 132.12, 131.80, 128.78, 128.37, 128.16, 128.02, 127.93, 127.51, 125.86, 125.49, 123.35, 122.48 (s), 100.39, 86.51, 86.47, 58.17, 52.99. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 11.6 min, t_2 (major) = 13.3 min. HRMS (ESI) calcd for $C_{25}H_{19}ON$ m/z $[M + Na]^+$: 372.1359; found: 372.1367.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	11.580	MM	1487.957	0.270	24084.021	96.175
2	13.265	MM	58.707	0.272	957.939	3.825



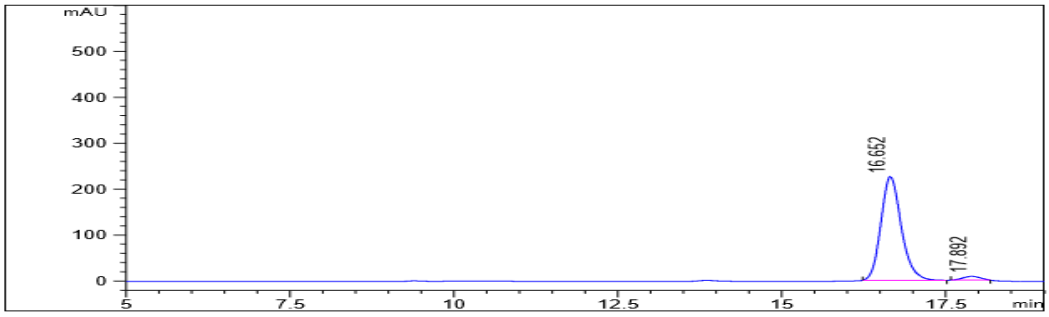
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	10.816	BB	204.501	0.204	2732.830	49.134
2	12.219	MM	191.587	0.246	2829.180	50.866



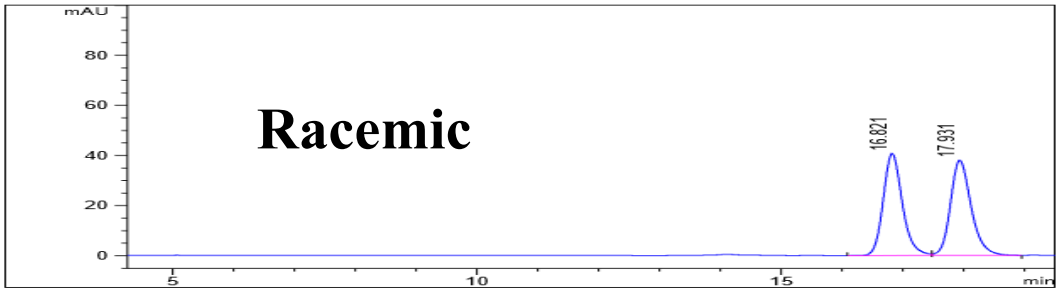
3b

(*S*)-1-phenyl-2-(1-(*p*-tolylethynyl)isoquinolin-2(1*H*)-yl)ethanone

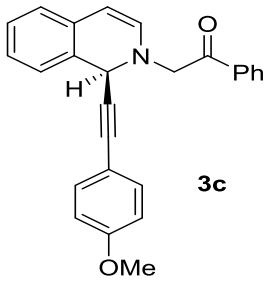
Yellow oil. Yield = 71%. $[\alpha]^{16}_{D}$ = -100.1 (c = 0.945, $CHCl_3$, 94% ee). ^1H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.2, 1H), 7.25 (d, *J* = 7.2, 2H), 7.17 (t, *J* = 6.8 Hz, 1H), 7.11 – 7.05 (m, 3H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.15 (d, *J* = 7.6 Hz, 1H), 5.70 (s, 1H), 5.55 (d, *J* = 7.6 Hz, 1H), 5.00 (d, *J* = 17.6 Hz, 1H), 4.48 (d, *J* = 17.6 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.52, 138.51, 136.90, 135.30, 133.58, 132.12, 131.68, 128.91, 128.77, 127.96, 127.93, 127.59, 125.86, 125.46, 123.30, 119.36, 100.35, 86.69, 85.65, 58.13, 52.98, 21.42. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 16.7 min, t_2 (major) = 17.9 min. HRMS (ESI) calcd for $C_{26}H_{21}ON$ m/z $[M + Na]^+$: 386.1515; found: 386.1532.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.652	MM	225.096	0.360	4857.834	96.980
2	17.892	MM	8.171	0.309	151.274	3.020



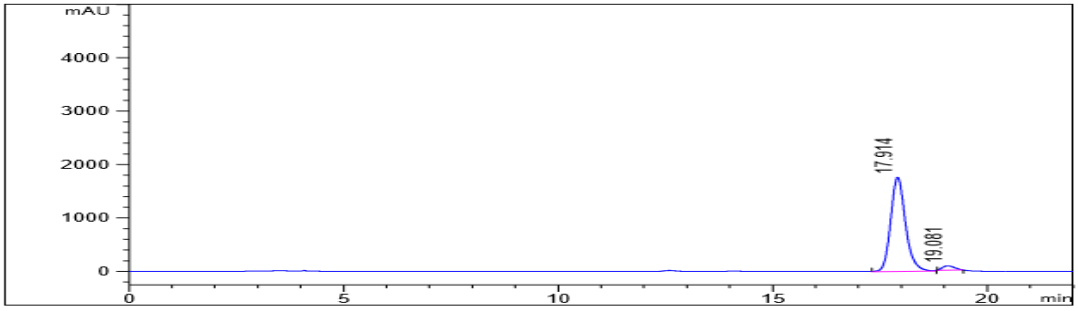
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.821	BV	40.652	0.336	890.679	49.815
2	17.931	VB	37.957	0.360	897.291	50.185



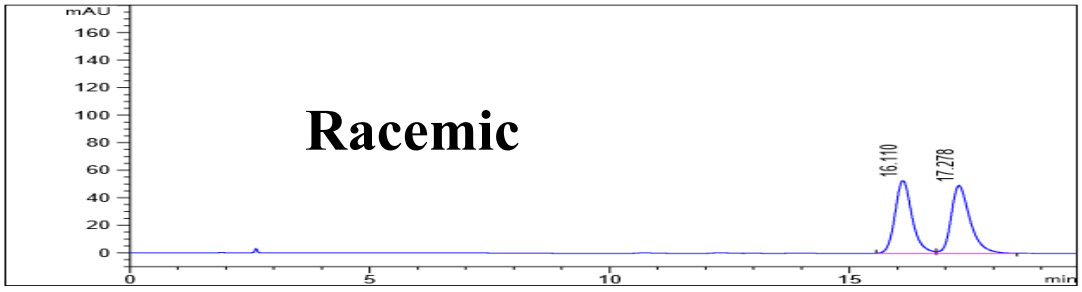
3c

(*S*)-2-(1-((4-methoxyphenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

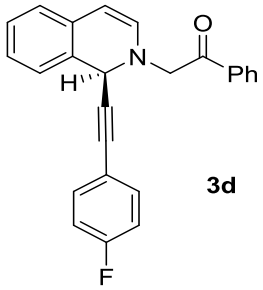
Yellow oil. Yield = 69%. $[\alpha]^{16}_{D}$ = -103.8 (*c* = 1.0, $CHCl_3$, 93% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.29 – 7.27 (m, 3H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.08 (t, *J* = 10.6, 4.2 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 2H), 6.14 (d, *J* = 7.6 Hz, 1H), 5.69 (s, 1H), 5.54 (d, *J* = 7.6 Hz, 1H), 4.97 (d, *J* = 17.6 Hz, 1H), 4.47 (d, *J* = 17.6 Hz, 1H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.55, 159.62, 136.91, 135.35, 133.54, 133.24, 132.15, 128.75, 127.93, 125.85, 125.43, 123.27, 114.55, 113.77, 100.29, 86.51, 84.99, 58.14, 55.21, 53.02. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 17.9 min, t_2 (major) = 19.1 min. HRMS (ESI) calcd for $C_{26}H_{21}O_2N$ m/z $[M + Na]^+$: 402.1465; found: 404.1472.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.914	MM	1764.985	0.401	42493.570	96.395
2	19.081	MM	80.635	0.329	1589.362	3.605



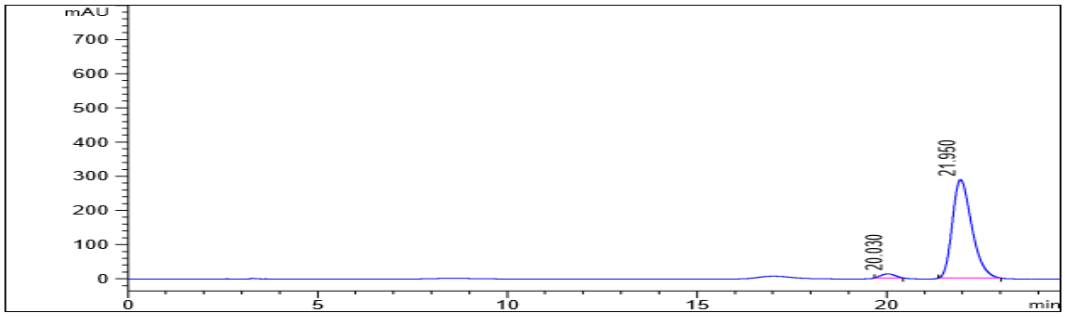
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.110	FM	52.943	0.412	1309.521	49.267
2	17.278	MF	49.281	0.456	1348.489	50.733



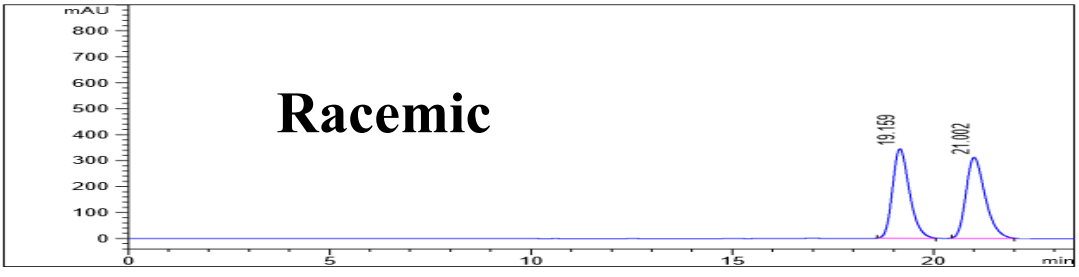
3d

(*S*)-2-(1-((4-fluorophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

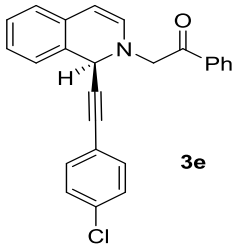
Yellow oil. Yield = 83%. $[\alpha]^{15}_{D}$ = -108.5 (c = 0.955, $CHCl_3$, 94% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.30 (m, 2H), 7.26 (d, *J* = 8.8 Hz, 1H), 7.18 (t, *J* = 6.8 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.98 – 6.92 (m, 3H), 6.15 (d, *J* = 7.6 Hz, 1H), 5.68 (s, 1H), 5.56 (d, *J* = 7.6 Hz, 1H), 4.95 (d, *J* = 18.0 Hz, 1H), 4.50 (d, *J* = 17.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.36, 163.70, 161.22, 136.73, 135.25, 133.89, 133.75, 133.66, 132.04, 128.79, 128.07, 127.91, 127.39, 125.83, 125.51, 123.41, 118.53, 115.53, 115.32, 100.38, 86.24, 85.32, 58.21, 52.90. HPLC (Daicel Chiralpak IC, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 20.0 min, t2 (major) = 22.0 min. HRMS (ESI) calcd for $C_{25}H_{18}ONF$ m/z $[M + Na]^+$: 390.1265; found: 390.1258.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.030	MM	12.328	0.418	309.352	2.939
2	21.950	FM	287.751	0.592	10218.126	97.061



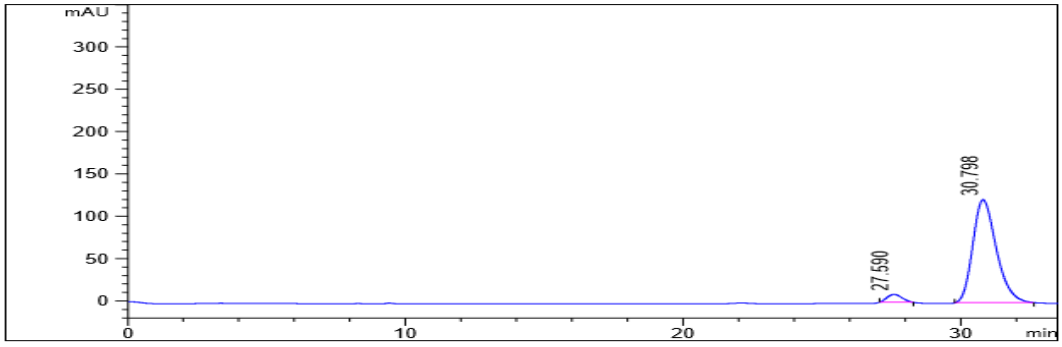
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	19.159	MF	345.373	0.488	10103.917	49.342
2	21.002	FM	312.366	0.553	10373.451	50.658



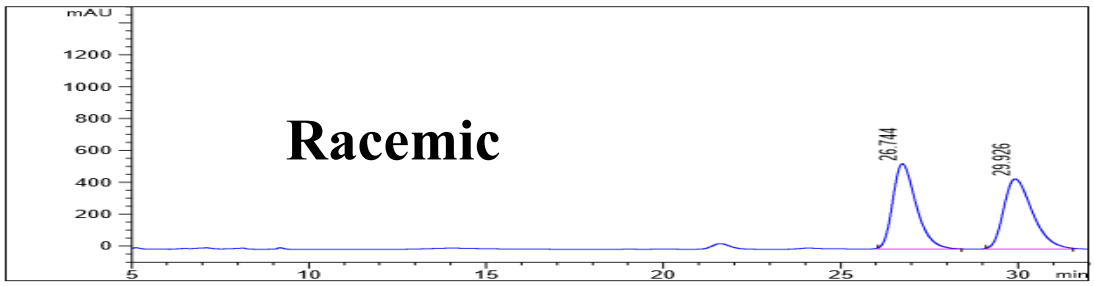
3e

(*S*)-2-(1-((4-chlorophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

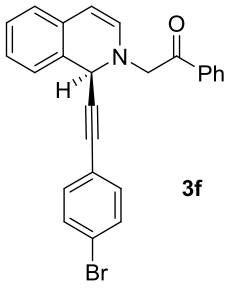
Yellow oil. Yield = 73%. $[\alpha]^{14}_{D}$ = -100.1 (c = 0.77, $CHCl_3$, 91% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.27 – 7.16 (m, 6H), 7.09 (td, *J* = 7.6, 1.2 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.13 (d, *J* = 7.6 Hz, 1H), 5.68 (s, 1H), 5.55 (d, *J* = 7.6 Hz, 1H), 4.92 (d, *J* = 18.0 Hz, 1H), 4.49 (d, *J* = 17.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.26, 136.69, 135.18, 134.34, 133.64, 133.00, 132.00, 128.79, 128.46, 128.10, 127.88, 127.23, 125.82, 125.52, 123.43, 120.91, 100.35, 87.58, 85.18, 58.21, 52.89. HPLC (Daicel Chiralpak IC, i-PrOH/hexane = 2/98, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 27.6 min, t_2 (major) = 30.8 min. HRMS (ESI) calcd for $C_{25}H_{18}ONCl$ m/z $[M + Na]^+$: 406.0969; found: 406.0976.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	27.590	MM	9.394	0.626	353.089	4.693
2	30.798	FM	121.621	0.983	7170.102	95.307



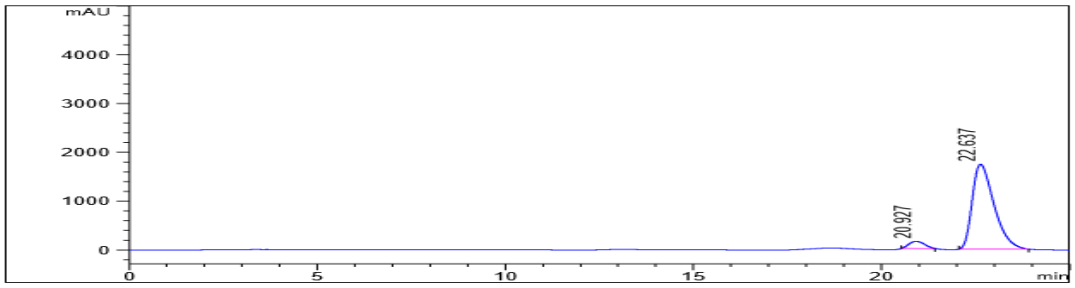
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	26.744	MF	533.408	0.765	24483.457	49.742
2	29.926	FM	438.378	0.940	24737.514	50.258



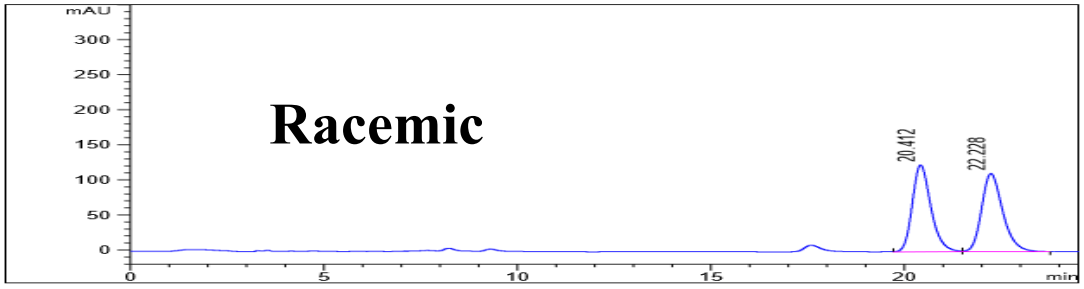
3f

(*S*)-2-(1-((4-bromophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

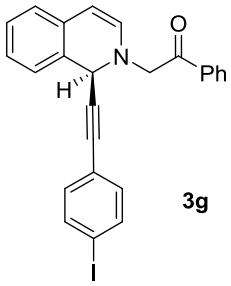
Yellow oil. Yield = 68%. $[\alpha]^{16}_{D}$ = -99.7 (c = 0.67, $CHCl_3$, 88% ee). ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.18 (t, *J* = 8.4 Hz, 3H), 7.09 (td, *J* = 7.6, 1.6 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.14 (d, *J* = 7.6 Hz, 1H), 5.67 (s, 1H), 5.55 (d, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 18.0 Hz, 1H), 4.49 (d, *J* = 17.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.30, 136.66, 135.29, 133.67, 133.24, 132.04, 131.42, 128.83, 128.13, 127.93, 127.26, 125.85, 125.56, 123.48, 122.63, 121.45, 100.44, 87.82, 85.29, 58.26, 52.96. HPLC (Daicel Chiralpak IC, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 20.9 min, t_2 (major) = 22.6 min. HRMS (ESI) calcd for $C_{25}H_{18}ONBr$ m/z $[M + Na]^+$: 450.0464; found: 450.0450.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.927	MM	150.678	0.487	4398.618	5.913
2	22.637	FM	1738.592	0.671	69993.273	94.087



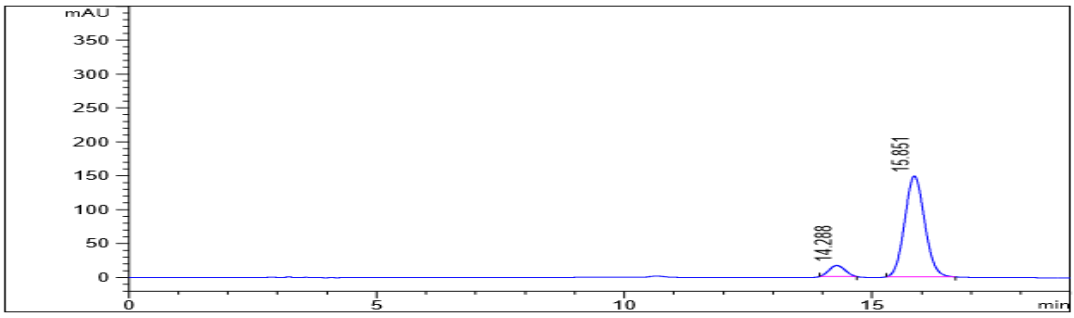
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.412	FM	123.949	0.559	4153.662	49.324
2	22.228	MF	111.723	0.637	4267.511	50.676



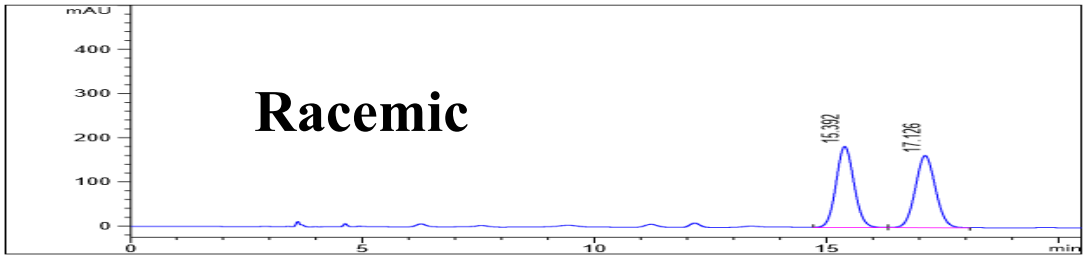
3g

(*S*)-2-(1-((4-iodophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

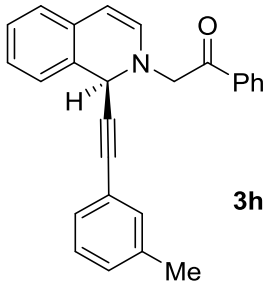
Yellow solid. Yield = 53%. $[\alpha]^{23}_{D}$ = -85.0 (c = 1.1, $CHCl_3$, 84% ee). ^1H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 3H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.18 (td, *J* = 7.8, 2 Hz, 1H), 7.09 (td, *J* = 7.2, 1.2 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 2H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.14 (d, *J* = 7.8 Hz, 1H), 5.67 (s, 1H), 5.55 (d, *J* = 7.8 Hz, 1H), 4.91 (d, *J* = 18.0 Hz, 1H), 4.49 (d, *J* = 18.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.30, 137.33, 136.64, 135.32, 133.65, 133.30, 132.05, 128.82, 128.80, 128.12, 127.93, 127.90, 127.26, 125.84, 125.56, 123.48, 122.03, 100.44, 88.12, 85.44, 58.27, 53.03. HPLC (Daicel Chiralpak IG, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 14.3 min, t_2 (major) = 15.9 min. HRMS (ESI) calcd for $C_{25}H_{18}ONI$ m/z $[M + Na]^+$: 498.0325; found: 498.0330.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	14.288	MF	16.304	0.372	364.256	8.070
2	15.851	FM	148.409	0.466	4149.724	91.930



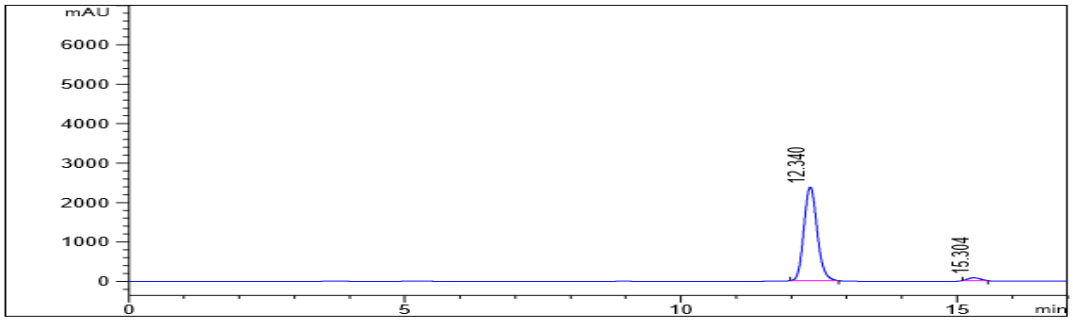
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	15.392	FM	183.927	0.451	4972.913	50.175
2	17.126	MF	163.277	0.504	4938.318	49.825



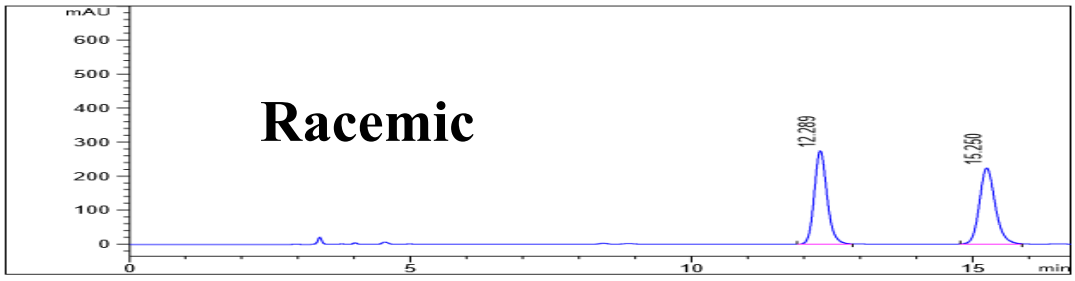
3h

(*S*)-1-phenyl-2-(1-(*m*-tolylethynyl)isoquinolin-2(1*H*)-yl)ethanone

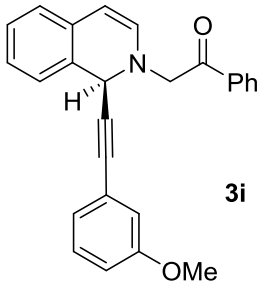
Yellow oil. Yield = 74%. $[\alpha]^{16}_{D}$ = -113.6 (c = 0.875, $CHCl_3$, 95% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.19 – 7.14 (m, 4H), 7.09 (t, *J* = 7.6 Hz, 2H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.15 (d, *J* = 7.6 Hz, 1H), 5.70 (s, 1H), 5.55 (d, *J* = 7.2 Hz, 1H), 4.99 (d, *J* = 18.0 Hz, 1H), 4.48 (d, *J* = 18.8 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.48, 137.84, 136.88, 135.30, 133.58, 132.38, 132.12, 129.25, 128.82, 128.76, 128.05, 127.98, 127.94, 127.54, 125.84, 125.47, 123.31, 122.24, 100.37, 86.74, 86.00, 58.14, 52.97, 21.10. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 12.3 min, t_2 (major) = 15.3 min. HRMS (ESI) calcd for $C_{26}H_{21}ON$ m/z $[M + Na]^+$: 386.1515; found: 386.1528.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	12.340	MF	2372.381	0.279	39752.574	97.334
2	15.304	FM	72.678	0.250	1088.859	2.666



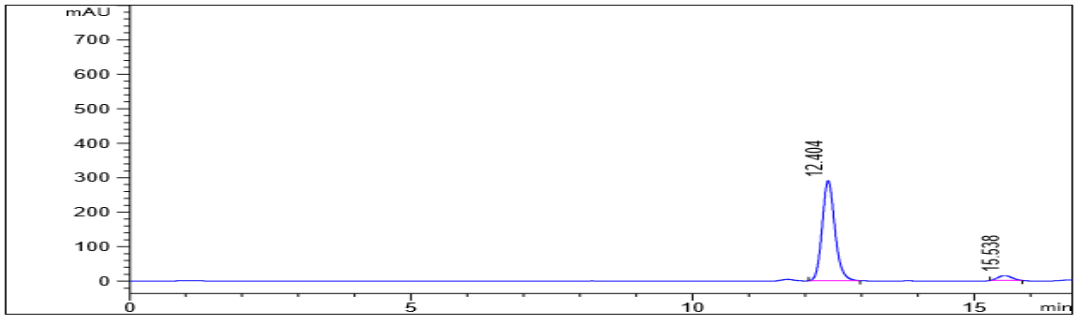
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	12.289	FM	274.895	0.264	4357.085	49.690
2	15.250	MF	224.171	0.328	4411.367	50.310



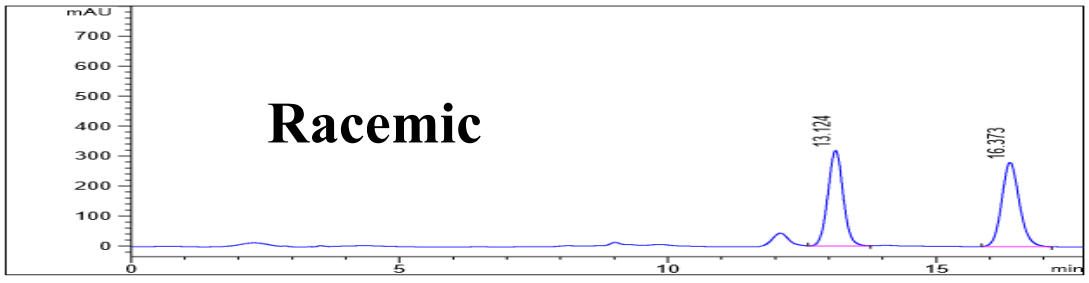
3i

(*S*)-2-(1-((3-methoxyphenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

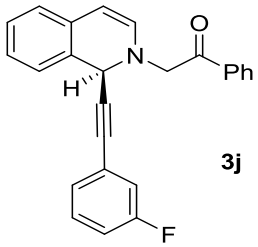
Yellow oil. Yield = 84%. $[\alpha]^{16}_{D}$ = -86.7 (c = 0.75, $CHCl_3$, 90% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.20 – 7.14 (m, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.00 – 6.95 (m, 2H), 6.88 – 6.83 (m, 2H), 6.15 (d, *J* = 7.6 Hz, 1H), 5.71 (s, 1H), 5.57 (d, *J* = 7.2 Hz, 1H), 4.98 (d, *J* = 18.0 Hz, 1H), 4.50 (d, *J* = 17.6 Hz, 1H), 3.74 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.47, 159.20, 136.82, 135.35, 133.61, 132.13, 129.25, 128.81, 128.05, 127.95, 127.48, 125.89, 125.52, 124.38, 123.49, 123.38, 116.57, 115.08, 100.41, 86.43, 86.30, 58.20, 55.24, 53.00. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 12.4 min, t_2 (major) = 15.5 min. HRMS (ESI) calcd for $C_{26}H_{21}O_2N$ m/z $[M + Na]^+$: 402.1465; found: 402.1466.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	12.404	MF	289.693	0.262	4557.270	94.943
2	15.538	FM	14.259	0.284	242.721	5.057



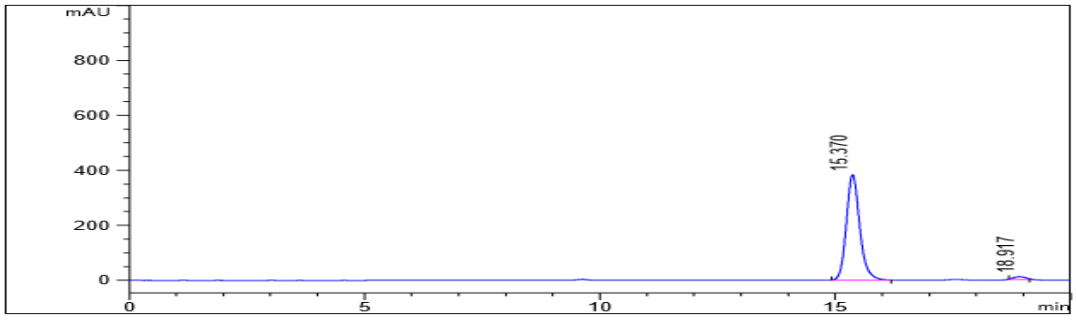
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	13.124	MM	318.551	0.328	6276.138	49.495
2	16.373	MM	280.540	0.380	6404.181	50.505



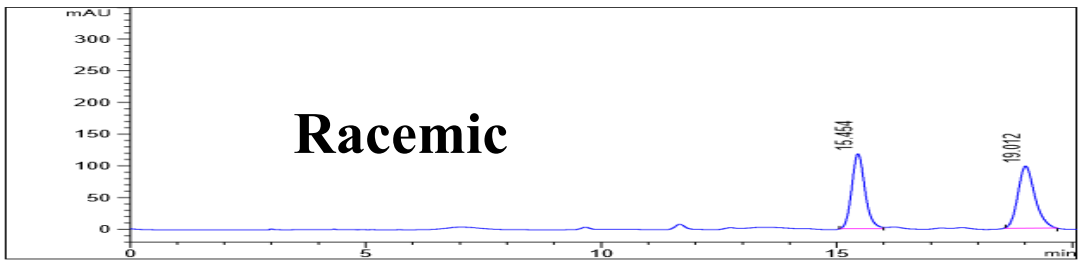
3j

(*S*)-2-(1-((3-fluorophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

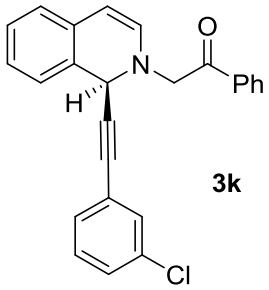
Yellow oil. Yield = 71%. $[\alpha]^{16}_{D}$ = -128.4 (c = 1.2, $CHCl_3$, 96% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.6 Hz, 2H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 5.6 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.20 – 7.15 (m, 2H), 7.09 (d, *J* = 9.6 Hz, 1H), 7.04 (d, *J* = 7.6 Hz, 2H), 6.21 (d, *J* = 7.2 Hz, 1H), 5.75 (s, 1H), 5.62 (d, *J* = 7.2 Hz, 1H), 5.00 (d, *J* = 18.0 Hz, 1H), 4.57 (d, *J* = 18.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.27, 163.39, 160.94, 136.66, 135.24, 133.68, 132.03, 129.78, 129.70, 128.82, 128.14, 127.92, 127.69, 127.67, 127.21, 125.85, 125.57, 124.34, 124.25, 123.48, 118.70, 118.47, 115.83, 115.62, 100.45, 87.59, 85.08, 58.23, 52.90. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 15.4 min, t_2 (major) = 18.9 min. HRMS (ESI) calcd for $C_{25}H_{18}ONF$ m/z $[M + Na]^+$: 390.1265; found: 390.1253.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	15.370	MF	383.123	0.330	7583.152	97.821
2	18.917	MM	9.867	0.285	168.888	2.179



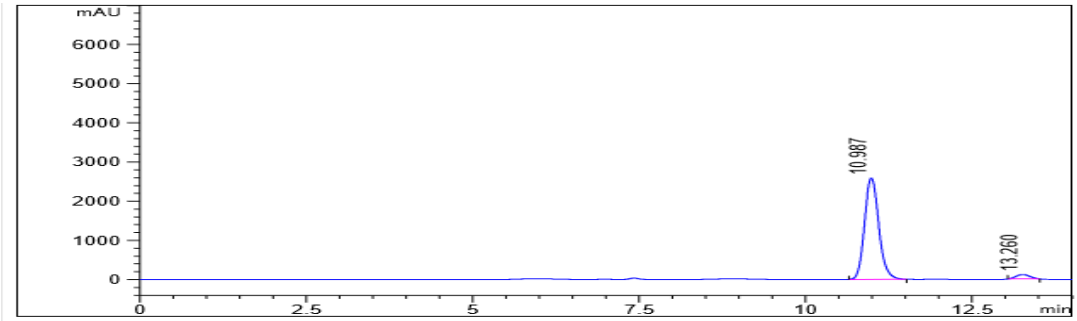
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	15.454	MF	118.064	0.324	2294.926	48.341
2	19.012	FM	98.004	0.417	2452.448	51.659



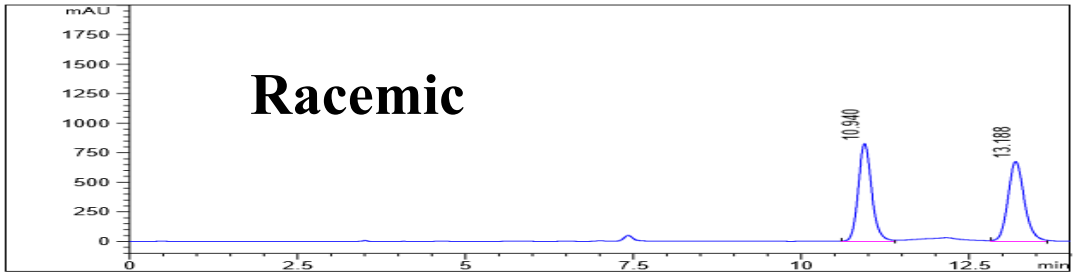
3k

(*S*)-2-(1-((3-chlorophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

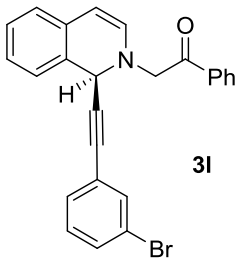
Yellow oil. Yield = 76%. $[\alpha]^{16}_{D}$ = -154.3 (c = 0.98, $CHCl_3$, 92% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.30 (s, 1H), 7.25 – 7.20 (m, 3H), 7.18 – 7.14 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.14 (d, *J* = 7.2 Hz, 1H), 5.68 (s, 1H), 5.56 (d, *J* = 7.6 Hz, 1H), 4.92 (d, *J* = 18.0 Hz, 1H), 4.50 (d, *J* = 18.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.23, 136.65, 135.19, 133.93, 133.68, 132.00, 131.61, 129.88, 129.38, 128.81, 128.61, 128.13, 127.90, 127.16, 125.82, 125.55, 124.14, 123.47, 100.41, 87.89, 84.89, 58.21, 52.88. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 11.0 min, t_2 (major) = 13.3 min. HRMS (ESI) calcd for $C_{25}H_{18}ONCl$ m/z $[M + Na]^+$: 406.0969; found: 406.0975.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	10.987	MF	2586.282	0.248	38537.355	95.951
2	13.260	FM	112.716	0.240	1626.042	4.049



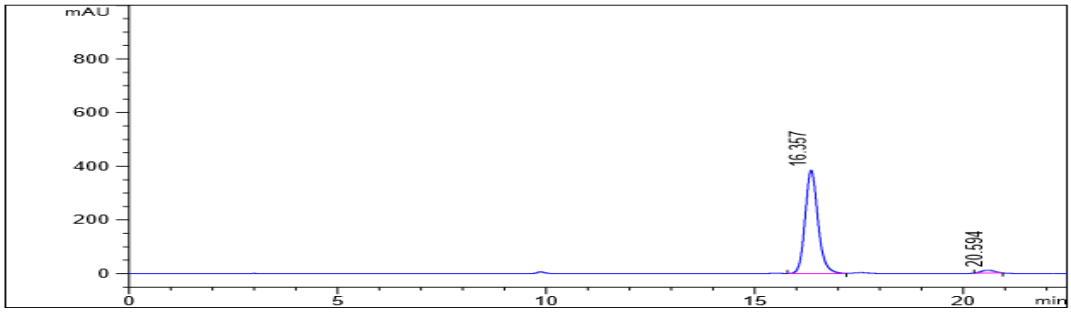
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	10.940	MF	828.841	0.234	11612.335	50.135
2	13.188	MF	677.579	0.284	11549.840	49.865



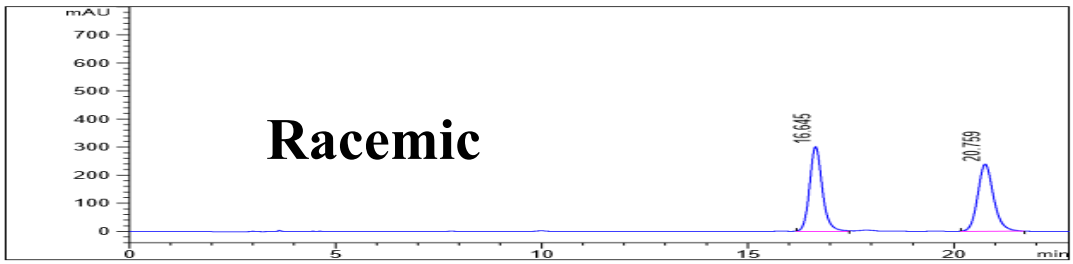
3l

(*S*)-2-(1-((3-bromophenyl)ethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

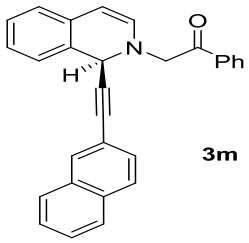
Yellow oil. Yield = 77%. $[\alpha]^{16}_{D}$ = -100.5 (c = 1.5, $CHCl_3$, 95% ee). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 6.8 Hz, 1H), 7.50 – 7.47 (m, 3H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 10.4 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.12 – 7.09 (m, 2H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.14 (d, *J* = 7.6 Hz, 1H), 5.68 (s, 1H), 5.56 (d, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 17.6 Hz, 1H), 4.50 (d, *J* = 17.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.23, 136.63, 135.21, 134.48, 133.69, 131.99, 131.50, 130.32, 129.59, 128.82, 128.14, 127.91, 127.16, 125.83, 125.57, 124.43, 123.49, 121.93, 100.43, 88.02, 84.75, 58.22, 52.89. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 16.4 min, t_2 (major) = 20.6 min. HRMS (ESI) calcd for $C_{25}H_{18}ONBr$ m/z $[M + Na]^+$: 450.0464; found: 450.0461.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.357	MM	385.295	0.358	8276.982	97.260
2	20.594	FM	10.713	0.363	233.207	2.740



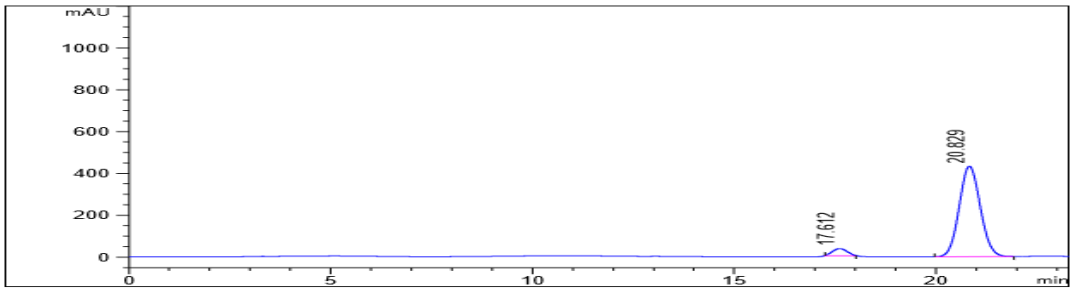
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.645	MF	301.457	0.359	6498.873	50.549
2	20.759	FM	238.769	0.444	6357.735	49.451



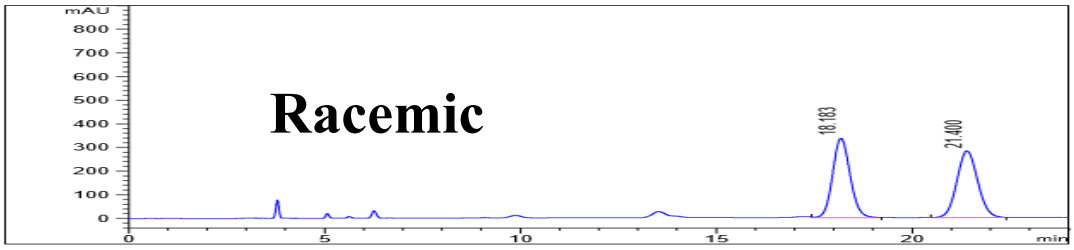
3m

(*S*)-2-(1-(naphthalen-2-ylethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

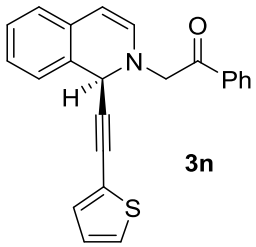
Yellow oil. Yield = 53%. $[\alpha]^{19}_{D}$ = -83.4 (c = 0.885, $CHCl_3$, 90% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.2 Hz, 2H), 7.85 (s, 1H), 7.78 – 7.76 (m, 1H), 7.72 – 7.70 (m, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.48 – 7.45 (m, 4H), 7.39 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.33 (d, *J* = 7.2 Hz, 1H), 7.19 (td, *J* = 7.2, 1.2 Hz, 1H), 7.12 (td, *J* = 7.2, 1.2 Hz, 1H), 6.98 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.18 (d, *J* = 7.8 Hz, 1H), 5.75 (s, 1H), 5.58 (d, *J* = 7.2 Hz, 1H), 5.02 (d, *J* = 17.4 Hz, 1H), 4.52 (d, *J* = 18.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.50, 136.83, 135.42, 133.61, 132.81, 132.17, 131.78, 128.82, 128.46, 128.07, 128.00, 127.83, 127.69, 127.66, 126.69, 126.50, 125.92, 125.56, 123.43, 119.80, 100.46, 86.89, 86.83, 58.28, 53.14. HPLC (Daicel Chiralpak IG, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 17.6 min, t_2 (major) = 20.8 min. HRMS (ESI) calcd for $C_{29}H_{21}ON$ m/z $[M + Na]^+$: 422.1515; found: 422.1509.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.612	MM	34.140	0.413	845.625	5.112
2	20.829	MM	432.228	0.605	15695.371	94.888



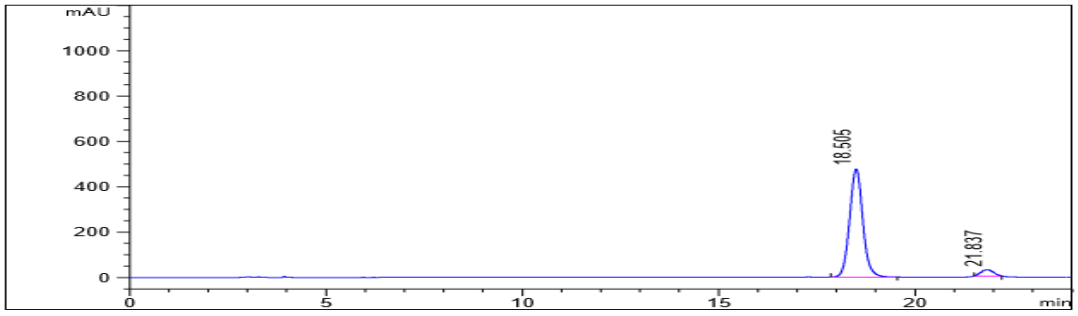
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.183	MF	335.068	0.513	10321.769	50.018
2	21.400	MF	281.318	0.611	10314.382	49.982



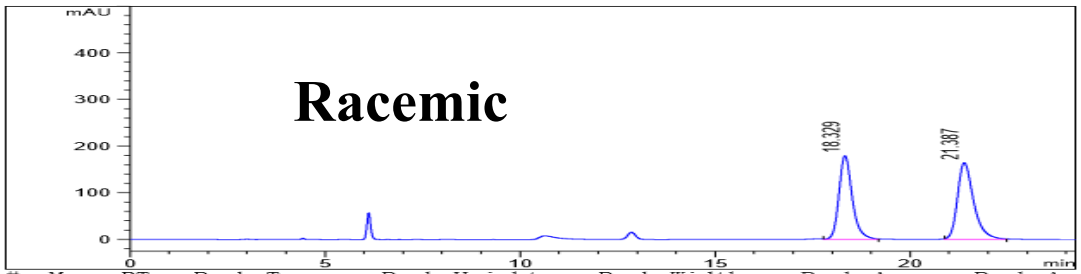
3n

(*S*)-1-phenyl-2-(1-(thiophen-2-ylethynyl)isoquinolin-2(1*H*)-yl)ethanone

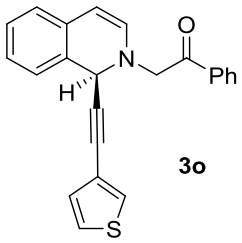
Yellow oil. Yield = 48%. $[\alpha]^{27}_{D}$ = -102.6 (c = 1.285, $CHCl_3$, 90% ee).^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.60 – 7.57 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.24 (d, *J* = 6.6 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.12 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.09 (td, *J* = 7.2, 1.2 Hz, 1H), 6.96 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.92 – 6.90 (m, 1H), 6.13 (d, *J* = 7.8 Hz, 1H), 5.71 (s, 1H), 5.54 (d, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 17.4 Hz, 1H), 4.48 (d, *J* = 17.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.34, 136.65, 135.34, 133.60, 132.38, 132.07, 128.78, 128.10, 127.95, 127.88, 127.21, 126.83, 125.94, 125.55, 123.46, 100.41, 90.56, 79.59, 58.23, 53.19. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 18.5 min, t_2 (major) = 21.8 min. HRMS (ESI) calcd for $C_{23}H_{17}ONS$ m/z $[M + Na]^+$: 378.0923; found: 378.0911.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.505	MM	477.828	0.392	11250.387	94.911
2	21.837	MM	27.608	0.364	603.175	5.089



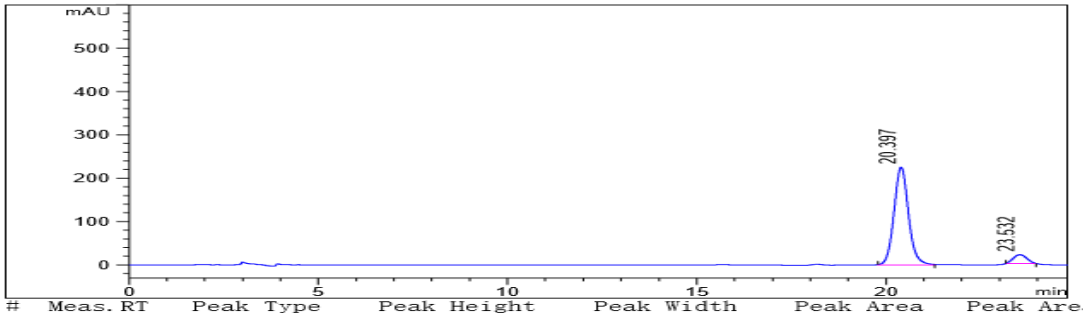
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.329	MF	179.594	0.398	4283.644	47.519
2	21.387	FM	164.340	0.480	4730.865	52.481



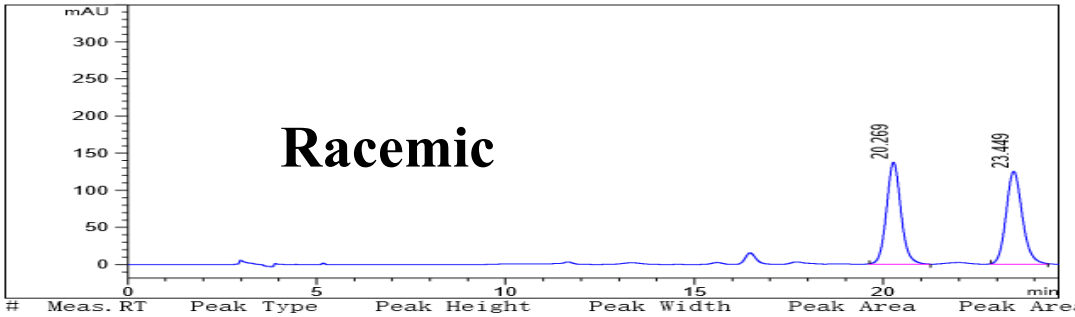
3o

(*S*)-1-phenyl-2-(1-(thiophen-3-ylethynyl)isoquinolin-2(1*H*)-yl)ethanone

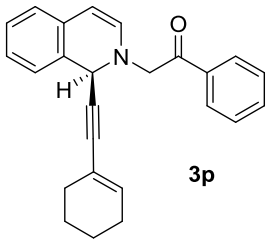
Yellow oil. Yield = 60%. $[\alpha]^{26}_{D}$ = -101.7 (c = 0.813, $CHCl_3$, 84% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 – 7.97 (m, 2H), 7.59 – 7.56 (m, 1H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.34 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.20 – 7.15 (m, 2H), 7.08 (td, *J* = 7.2, 1.2 Hz, 1H), 7.01 (dd, *J* = 5.4, 1.2 Hz, 1H), 6.96 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.13 (d, *J* = 7.8 Hz, 1H), 5.68 (s, 1H), 5.54 (d, *J* = 7.8 Hz, 1H), 4.94 (d, *J* = 17.4 Hz, 1H), 4.48 (d, *J* = 17.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.41, 136.75, 135.36, 133.58, 132.09, 129.94, 129.12, 128.78, 128.02, 127.94, 127.88, 125.89, 125.49, 125.14, 123.38, 100.34, 86.16, 81.55, 58.21, 53.03. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 20.4 min, t_2 (major) = 23.5 min. HRMS (ESI) calcd for $C_{23}H_{17}ONS$ m/z $[M + Na]^+$: 378.0923; found: 378.0905.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.397	MF	225.382	0.442	5972.778	92.178
2	23.532	MM	20.417	0.414	506.809	7.822



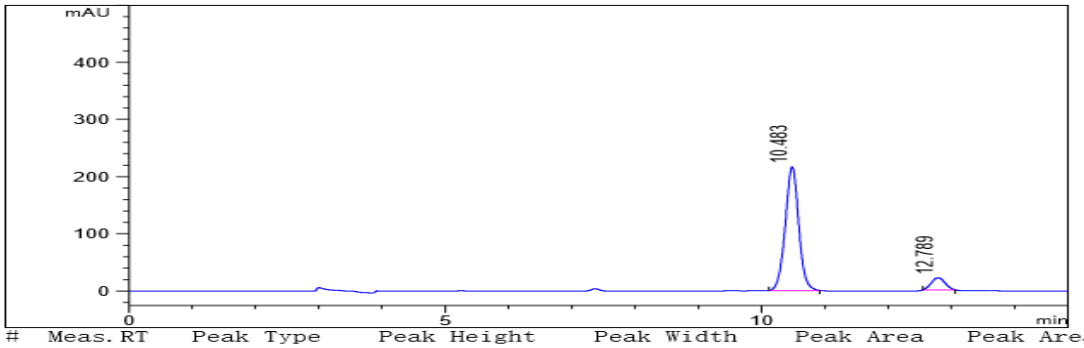
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.269	FM	137.194	0.444	3655.200	49.432
2	23.449	FM	125.108	0.498	3739.167	50.568



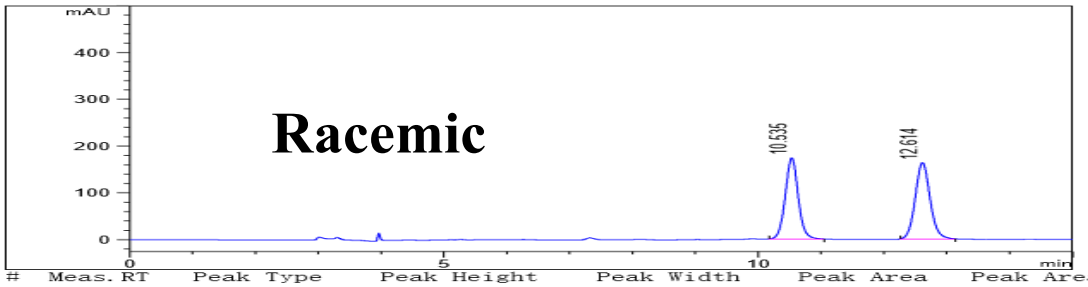
3p

(*S*)-2-(1-(cyclohex-1-en-1-ylethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

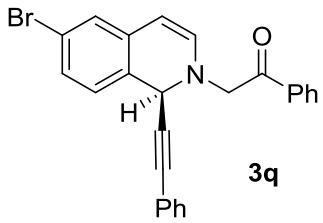
Yellow oil. Yield = 57%. $[\alpha]^{27}_{D}$ = -55.6 (c = 1.219, $CHCl_3$, 82% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.2 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.15 (t, *J* = 7.2 Hz, 1H), 7.07 (t, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 7.2 Hz, 1H), 6.12 (d, *J* = 7.2 Hz, 1H), 6.04 – 6.03 (m, 1H), 5.58 (s, 1H), 5.51 (d, *J* = 7.8 Hz, 1H), 4.92 (d, *J* = 17.4 Hz, 1H), 4.43 (d, *J* = 18.0 Hz, 1H), 2.05 – 2.02 (m, 4H), 1.60 – 1.57 (m, 2H), 1.54 – 1.51 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.66, 136.93, 135.48, 135.40, 133.52, 132.18, 128.75, 127.98, 127.90, 127.84, 125.78, 125.39, 123.20, 120.08, 100.33, 88.67, 83.47, 58.08, 53.01, 29.12, 25.55, 22.18, 21.39. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 10.5 min, t_2 (major) = 12.8 min. HRMS (ESI) calcd for $C_{25}H_{23}ON$ m/z [M + Na]$^+$: 376.1672; found: 376.1660.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	10.483	MF	216.491	0.247	3212.319	91.153
2	12.789	MM	21.151	0.246	311.791	8.847



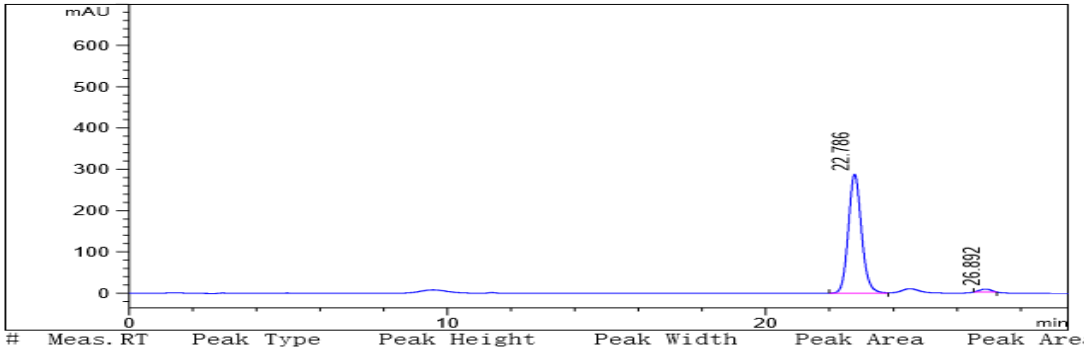
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	10.535	MF	173.501	0.238	2475.802	48.141
2	12.614	FM	163.055	0.273	2666.991	51.859



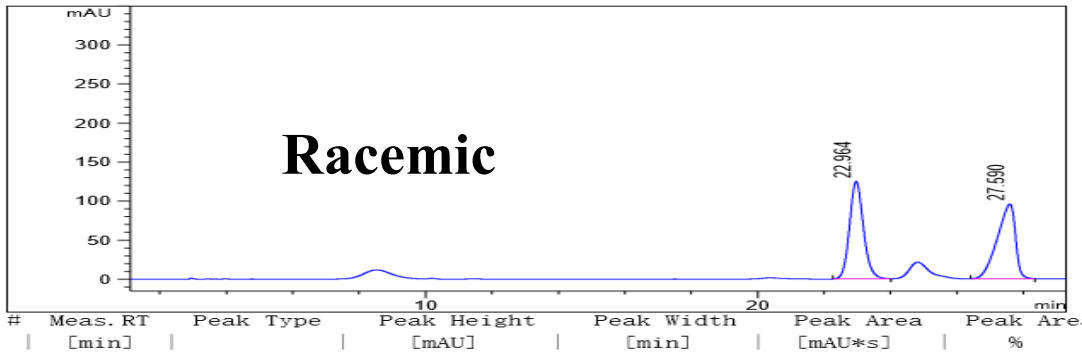
3q

(*S*)-2-(6-bromo-1-(phenylethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

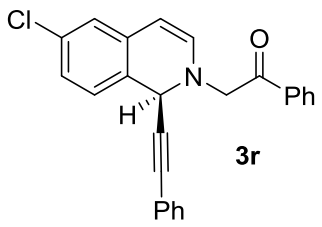
Yellow oil. Yield = 84%. $[\alpha]^{16}_{D}$ = -103.4 (c = 1.23, $CHCl_3$, 96% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 6.6 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.18 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 7.08 (s, 1H), 6.16 (d, *J* = 7.8 Hz, 1H), 5.66 (s, 1H), 5.44 (d, *J* = 7.8 Hz, 1H), 4.98 (d, *J* = 17.4 Hz, 1H), 4.48 (d, *J* = 18.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.13, 138.07, 135.13, 134.35, 133.69, 131.77, 128.81, 128.54, 128.20, 127.93, 127.86, 127.45, 126.08, 125.78, 122.17, 121.98, 98.85, 86.79, 85.86, 58.06, 52.55. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 22.8 min, t_2 (major) = 26.9 min. HRMS (ESI) calcd for $C_{25}H_{18}ONBr$ m/z $[M + Na]^+$: 450.0464; found: 450.0442.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	22.786	MM	288.159	0.481	8309.366	97.840
2	26.892	MM	7.315	0.418	183.458	2.160



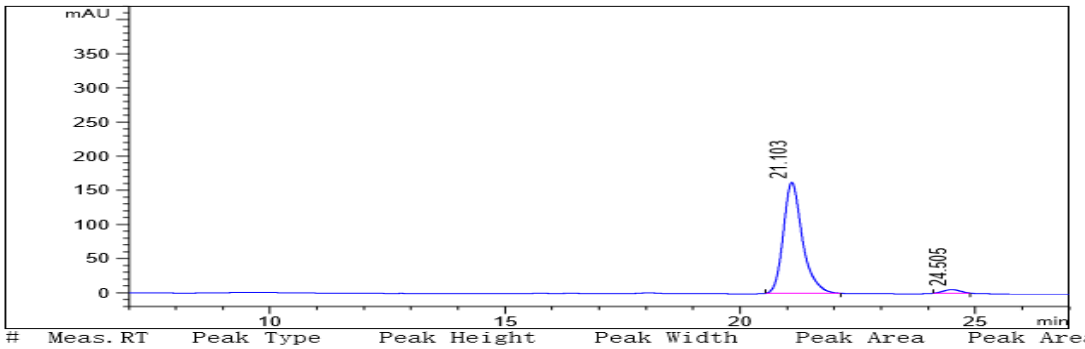
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	22.964	MF	124.890	0.488	3654.131	50.131
2	27.590	FM	95.562	0.634	3635.035	49.869



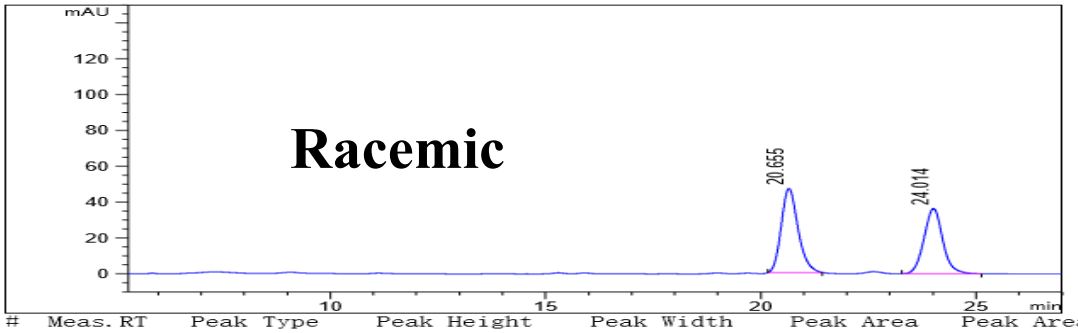
3r

(*S*)-2-(6-chloro-1-(phenylethynyl)isoquinolin-2(1*H*)-yl)-1-phenylethanone

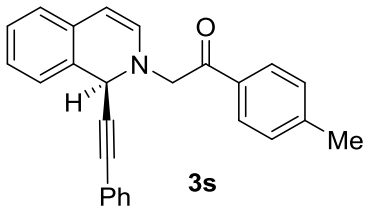
Yellow oil. Yield = 44%. $[\alpha]^{16}_{D}$ = -74.4 (c = 0.54, $CHCl_3$, 95% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 7.8 Hz, 2H), 7.28 – 7.24 (m, 3H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.03 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.93 (s, 1H), 6.17 (d, *J* = 7.8 Hz, 1H), 5.68 (s, 1H), 5.45 (d, *J* = 7.2 Hz, 1H), 4.98 (d, *J* = 17.4 Hz, 1H), 4.49 (d, *J* = 18 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.16, 138.05, 135.16, 134.00, 133.75, 133.70, 131.78, 128.81, 128.54, 128.20, 127.88, 127.15, 125.62, 125.03, 122.91, 122.20, 99.02, 86.78, 85.95, 58.07, 52.53. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 21.1 min, t_2 (major) = 24.5 min. HRMS (ESI) calcd for $C_{25}H_{18}ONCl$ m/z $[M + Na]^+$: 406.0969; found: 406.0987.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	21.103	MF	162.499	0.472	4606.290	97.337
2	24.505	FM	5.144	0.408	126.018	2.663



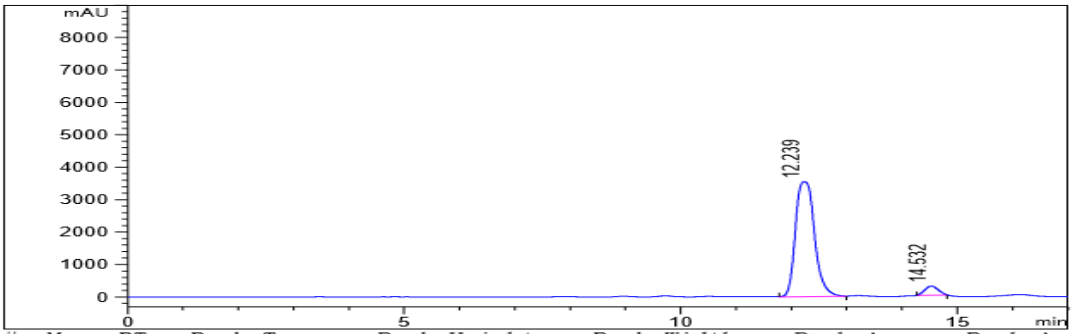
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.655	MM	46.936	0.454	1277.266	53.597
2	24.014	MM	36.375	0.507	1105.829	46.403



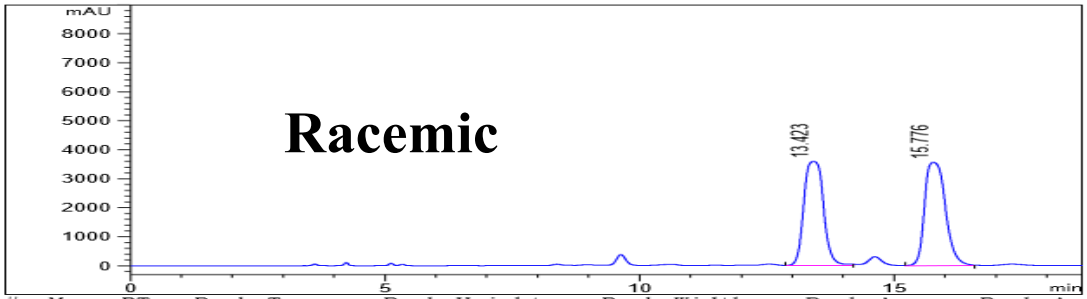
3s

(*S*)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)-1-(*p*-tolyl)ethanone

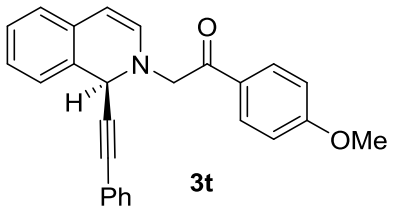
Yellow oil. Yield = 85%. $[\alpha]^{27}_{D}$ = -82.2 (c = 1.0, $CHCl_3$, 90% ee). ^{1}H NMR (600 MHz, CDCl3) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.36 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.27 – 7.24 (m, 6H), 7.17 (td, *J* = 7.8, 1.2 Hz, 1H), 7.09 (td, *J* = 7.8, 1.2 Hz, 1H), 6.96 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.14 (d, *J* = 7.2 Hz, 1H), 5.70 (s, 1H), 5.54 (d, *J* = 7.8 Hz, 1H), 4.95 (d, *J* = 17.4 Hz, 1H), 4.46 (d, *J* = 18 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.12, 144.54, 136.95, 132.93, 132.22, 131.86, 129.50, 128.39, 128.20, 128.11, 128.05, 127.59, 125.92, 125.50, 123.38, 122.60, 100.34, 86.60, 86.51, 58.13, 53.07, 21.74. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 12.2 min, t_2 (major) = 14.5 min. HRMS (ESI) calcd for $C_{26}H_{21}ON$ m/z $[M + Na]^+$: 386.1515; found: 386.1524.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	12.239	MF	3548.173	0.398	84796.898	94.763
2	14.532	FM	278.947	0.280	4686.304	5.237



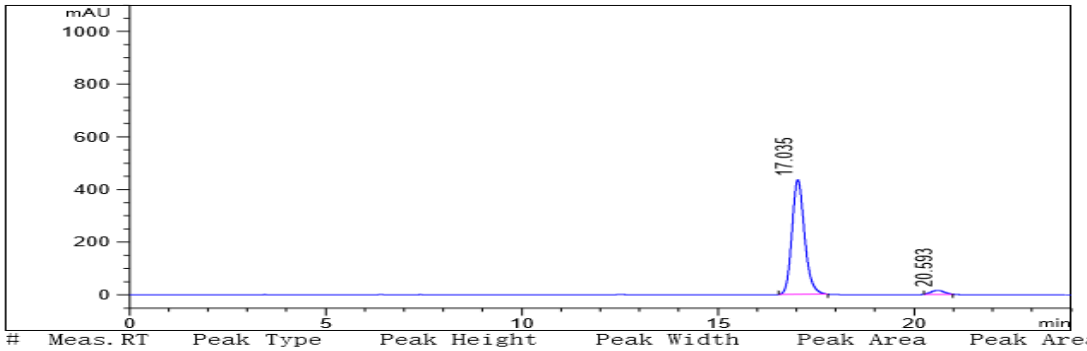
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	13.423	MF	3587.928	0.446	96059.336	48.700
2	15.776	MM	3564.105	0.473	101186.695	51.300



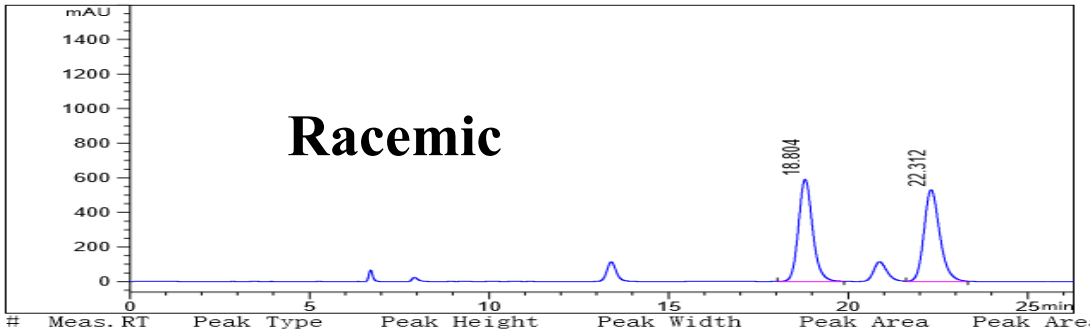
3t

(*S*)-1-(4-methoxyphenyl)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

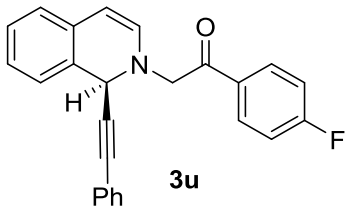
Yellow oil. Yield = 80%. $[\alpha]^{15}_{D}$ = -59.2 (c = 0.71, $CHCl_3$, 93% ee).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.8, 2H), 7.37 – 7.35 (m, 2H), 7.29 – 7.23 (m, 4H), 7.17 (td *J* = 6.8, 1.6 Hz, 1H), 7.08 (td, *J* = 7.6, 1.6 Hz, 1H), 6.97 – 6.91 (m, 3H), 6.15 (d, *J* = 7.6 Hz, 1H), 5.70 (s, 1H), 5.54 (d, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 17.6 Hz, 1H), 4.44 (d, *J* = 17.6 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.91, 163.81, 136.95, 132.18, 131.80, 130.26, 128.34, 128.15, 127.98, 127.52, 125.86, 125.42, 123.30, 122.54, 113.93, 100.23, 86.56, 86.42, 57.86, 55.46, 53.01. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 17.3 min, t_2 (major) = 20.6 min. HRMS (ESI) calcd for $C_{26}H_{21}O_2N$ m/z $[M + Na]^+$: 402.1465; found: 402.1476.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.035	MM	435.258	0.373	9737.745	96.351
2	20.593	MM	15.611	0.394	368.832	3.649



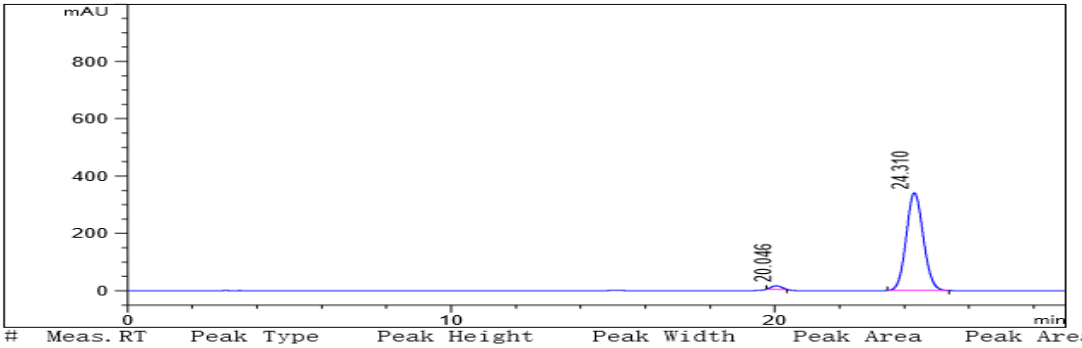
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.804	FM	591.210	0.456	16188.455	49.803
2	22.312	MF	531.636	0.512	16316.716	50.197



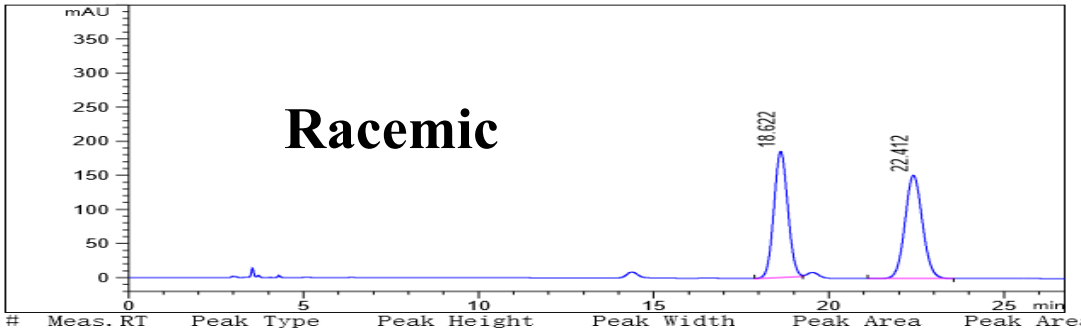
3u

(*S*)-1-(4-fluorophenyl)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

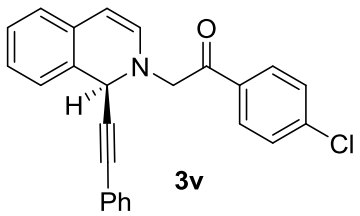
Yellow oil. Yield = 80%. $[\alpha]^{22}_{D}$ = -100.3 (c = 1.3, $CHCl_3$, 96% ee).^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 – 8.00 (m, 2H), 7.35 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.29 – 7.25 (m, 4H), 7.17 (td, *J* = 7.8, 1.8 Hz, 1H), 7.14 – 7.08 (m, 3H), 6.96 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.13 (d, *J* = 7.2 Hz, 1H), 5.67 (s, 1H), 5.56 (d, *J* = 7.8 Hz, 1H), 4.91 (d, *J* = 18.0 Hz, 1H), 4.45 (d, *J* = 17.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 193.97, 166.80, 165.11, 136.65, 132.05, 131.78, 130.71, 130.64, 128.44, 128.20, 128.07, 127.51, 125.85, 125.58, 123.41, 122.43, 116.01, 115.87, 100.64, 86.64, 86.38, 58.16, 53.06. HPLC (Daicel Chiralpak IG, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 20.0 min, t_2 (major) = 24.3 min. HRMS (ESI) calcd for $C_{25}H_{18}ONF$ m/z $[M + Na]^+$: 390.1265; found: 390.1280.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	20.046	MM	12.302	0.363	268.260	2.099
2	24.310	MM	340.850	0.612	12510.547	97.901



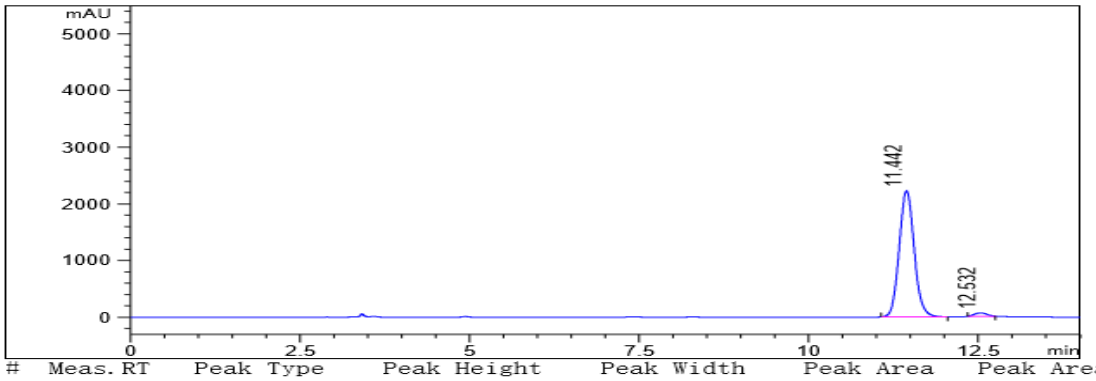
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.622	MM	184.852	0.461	5117.918	49.384
2	22.412	MF	151.340	0.578	5245.544	50.616



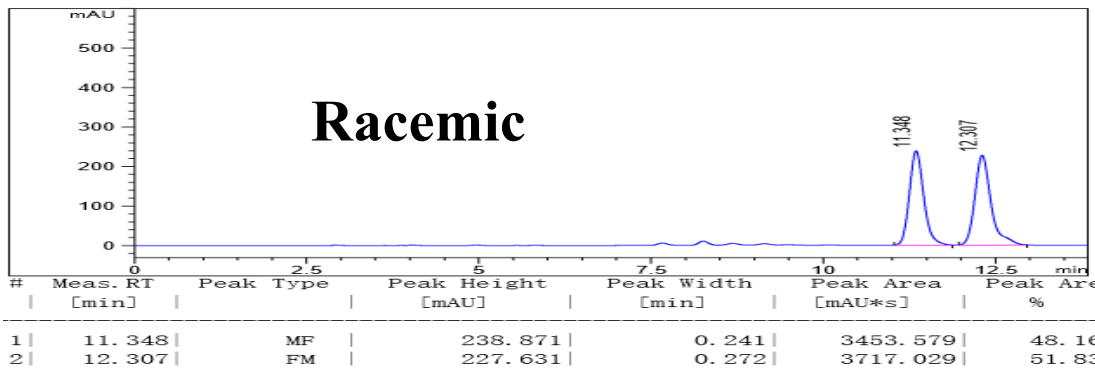
3v

(*S*)-1-(4-chlorophenyl)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

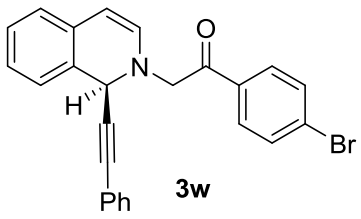
Yellow oil. Yield = 42%. $[\alpha]^{15}_{D}$ = -53.8 (c = 0.595, $CHCl_3$, 96% ee).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.36 – 7.34 (m, 2H), 7.29 – 7.24 (m, 4H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.12 (d, *J* = 7.2 Hz, 1H), 5.66 (s, 1H), 5.56 (d, *J* = 7.6 Hz, 1H), 4.90 (d, *J* = 17.6 Hz, 1H), 4.45 (d, *J* = 17.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.41, 140.05, 136.61, 133.52, 131.98, 131.77, 129.37, 129.09, 128.46, 128.20, 128.08, 127.44, 125.84, 125.59, 123.41, 122.34, 100.69, 86.63, 86.29, 58.19, 52.97. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 11.4 min, t_2 (major) = 12.5 min. HRMS (ESI) calcd for $C_{25}H_{18}ONCl$ m/z $[M + Na]^+$: 406.0969; found: 406.0979.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	11.442	MM	2224.301	0.257	34297.633	97.781
2	12.532	MM	59.620	0.218	778.202	2.219



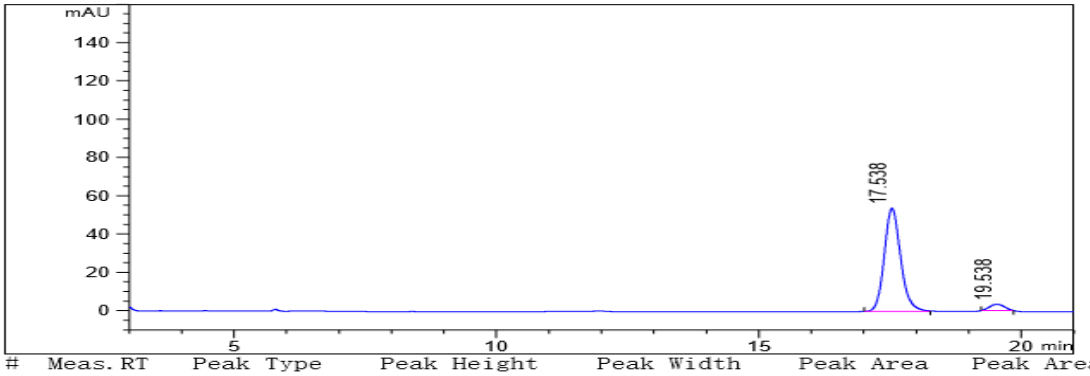
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	11.348	MF	238.871	0.241	3453.579	48.163
2	12.307	FM	227.631	0.272	3717.029	51.837



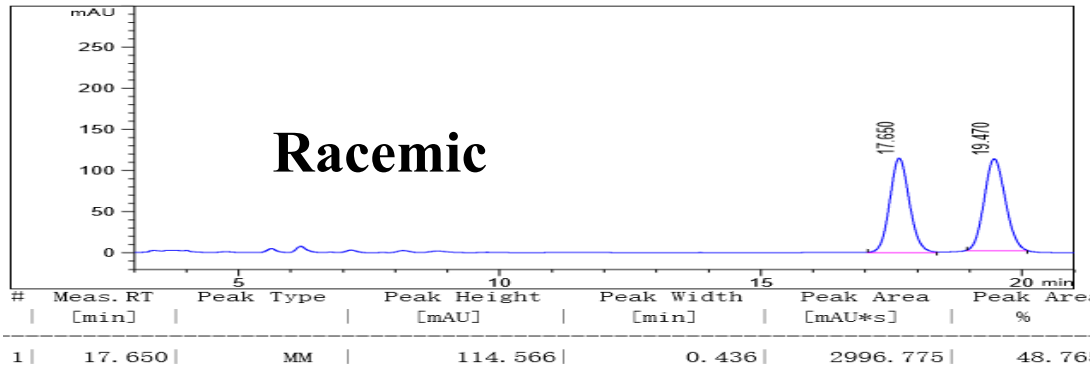
3w

(*S*)-1-(4-bromophenyl)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

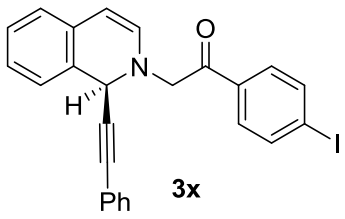
Yellow oil. Yield = 64%. $[\alpha]^{27}_{D}$ = -49.4 (c = 0.888, $CHCl_3$, 90% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 7.2 Hz, 2H), 7.28 – 7.24 (m, 4H), 7.17 (t, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 7.8 Hz, 1H), 6.12 (d, *J* = 7.8 Hz, 1H), 5.66 (s, 1H), 5.55 (d, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 17.4 Hz, 1H), 4.44 (d, *J* = 18 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 194.70, 136.60, 134.09, 132.15, 132.06, 131.83, 129.53, 128.86, 128.51, 128.25, 128.13, 127.55, 125.89, 125.66, 123.48, 122.45, 100.80, 86.76, 86.38, 58.27, 53.11. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 17.5 min, t_2 (major) = 19.5 min. HRMS (ESI) calcd for $C_{25}H_{18}ONBr$ m/z $[M + Na]^+$: 450.0464; found: 450.0454.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.538	MF	53.990	0.363	1176.575	94.764
2	19.538	MM	3.306	0.328	65.009	5.236



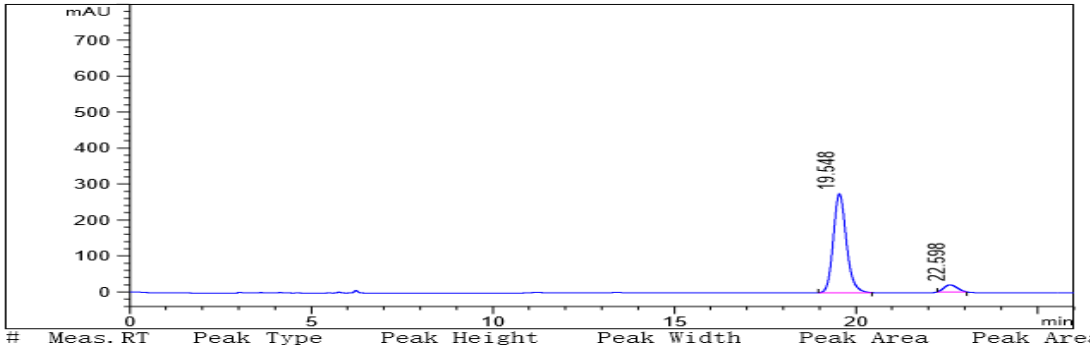
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.650	MM	114.566	0.436	2996.775	48.765
2	19.470	MM	111.571	0.470	3148.562	51.235



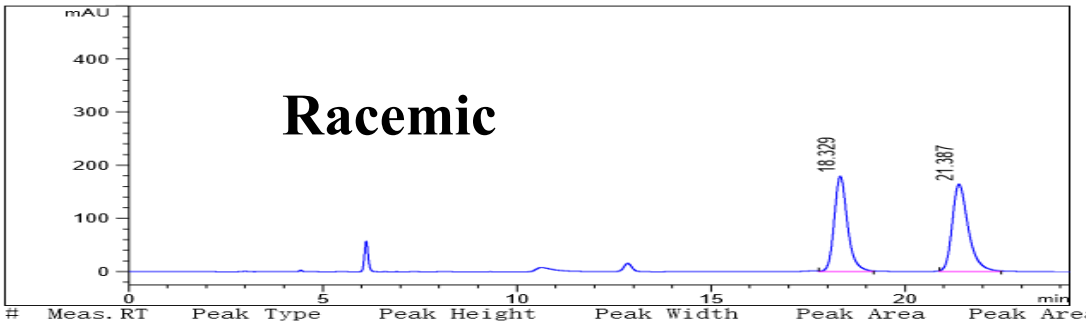
3x

(*S*)-1-(4-iodophenyl)-2-(1-(phenylethynyl)isoquinolin-2(1*H*)-yl)ethanone

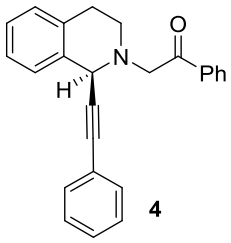
Yellow solid. Yield = 27%. $[\alpha]^{28}_{D}$ = -74.6 (c = 0.5, $CHCl_3$, 87% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.34 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.29 – 7.24 (m, 4H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.10 (td, *J* = 7.8, 1.2 Hz, 1H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.12 (d, *J* = 7.8 Hz, 1H), 5.65 (s, 1H), 5.55 (d, *J* = 7.2 Hz, 1H), 4.88 (d, *J* = 18 Hz, 1H), 4.44 (d, *J* = 17.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 195.02, 138.14, 136.58, 134.62, 132.05, 131.83, 129.35, 128.50, 128.25, 128.12, 127.55, 125.88, 125.65, 123.47, 122.44, 101.67, 100.80, 86.76, 86.37, 58.21, 53.10. HPLC (Daicel Chiralpak IG, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 19.5 min, t_2 (major) = 22.6 min. HRMS (ESI) calcd for $C_{25}H_{18}ONI$ m/z $[M + Na]^+$: 498.0325; found: 498.0325.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	19.548	MM	274.932	0.419	6907.184	93.292
2	22.598	MM	19.882	0.416	496.633	6.708



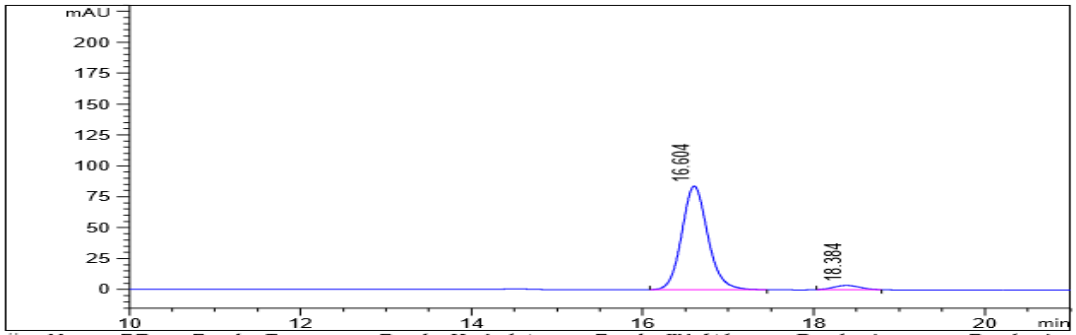
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	18.329	MF	179.594	0.398	4283.644	47.519
2	21.387	FM	164.340	0.480	4730.865	52.481



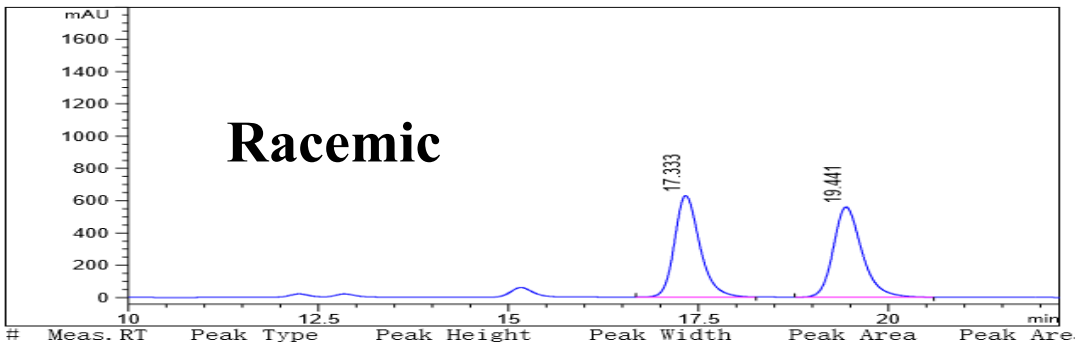
4

(*S*)-1-phenyl-2-(1-(phenylethynyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)ethan-1-one

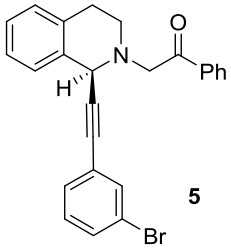
Yellow oil. Two step yield = 46%. $[\alpha]^{28}_{D}$ = +51.2 (c = 0.965, $CHCl_3$, 92% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.8 Hz, 2H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.41 – 7.39 (m, 2H), 7.34 – 7.33 (m, 1H), 7.26 – 7.24 (m, 3H), 7.18 – 7.16 (m, 2H), 7.12 – 7.10 (m, 1H), 5.13 (s, 1H), 4.26 (d, *J* = 16.8 Hz, 1H), 4.22 (d, *J* = 16.8 Hz, 1H), 3.18 – 3.12 (m, 1H), 3.09 –3.04 (m, 1H), 2.94 – 2.90 (m, 1H), 2.85 – 2.81 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.81, 136.20, 135.00, 133.72, 133.27, 131.82, 129.00, 128.61, 128.37, 128.27, 127.79, 127.08, 125.97, 122.94, 87.28, 86.97, 61.64, 55.22, 46.85, 28.91. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 16.6 min, t_2 (major) = 18.4 min. HRMS (ESI) calcd for $C_{25}H_{21}ON$ m/z $[M + Na]^+$: 374.1515; found: 374.1532.



#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	16.604	MF	83.830	0.353	1774.320	95.904
2	18.384	FM	3.497	0.361	75.785	4.096



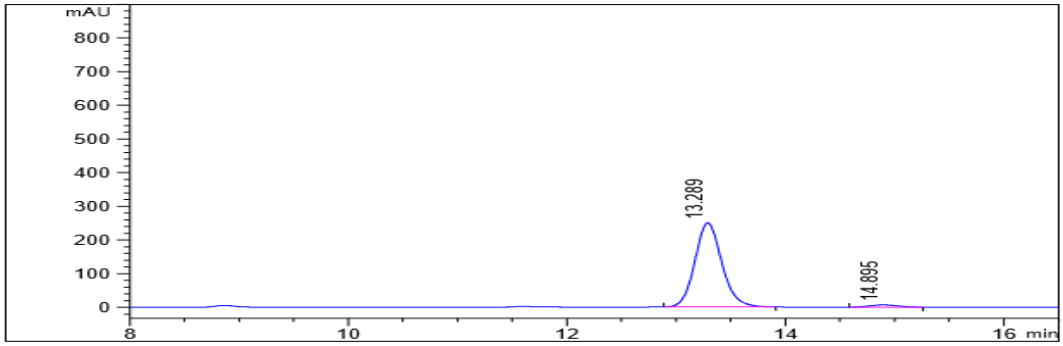
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	17.333	FM	629.904	0.387	14641.958	49.991
2	19.441	MF	558.666	0.437	14647.081	50.009



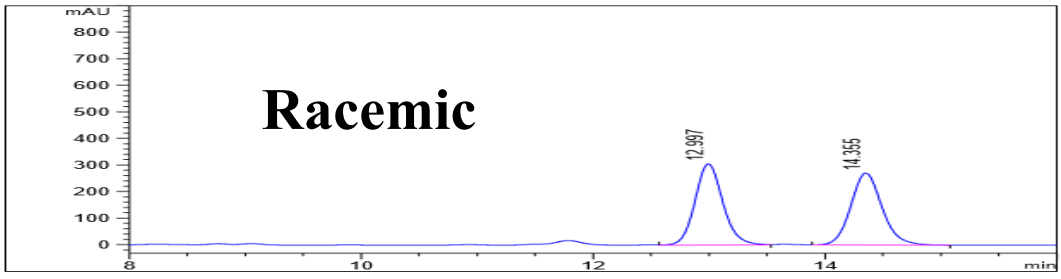
5

(*S*)-2-(1-((3-bromophenyl)ethynyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)-1-phenylethan-1-one

Yellow oil. Two step yield = 49%. $[\alpha]^{28}_{D}$ = +74.8 (c = 0.5, $CHCl_3$, 95% ee). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.2 Hz, 2H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 6.6 Hz, 2H), 7.19 – 7.16 (m, 2H), 7.11 (t, *J* = 8.4 Hz, 2H), 5.13 (s, 1H), 4.25 (d, *J* = 16.8 Hz, 1H), 4.18 (d, *J* = 16.2 Hz, 1H), 3.16 – 3.12 (m, 1H), 3.10 – 3.05 (m, 1H), 2.96 – 2,92 (m, 1H), 2.84 –2.80 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.61, 136.12, 134.62, 134.53, 133.71, 133.33, 131.42, 130.36, 129.71, 129.05, 128.63, 128.32, 127.70, 127.20, 126.02, 124.89, 122.07, 88.77, 85.50, 61.57, 55.04, 46.84, 28.85. HPLC (Daicel Chiralpak IA, i-PrOH/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm): t_1 (minor) = 13.3 min, t_2 (major) = 14.9 min. HRMS (ESI) calcd for $C_{25}H_{20}ONBr$ m/z $[M + Na]^+$: 452.0620; found: 452.0630.



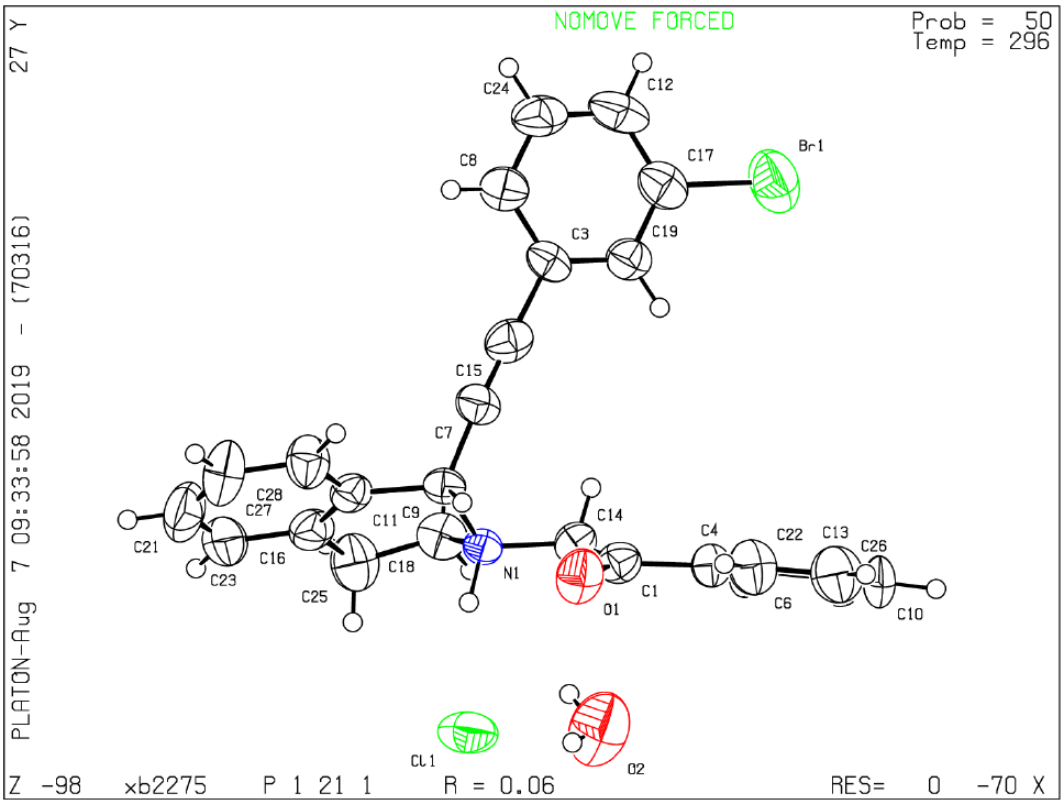
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	13.289	MF	249.520	0.286	4278.408	97.259
2	14.895	MM	6.736	0.298	120.565	2.741



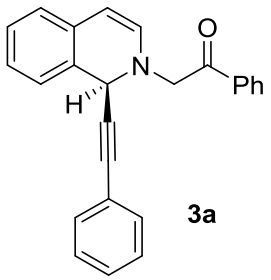
#	Meas. RT [min]	Peak Type	Peak Height [mAU]	Peak Width [min]	Peak Area [mAU*s]	Peak Area %
1	12.997	MM	305.849	0.279	5117.547	50.251
2	14.355	MF	270.826	0.312	5066.436	49.749

6. **X-Ray data of 5·HCl**

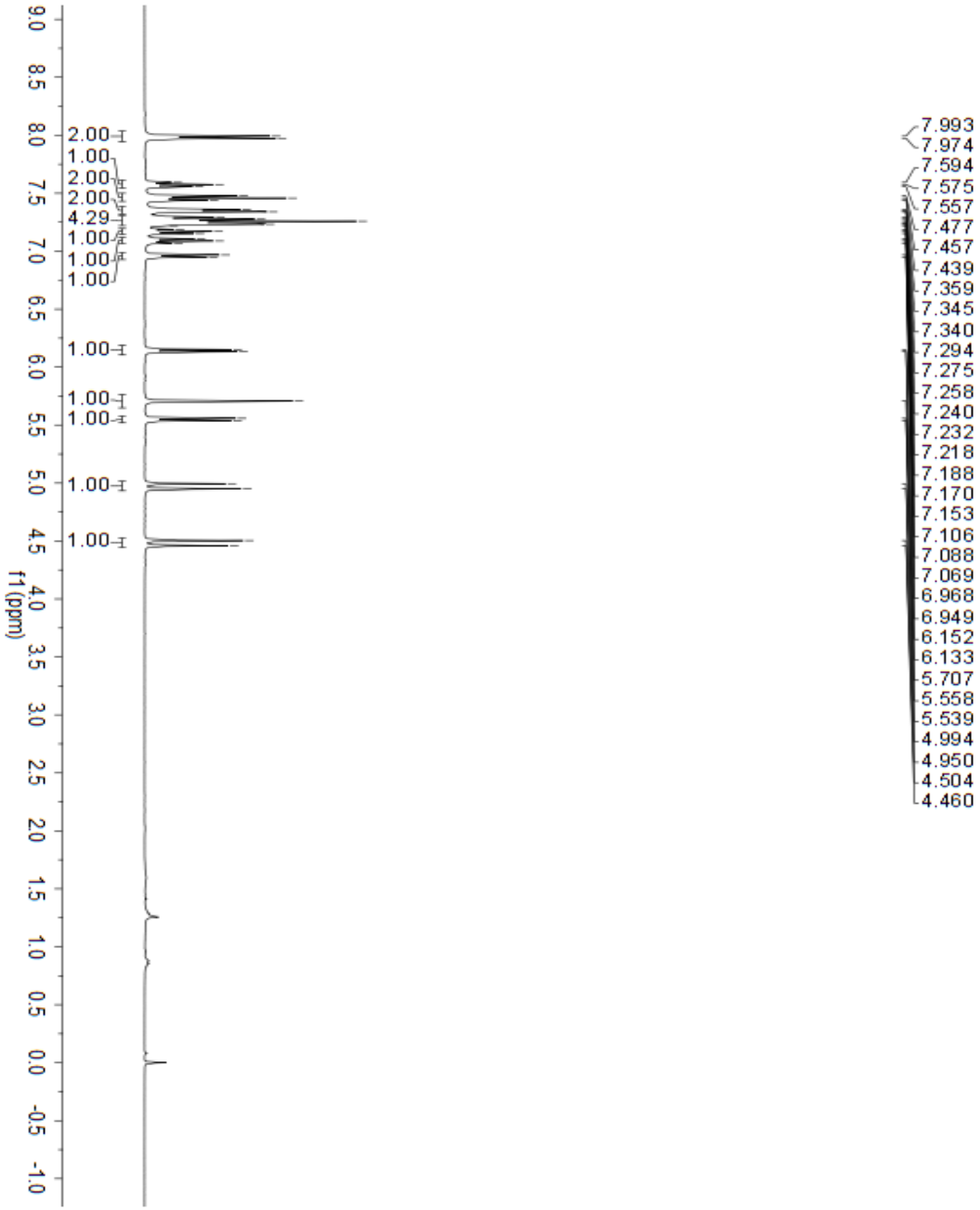
Crystal data and structure refinement for C:.		
Identification code	xb2275	
Empirical formula	C25 H23 Br Cl N O2	
Formula weight	484.80	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 12.376(3) Å	α= 90°.
	b = 5.3988(14) Å	β= 93.647(5)°.
	c = 16.964(4) Å	γ = 90°.
Volume	1131.1(5) $Å^3$	
Z	2	
Density (calculated)	1.423 Mg/m^3	
Absorption coefficient	1.956 mm^{-1}	
F(000)	496	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.978 to 24.999°.	
Index ranges	-14<=h<=14, -6<=k<=6, -11<=l<=20	
Reflections collected	5621	
Independent reflections	3557 [R(int) = 0.0555]	
Completeness to theta = 24.999°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.5849	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3557 / 37 / 271	
Goodness-of-fit on F^2	0.941	
Final R indices [I>2sigma(I)]	R1 = 0.0558, wR2 = 0.1231	
R indices (all data)	R1 = 0.1125, wR2 = 0.1506	
Absolute structure parameter	0.028(17)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.325 and -0.362 $e.Å^{-3}$	

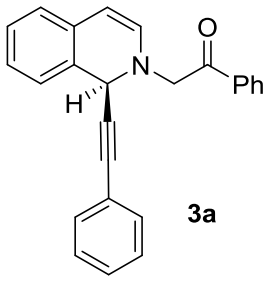

NOMOVE FORCED
Prob = 50
Temp = 296
27 Y
PLATON-Aug 7 09:33:58 2019 - (70316)
C24
C12
C8
C17
Br1
C3
C19
C15
C7
C28
C27
C11
C9
C14
C4
C22
C13
C26
C21
C16
C18
N1
C1
C6
C10
C23
C25
O1
CL1
O2
Z -98 xb2275 P 1 21 1 R = 0.06 RES= 0 -70 X

7. Copies of NMR Spectra.

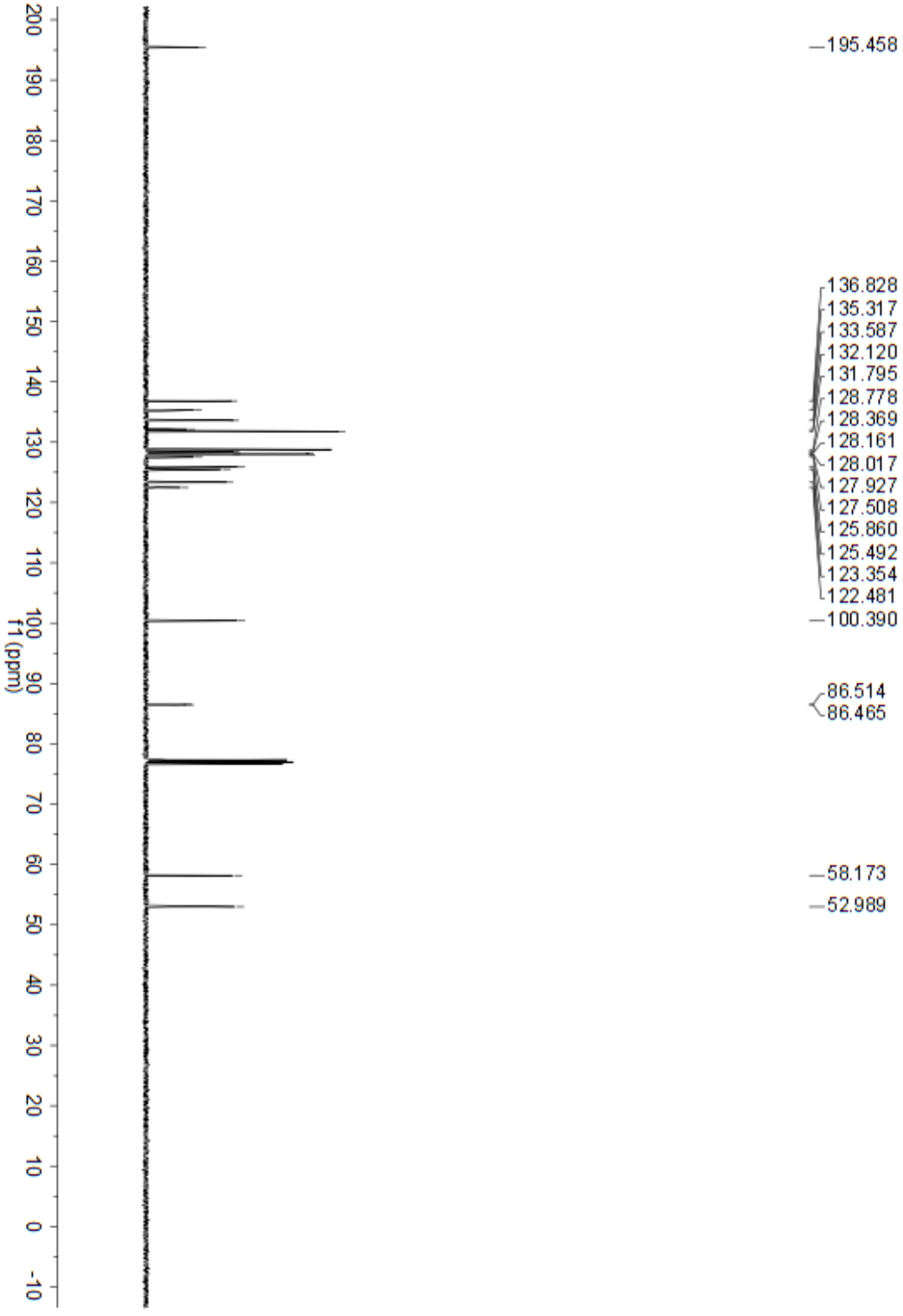


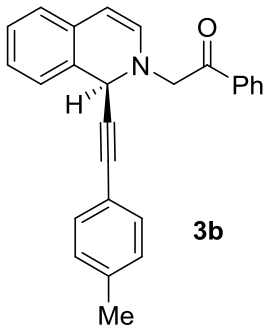
3a



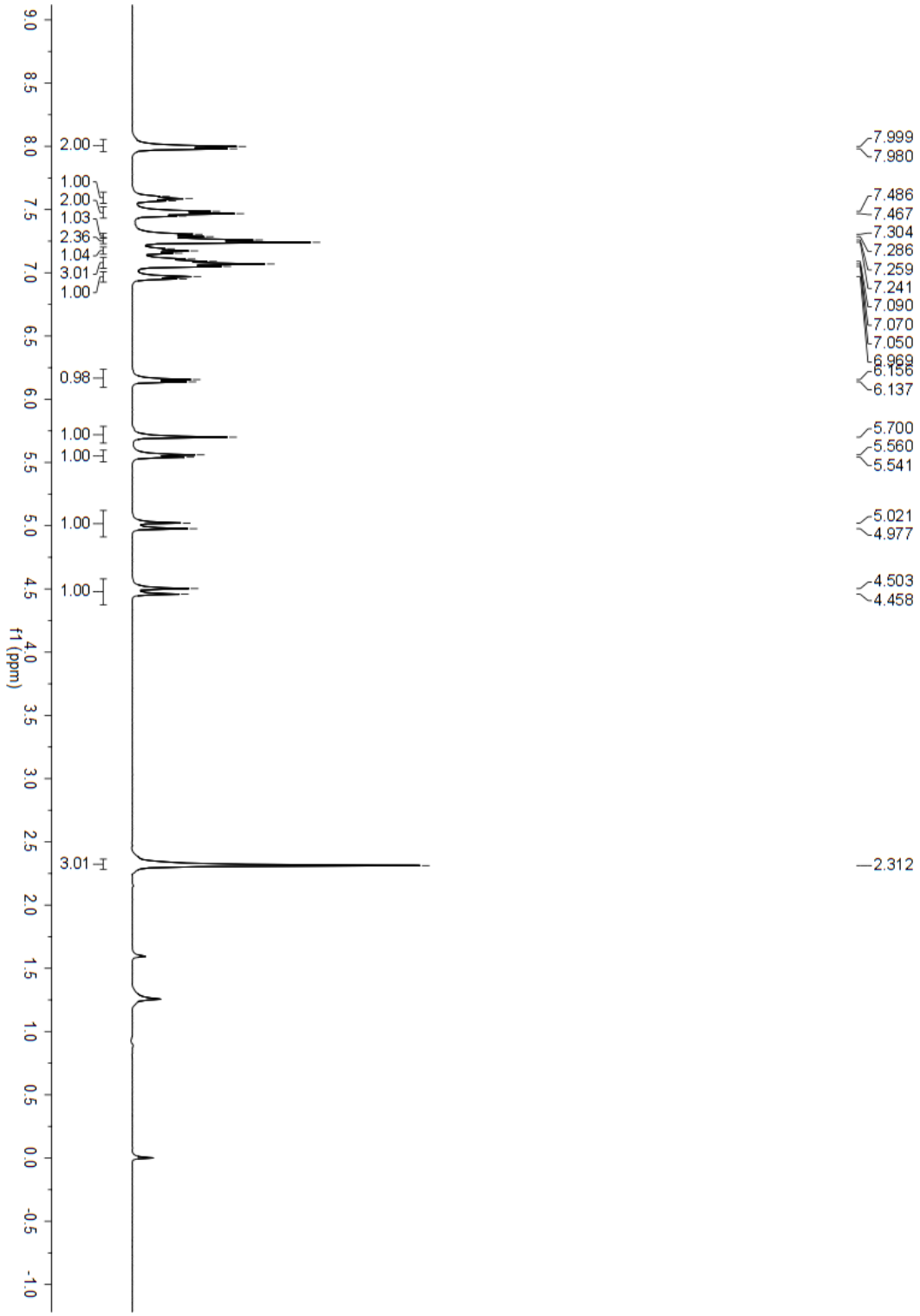

O
N
Ph
H

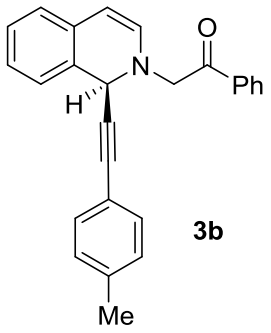
3a


195.458
136.828
135.317
133.587
132.120
131.795
128.778
128.369
128.161
128.017
127.927
127.508
125.860
125.492
123.354
122.481
100.390
86.514
86.465
58.173
52.989
f1 (ppm)

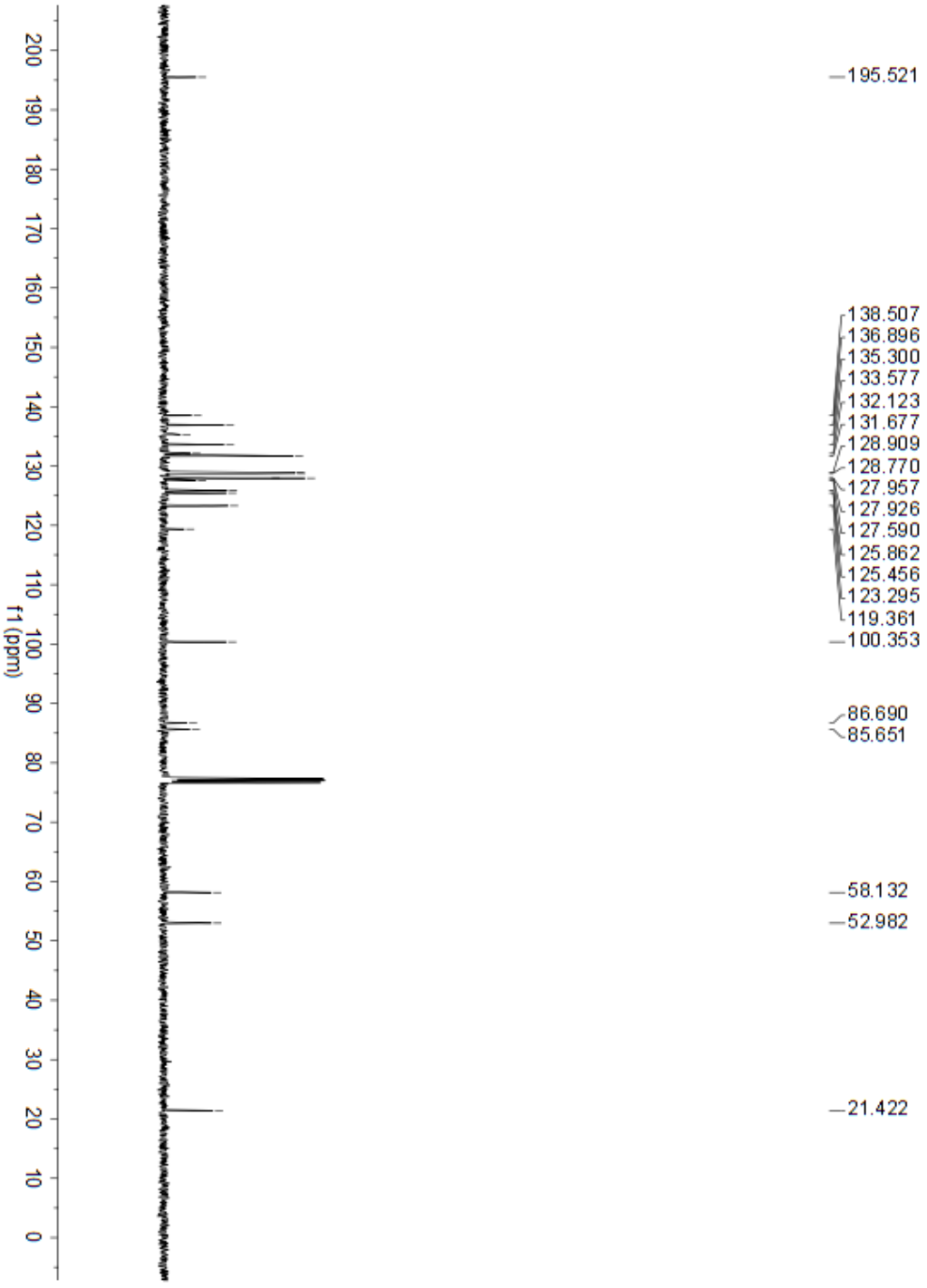

O
N
Ph
H
Me

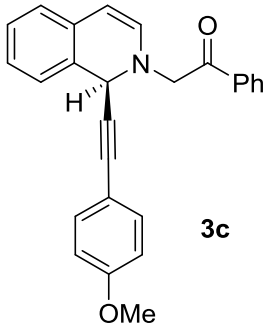
3b


f1 (ppm)
2.00
1.00
2.00
1.03
2.36
1.04
3.01
1.00
0.98
1.00
1.00
1.00
1.00
3.01
7.999
7.980
7.486
7.467
7.304
7.286
7.259
7.241
7.090
7.070
7.050
6.969
6.156
6.137
5.700
5.560
5.541
5.021
4.977
4.503
4.458
2.312

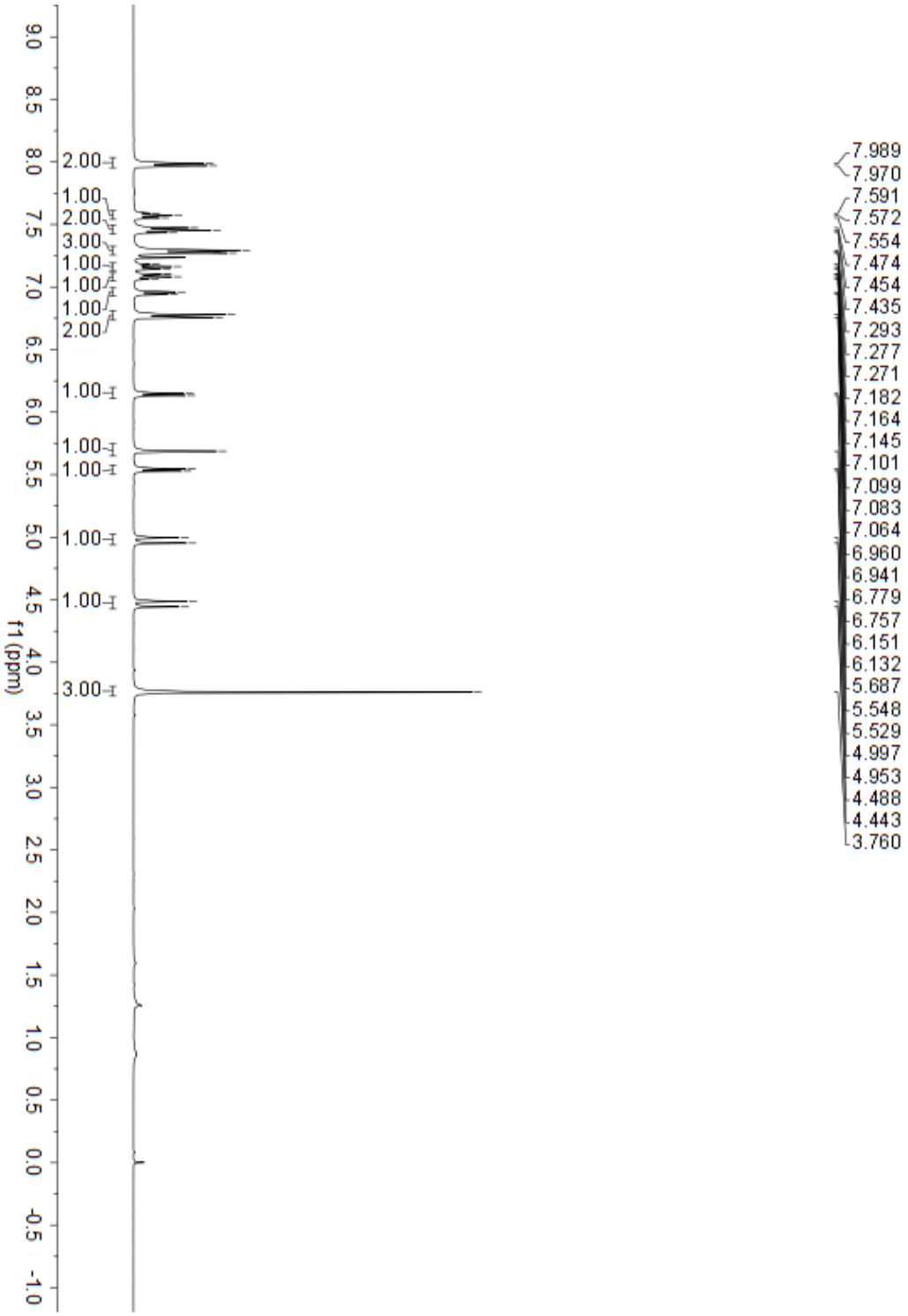

O
N
Ph
H
Me

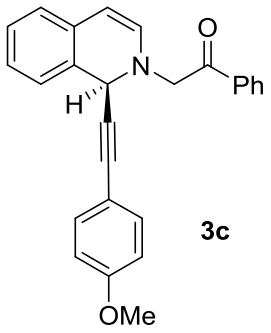
3b


f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
195.521
138.507
136.896
135.300
133.577
132.123
131.677
128.909
128.770
127.957
127.926
127.590
125.862
125.456
123.295
119.361
100.353
86.690
85.651
58.132
52.982
21.422

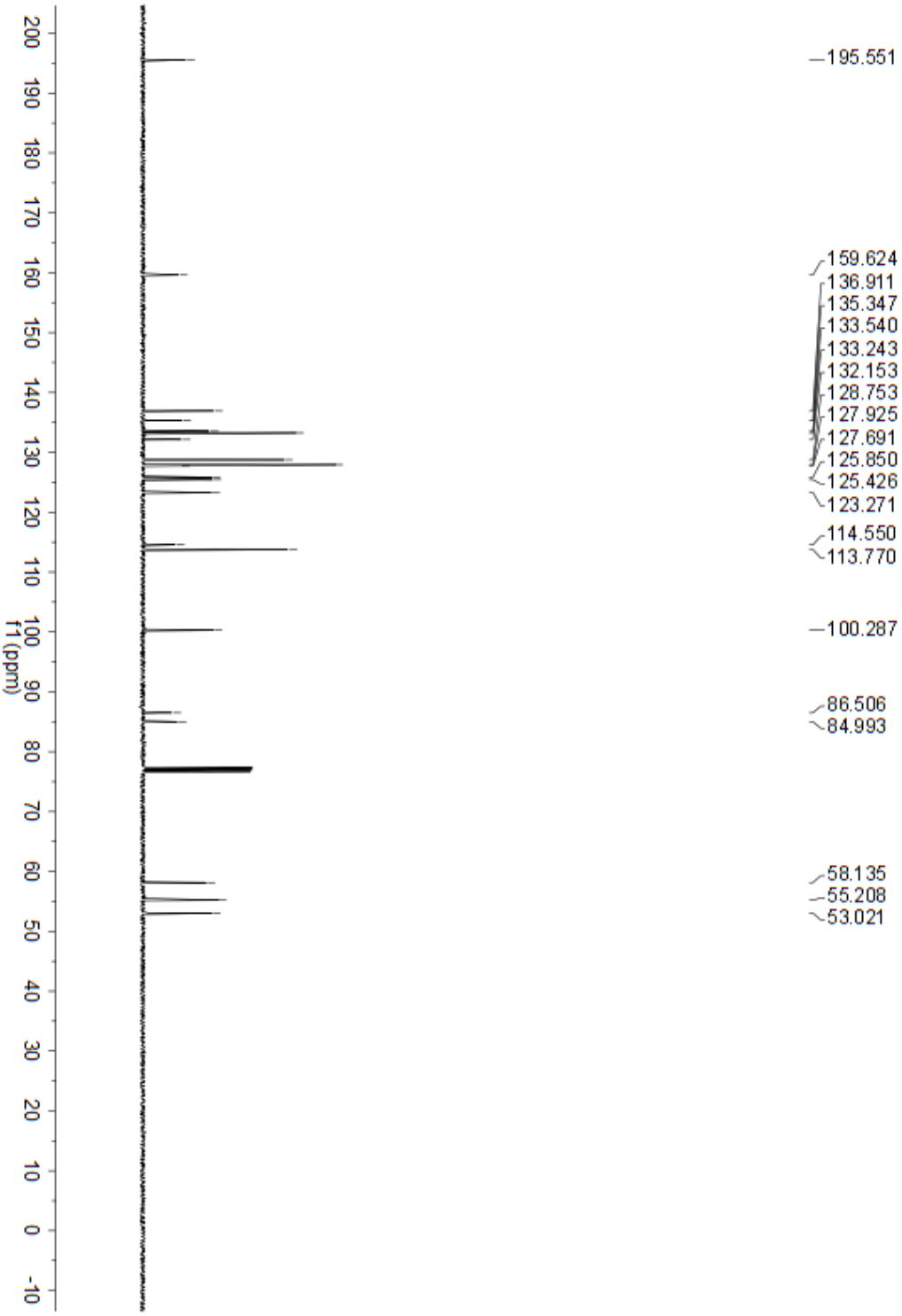

O
N
Ph
H
OMe

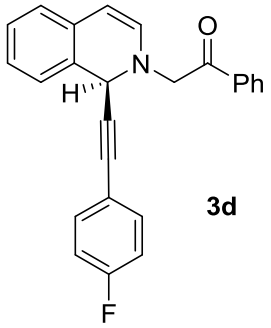
3c


f1 (ppm)
2.00
1.00
2.00
3.00
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
1.00
3.00
7.989
7.970
7.591
7.572
7.554
7.474
7.454
7.435
7.293
7.277
7.271
7.182
7.164
7.145
7.101
7.099
7.083
7.064
6.960
6.941
6.779
6.757
6.151
6.132
5.687
5.548
5.529
4.997
4.953
4.488
4.443
3.760

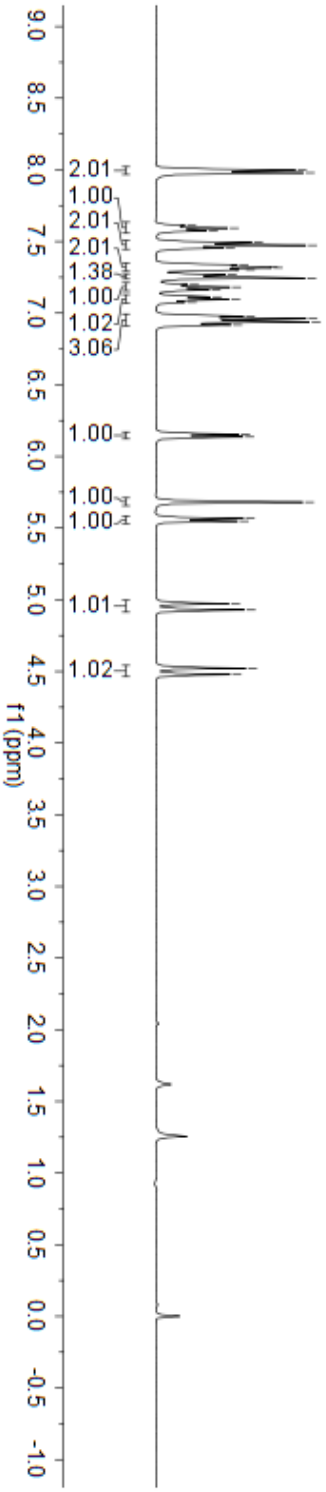

O
N
Ph
H
OMe

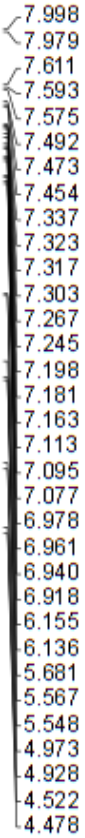
3c

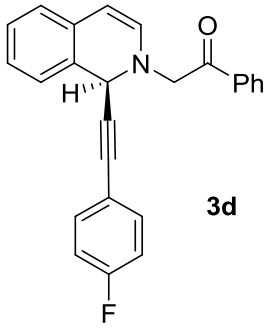

195.551
159.624
136.911
135.347
133.540
133.243
132.153
128.753
127.925
127.691
125.850
125.426
123.271
114.550
113.770
100.287
86.506
84.993
58.135
55.208
53.021
f1 (ppm)


O
N
Ph
H
F

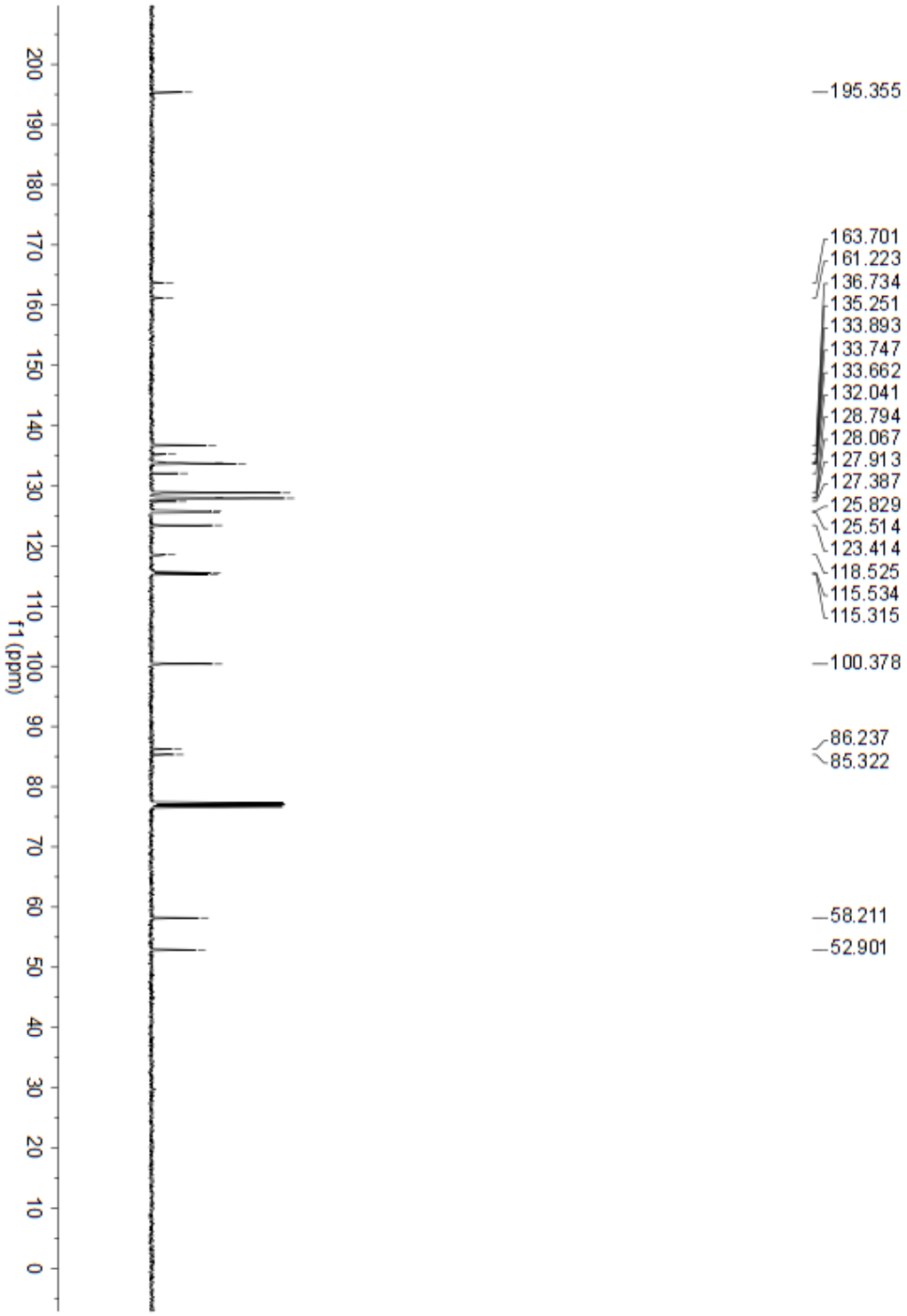
3d

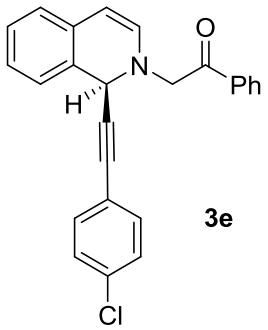

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
2.01
1.00
2.01
2.01
1.38
1.00
1.02
3.06
1.00
1.00
1.00
1.01
1.02


7.998
7.979
7.611
7.593
7.575
7.492
7.473
7.454
7.337
7.323
7.317
7.303
7.267
7.245
7.198
7.181
7.163
7.113
7.095
7.077
6.978
6.961
6.940
6.918
6.155
6.136
5.681
5.567
5.548
4.973
4.928
4.522
4.478

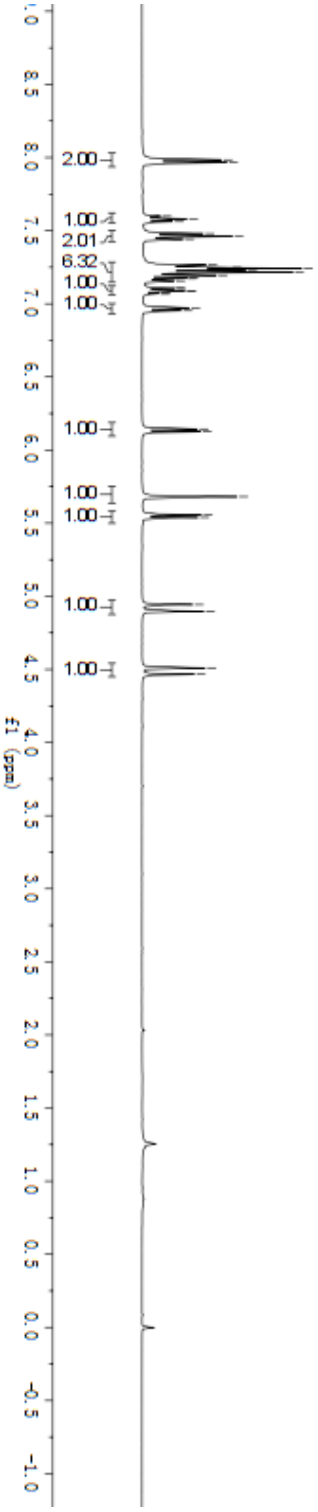

O
N
Ph
H
F

3d

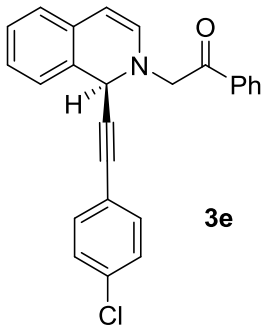

195.355
163.701
161.223
136.734
135.251
133.893
133.747
133.662
132.041
128.794
128.067
127.913
127.387
125.829
125.514
123.414
118.525
115.534
115.315
100.378
86.237
85.322
58.211
52.901
f1 (ppm)


O
N
Ph
H
Cl

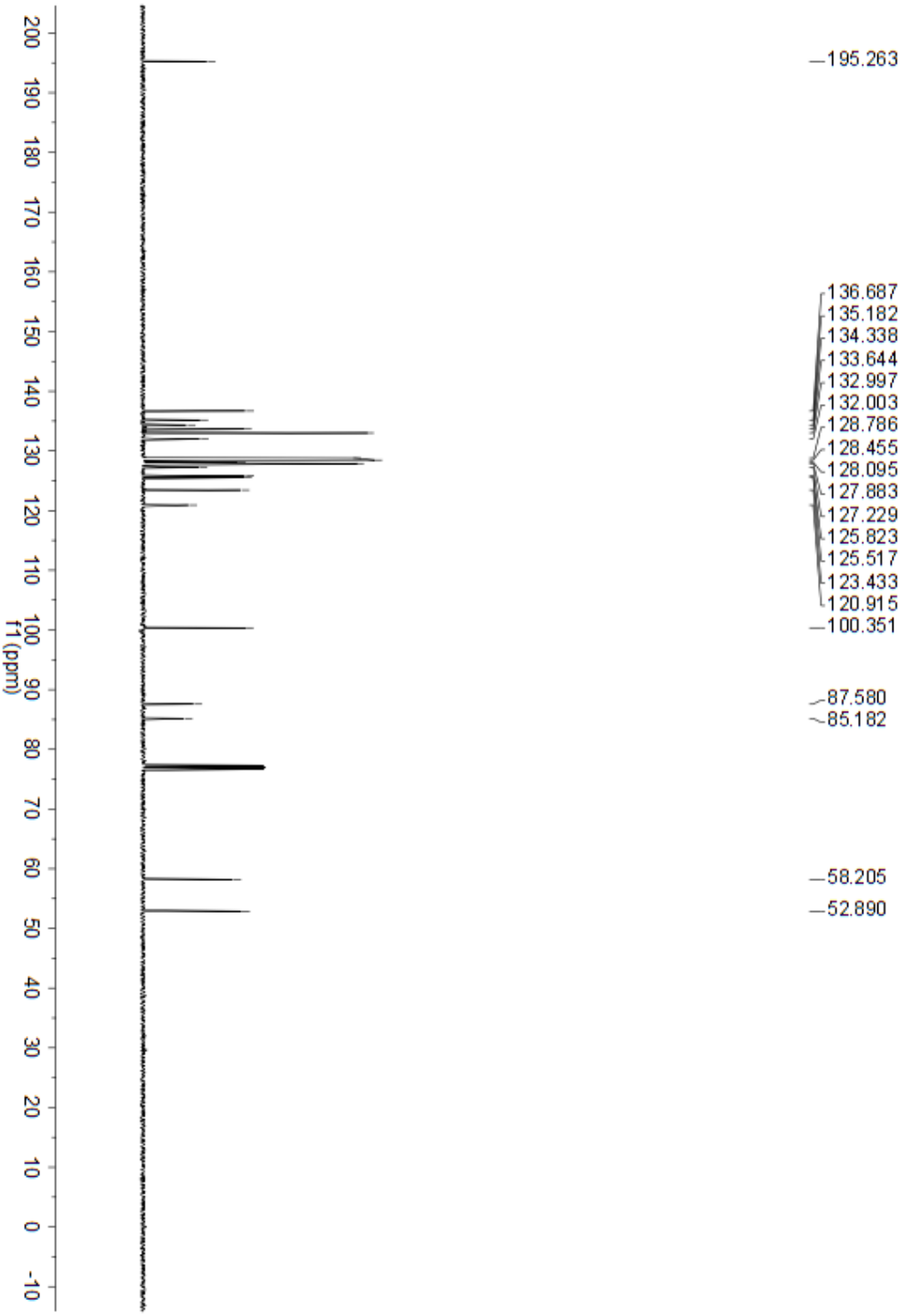
3e

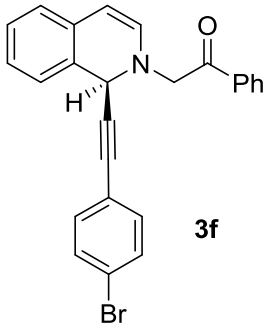

2.00
1.00
2.01
6.32
1.00
1.00
1.00
1.00
1.00
1.00
f1 (ppm)


7.984
7.966
7.599
7.581
7.562
7.480
7.461
7.442
7.265
7.260
7.248
7.243
7.234
7.216
7.194
7.175
7.173
7.157
7.108
7.105
7.089
7.087
7.071
7.068
6.972
6.953
6.144
6.125
5.681
5.557
5.538
4.943
4.898
4.510
4.486

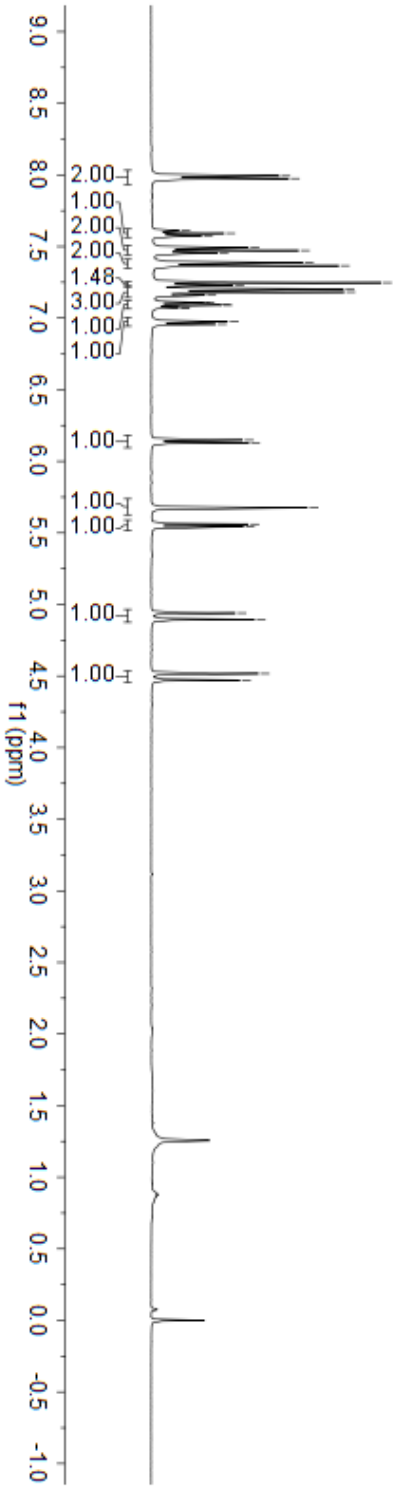

O
N
Ph
H
Cl

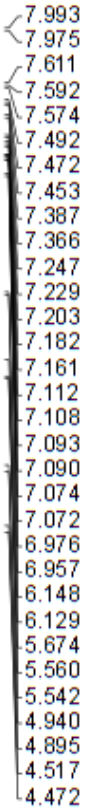
3e

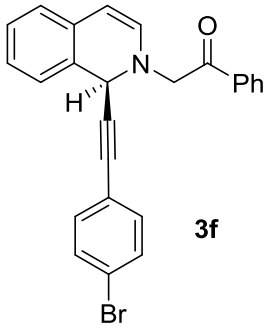

195.263
136.687
135.182
134.338
133.644
132.997
132.003
128.786
128.455
128.095
127.883
127.229
125.823
125.517
123.433
120.915
100.351
87.580
85.182
58.205
52.890
f1 (ppm)


O
N
Ph
H
Br

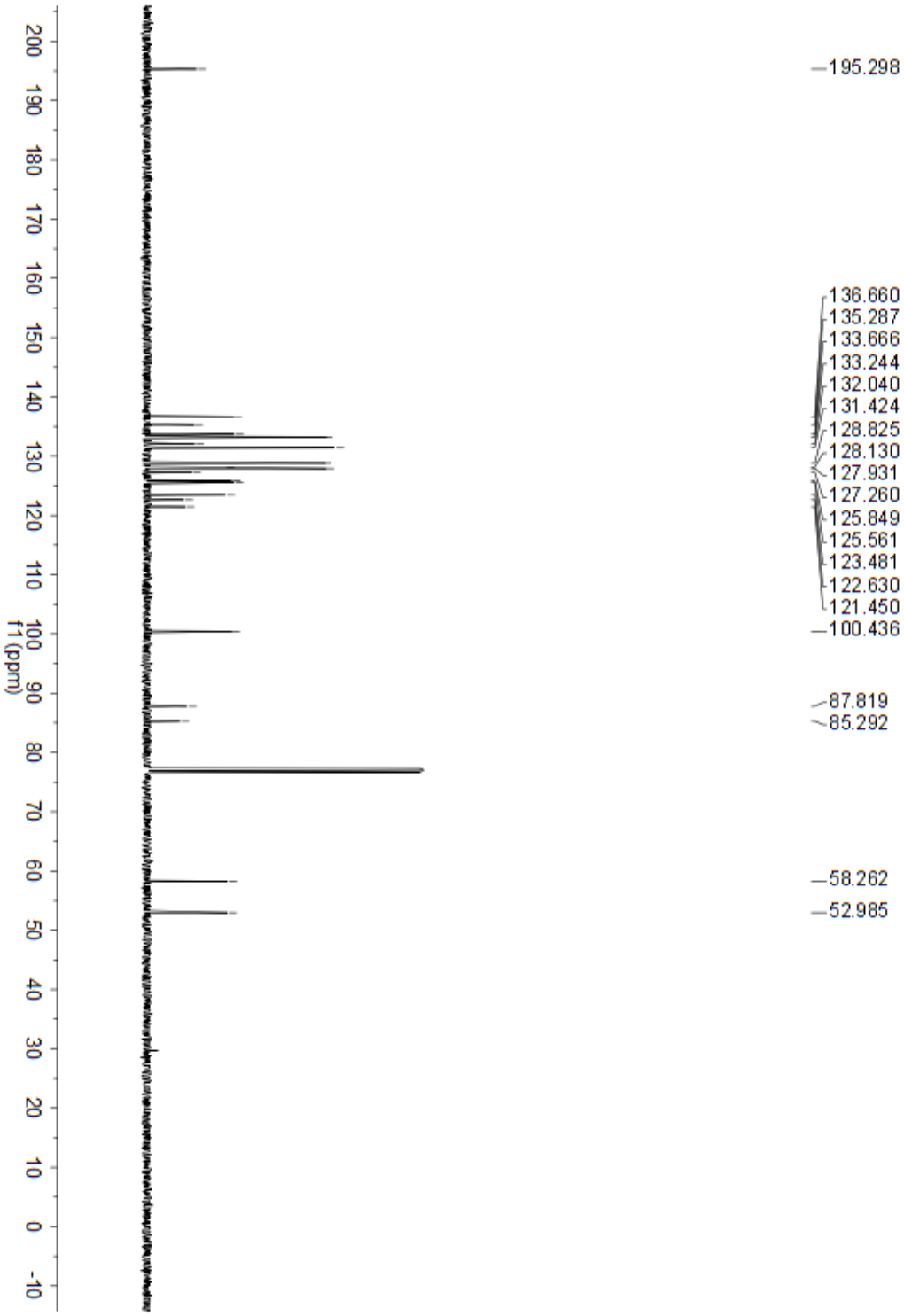
3f

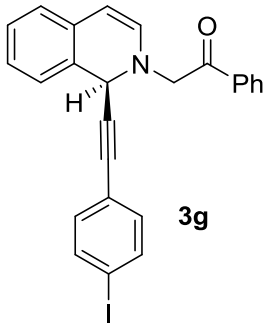

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
2.00
1.00
2.00
2.00
1.48
3.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00


7.993
7.975
7.611
7.592
7.574
7.492
7.472
7.453
7.387
7.366
7.247
7.229
7.203
7.182
7.161
7.112
7.108
7.093
7.090
7.074
7.072
6.976
6.957
6.148
6.129
5.674
5.560
5.542
4.940
4.895
4.517
4.472

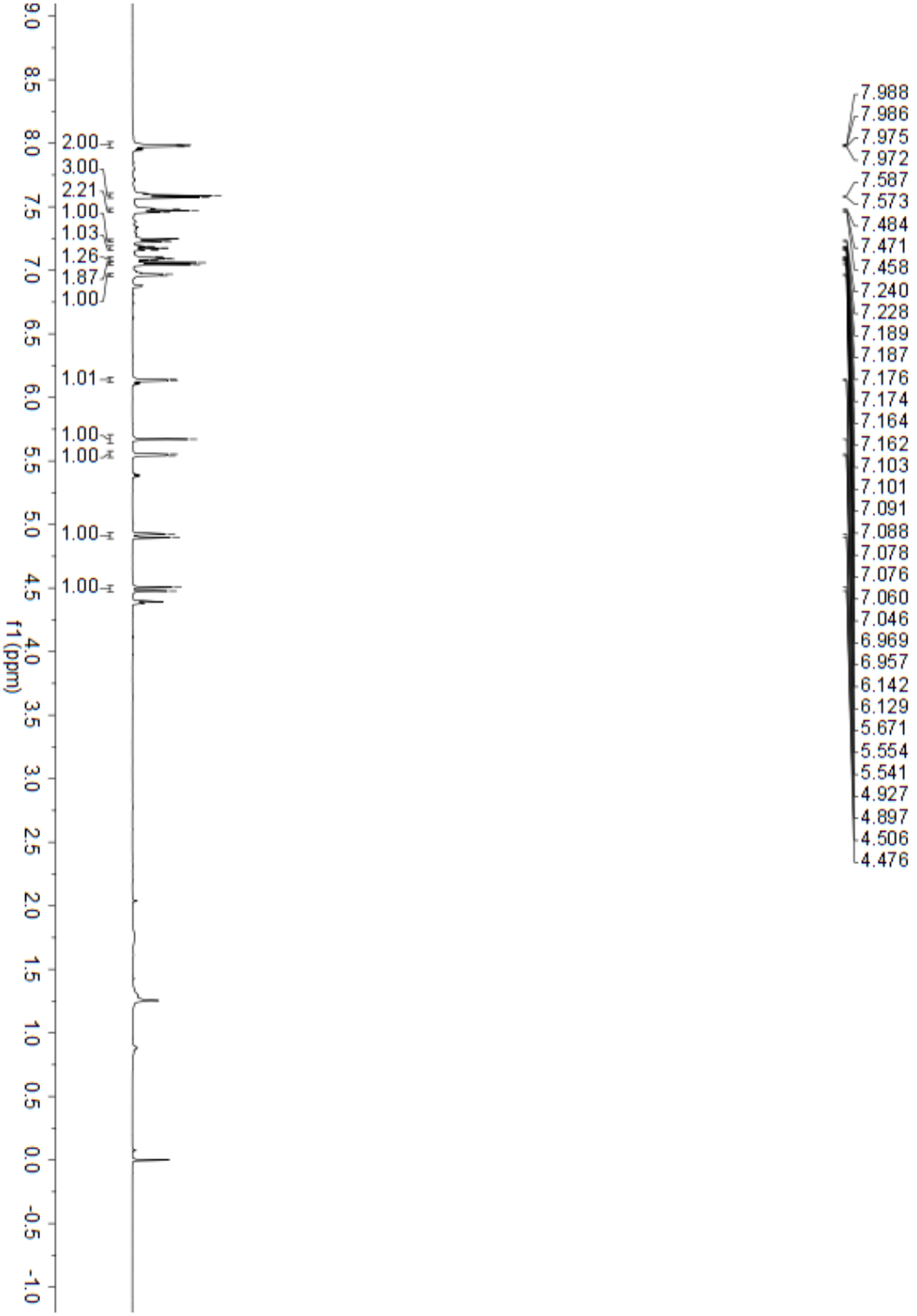

O
N
Ph
H
Br

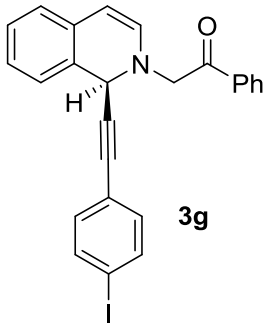
3f


195.298
136.660
135.287
133.666
133.244
132.040
131.424
128.825
128.130
127.931
127.260
125.849
125.561
123.481
122.630
121.450
100.436
87.819
85.292
58.262
52.985
f1 (ppm)

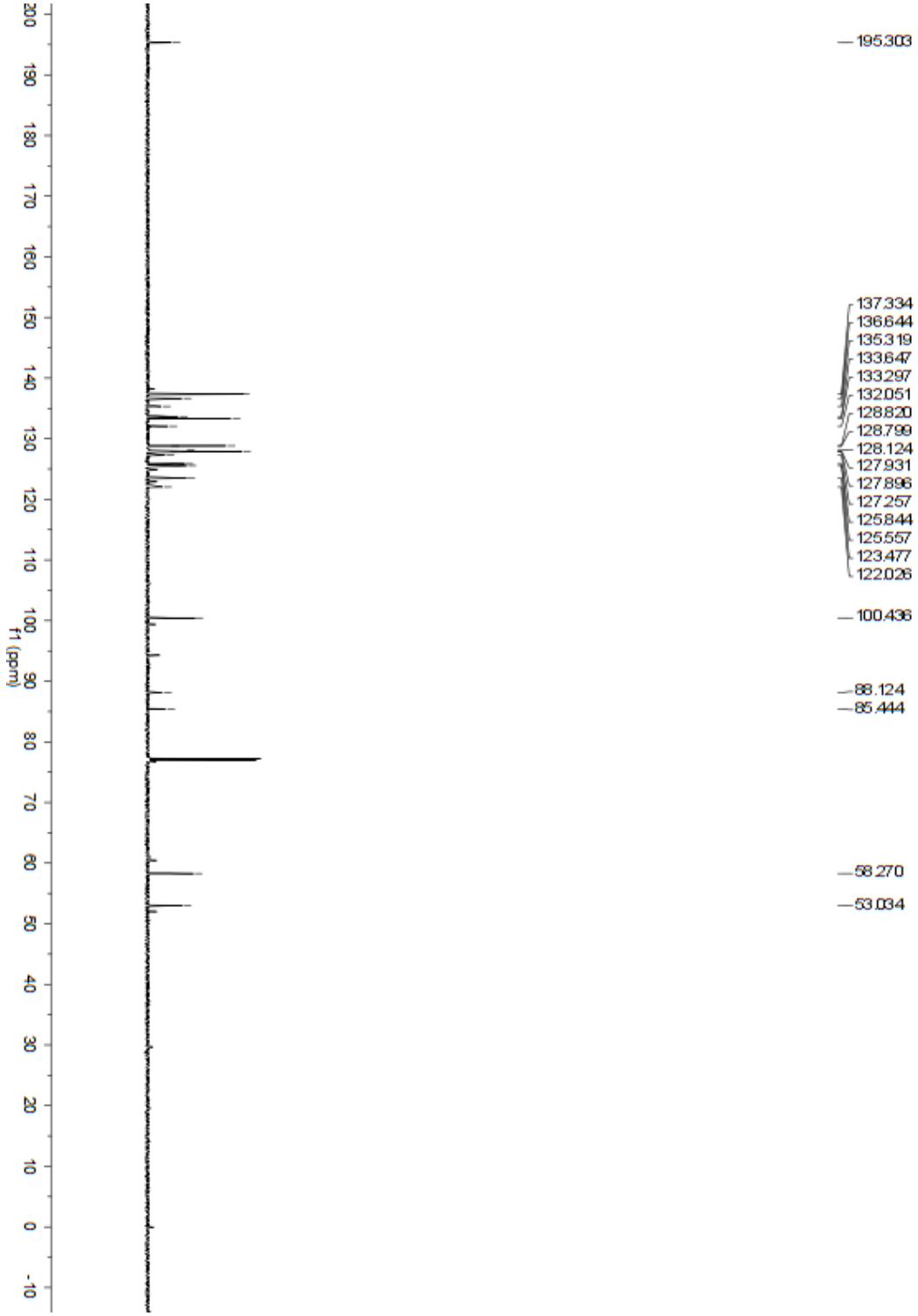

O
N
Ph
H
I

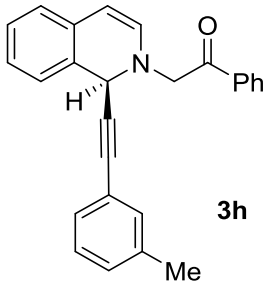
3g


9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
2.00
3.00
2.21
1.00
1.03
1.26
1.87
1.00
1.01
1.00
1.00
1.00
1.00
7.988
7.986
7.975
7.972
7.587
7.573
7.484
7.471
7.458
7.240
7.228
7.189
7.187
7.176
7.174
7.164
7.162
7.103
7.101
7.091
7.088
7.078
7.076
7.060
7.046
6.969
6.957
6.142
6.129
5.671
5.554
5.541
4.927
4.897
4.506
4.476

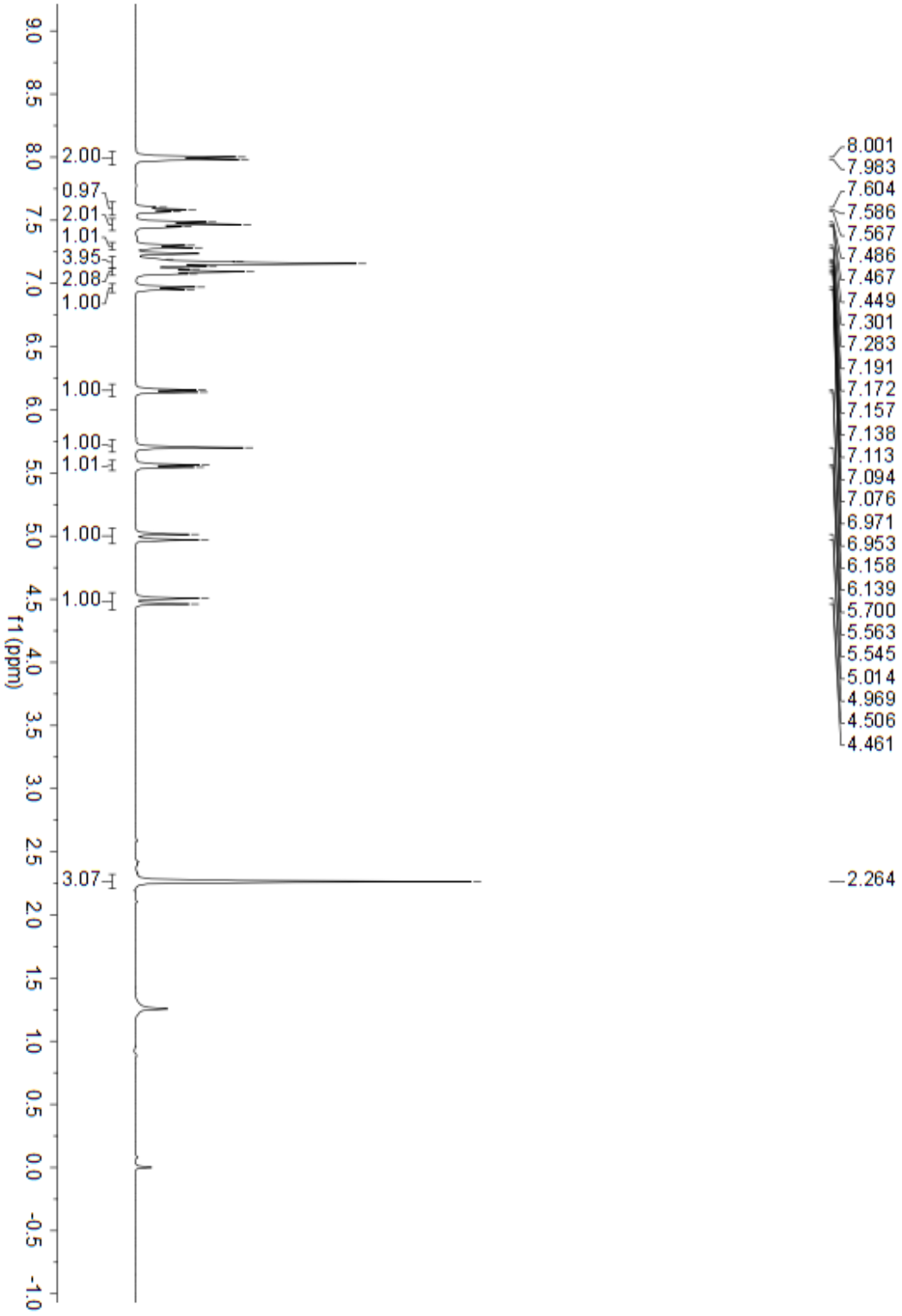

O
N
Ph
H
I

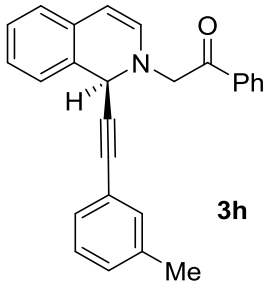
3g


195.303
137.334
136.644
135.319
133.647
133.297
132.051
128.820
128.799
128.124
127.931
127.896
127.257
125.844
125.557
123.477
122.026
100.436
88.124
85.444
58.270
53.034
f1 (ppm)

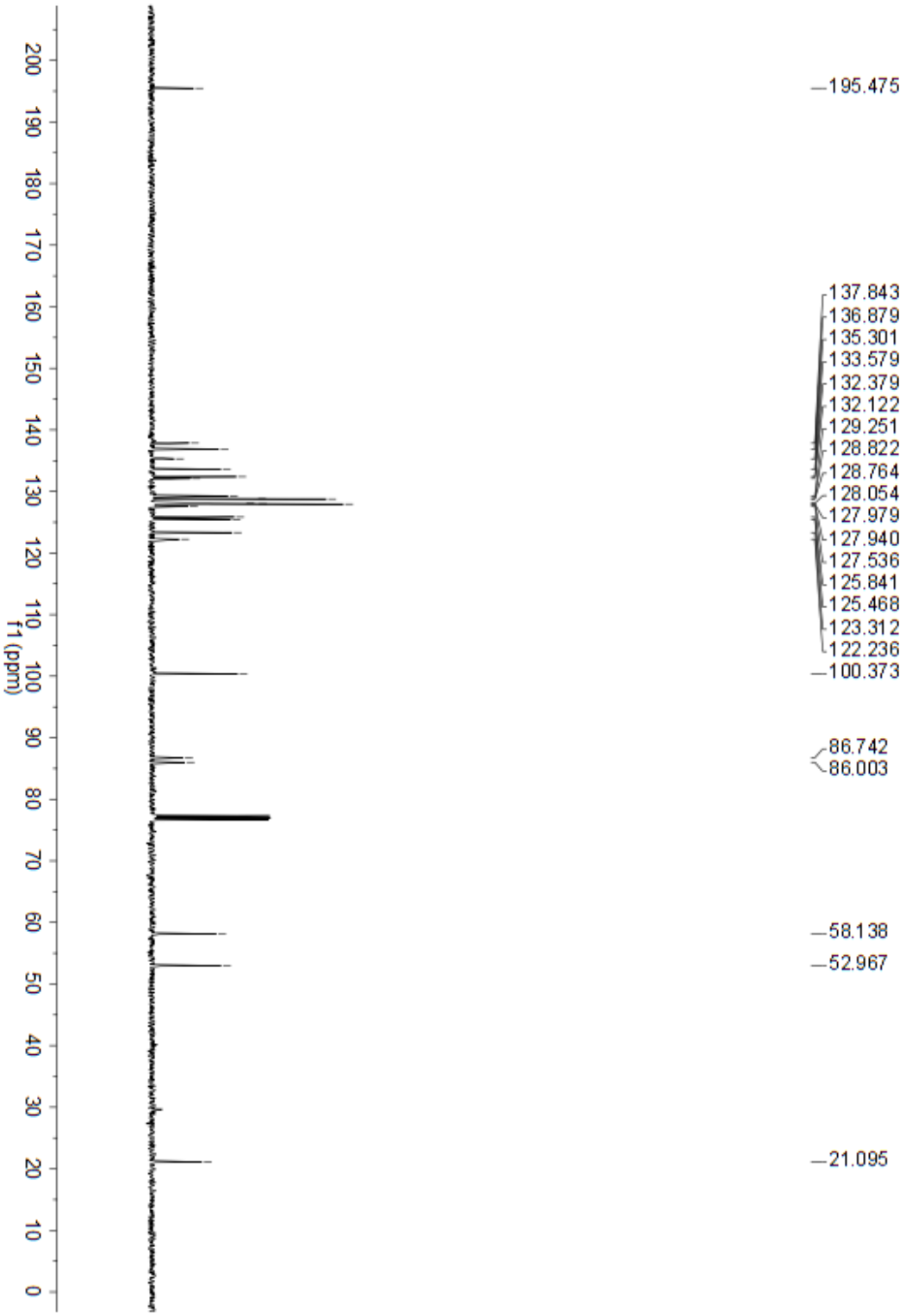

O
N
Ph
H
Me

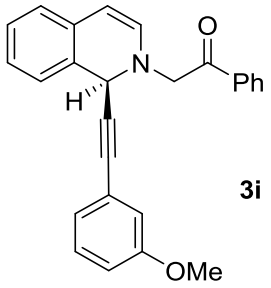
3h


2.00
0.97
2.01
1.01
3.95
2.08
1.00
1.00
1.00
1.01
1.00
1.00
3.07
f1 (ppm)
8.001
7.983
7.604
7.586
7.567
7.486
7.467
7.449
7.301
7.283
7.191
7.172
7.157
7.138
7.113
7.094
7.076
6.971
6.953
6.158
6.139
5.700
5.563
5.545
5.014
4.969
4.506
4.461
2.264

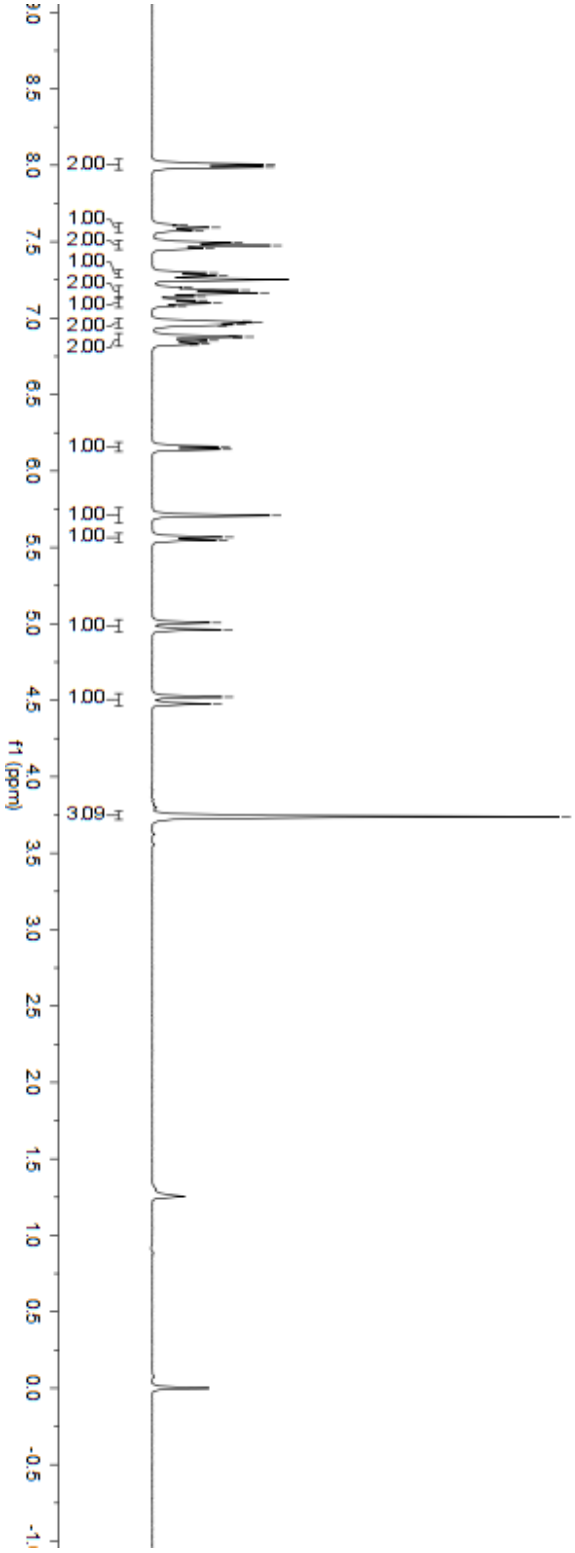

O
N
Ph
H
Me

3h

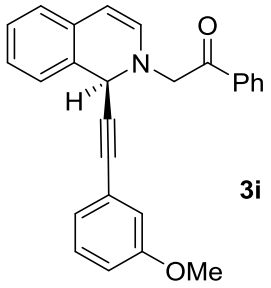

f1 (ppm)
195.475
137.843
136.879
135.301
133.579
132.379
132.122
129.251
128.822
128.764
128.054
127.979
127.940
127.536
125.841
125.468
123.312
122.236
100.373
86.742
86.003
58.138
52.967
21.095


O
N
Ph
H
OMe

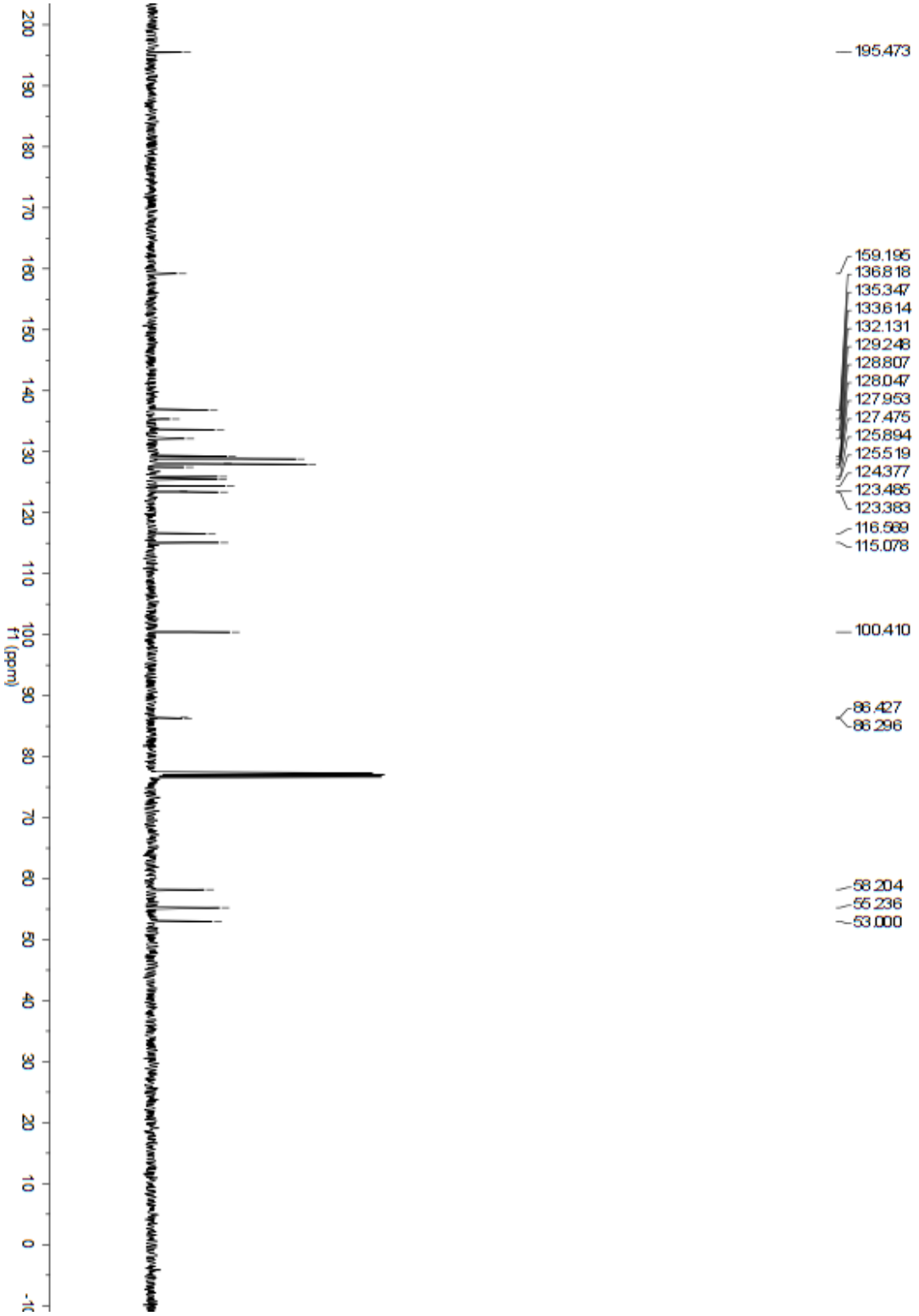
3i

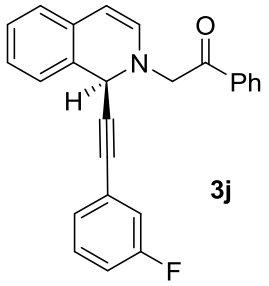

2.00
1.00
2.00
1.00
2.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
1.00
3.09
f1 (ppm)


8.006
7.987
7.611
7.592
7.574
7.494
7.475
7.456
7.296
7.277
7.199
7.182
7.163
7.144
7.117
7.098
7.079
6.978
6.974
6.969
6.958
6.950
6.882
6.877
6.873
6.854
6.847
6.833
6.826
6.160
6.141
5.708
5.566
5.548
5.007
4.962
4.521
4.477
3.739

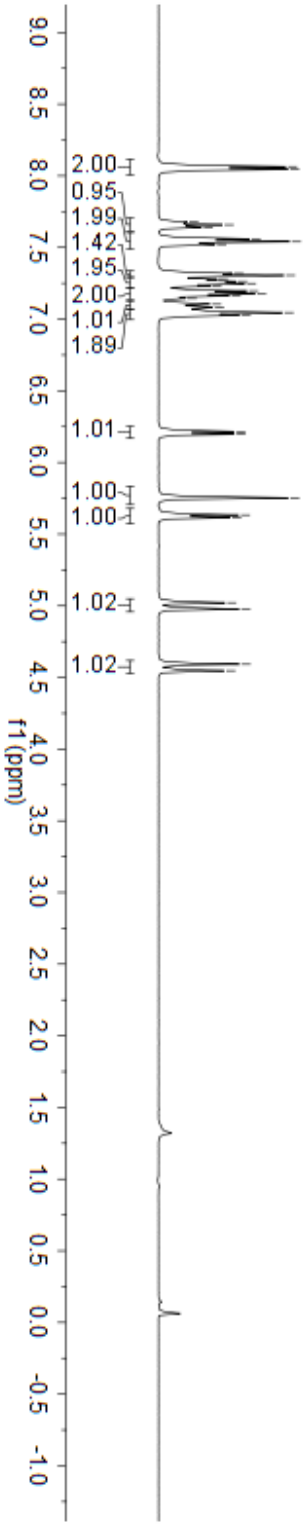

O
N
Ph
H
OMe

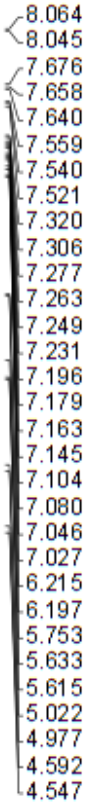
3i

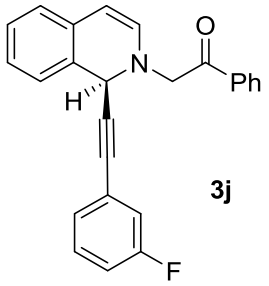

195.473
159.195
136.818
135.347
133.614
132.131
129.248
128.807
128.047
127.953
127.475
125.894
125.519
124.377
123.485
123.383
116.569
115.078
100.410
86.427
86.296
58.204
55.236
53.000
f1 (ppm)


O
N
Ph
H
F

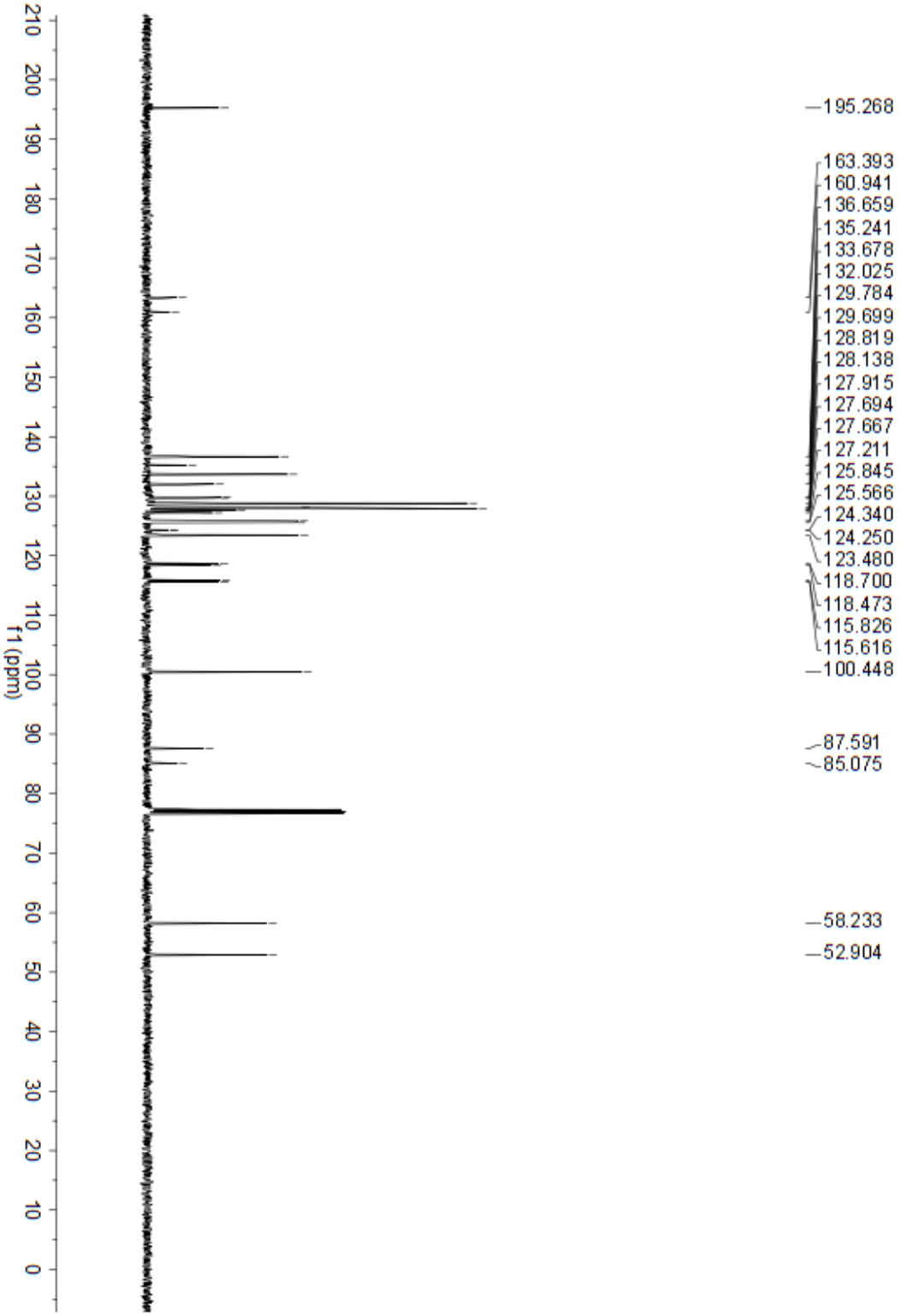
3j

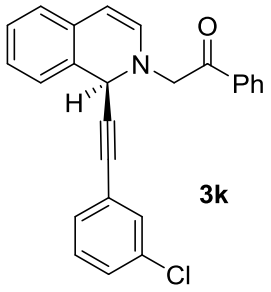

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)
2.00
0.95
1.99
1.42
1.95
2.00
1.01
1.89
1.01
1.00
1.00
1.02
1.02


8.064
8.045
7.676
7.658
7.640
7.559
7.540
7.521
7.320
7.306
7.277
7.263
7.249
7.231
7.196
7.179
7.163
7.145
7.104
7.080
7.046
7.027
6.215
6.197
5.753
5.633
5.615
5.022
4.977
4.592
4.547

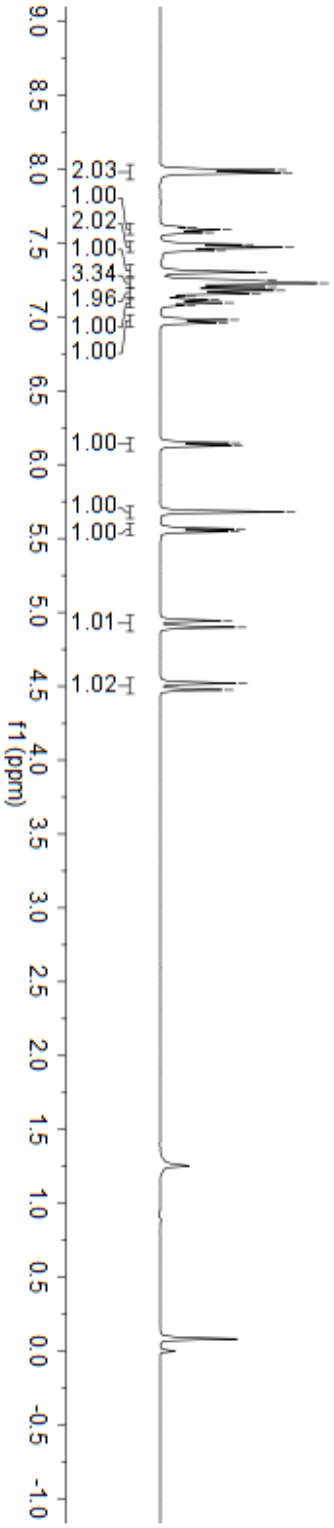

O
N
Ph
H
F

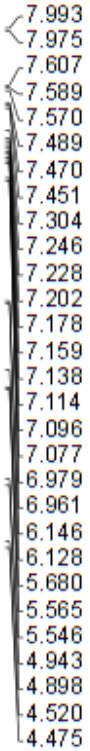
3j

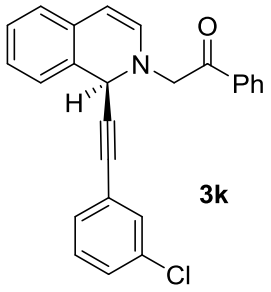

f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
195.268
163.393
160.941
136.659
135.241
133.678
132.025
129.784
129.699
128.819
128.138
127.915
127.694
127.667
127.211
125.845
125.566
124.340
124.250
123.480
118.700
118.473
115.826
115.616
100.448
87.591
85.075
58.233
52.904


O
N
Ph
H
Cl

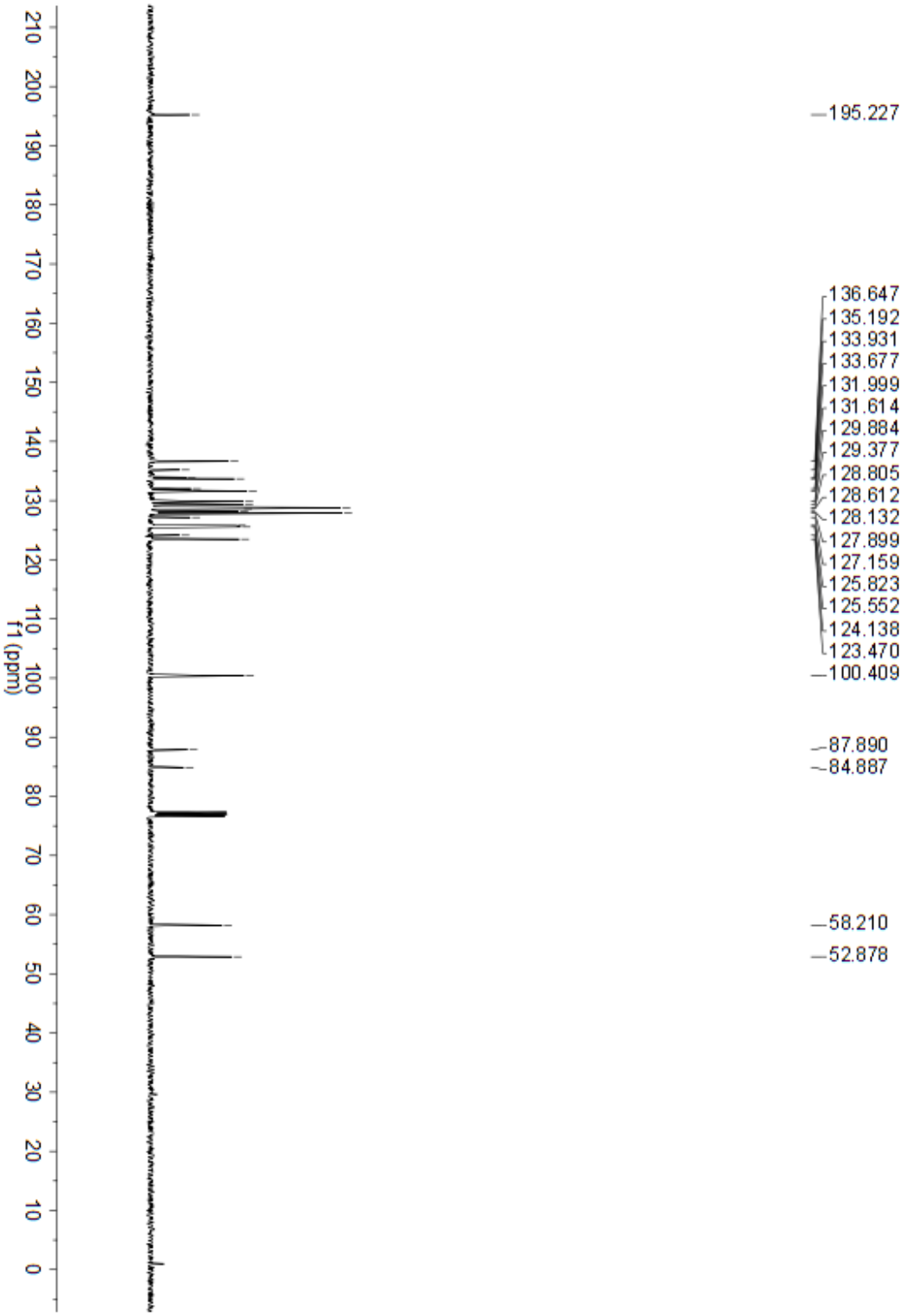
3k

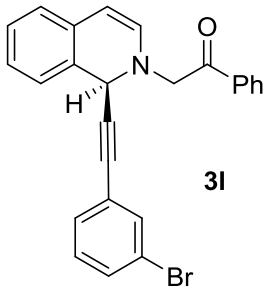

2.03
1.00
2.02
1.00
3.34
1.96
1.00
1.00
1.00
1.00
1.00
1.01
1.02
f1 (ppm)


7.993
7.975
7.607
7.589
7.570
7.489
7.470
7.451
7.304
7.246
7.228
7.202
7.178
7.159
7.138
7.114
7.096
7.077
6.979
6.961
6.146
6.128
5.680
5.565
5.546
4.943
4.898
4.520
4.475

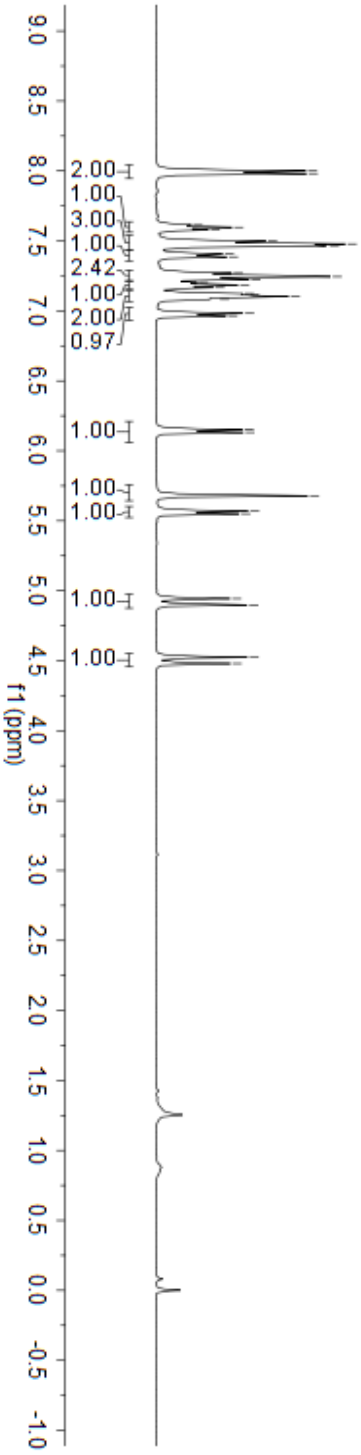

O
N
Ph
H
Cl

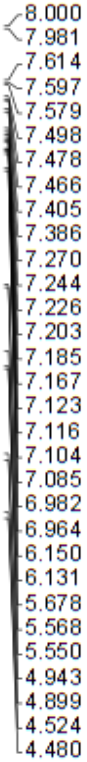
3k

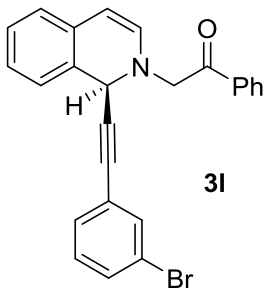

f1 (ppm)
195.227
136.647
135.192
133.931
133.677
131.999
131.614
129.884
129.377
128.805
128.612
128.132
127.899
127.159
125.823
125.552
124.138
123.470
100.409
87.890
84.887
58.210
52.878


O
N
Ph
H
Br

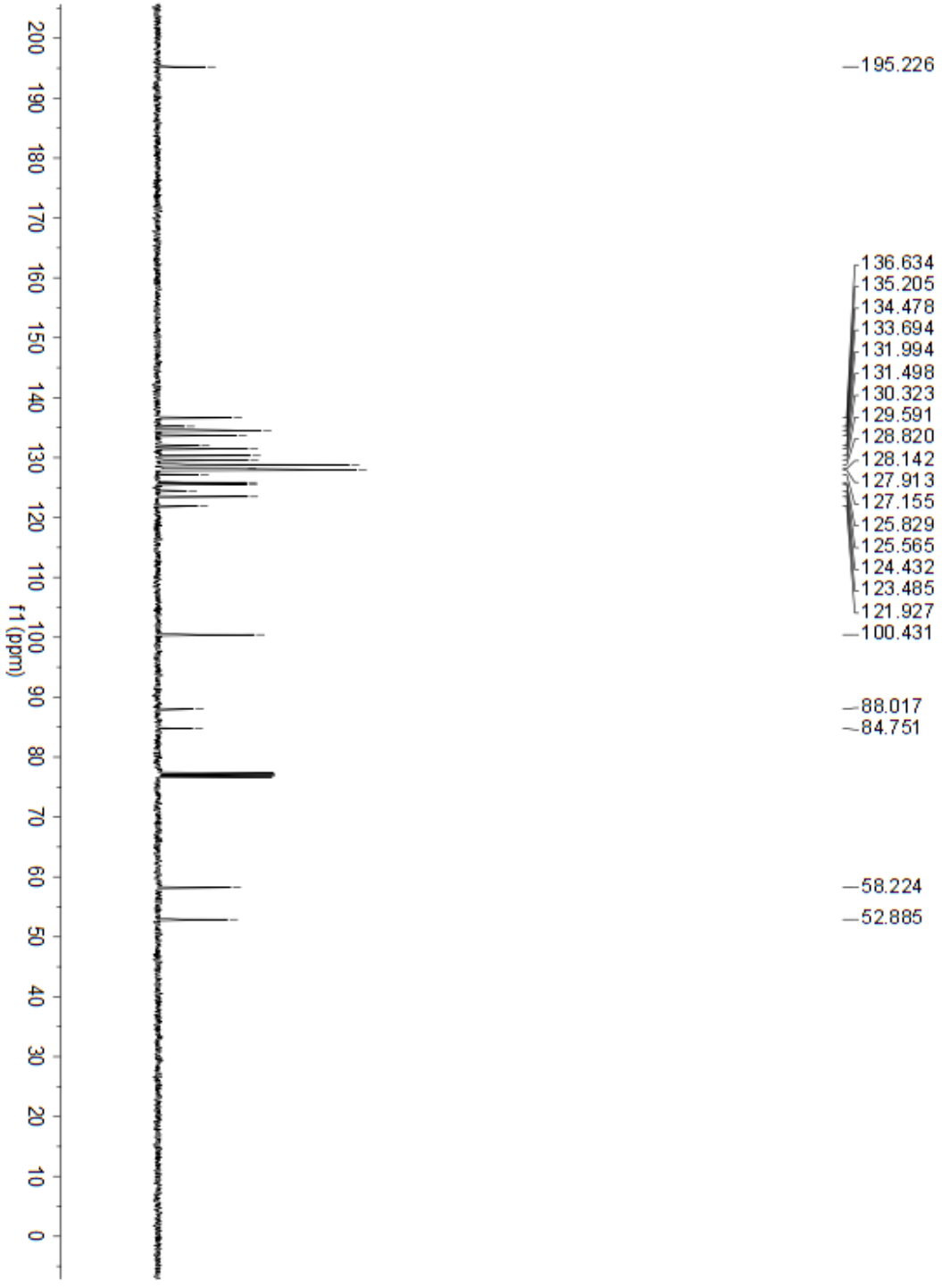
3l

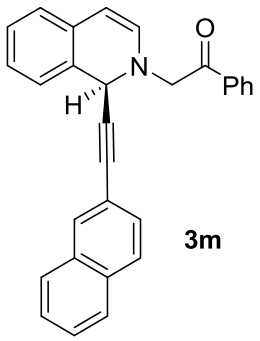

2.00
1.00
3.00
1.00
2.42
1.00
2.00
0.97
1.00
1.00
1.00
1.00
1.00
f1 (ppm)


8.000
7.981
7.614
7.597
7.579
7.498
7.478
7.466
7.405
7.386
7.270
7.244
7.226
7.203
7.185
7.167
7.123
7.116
7.104
7.085
6.982
6.964
6.150
6.131
5.678
5.568
5.550
4.943
4.899
4.524
4.480

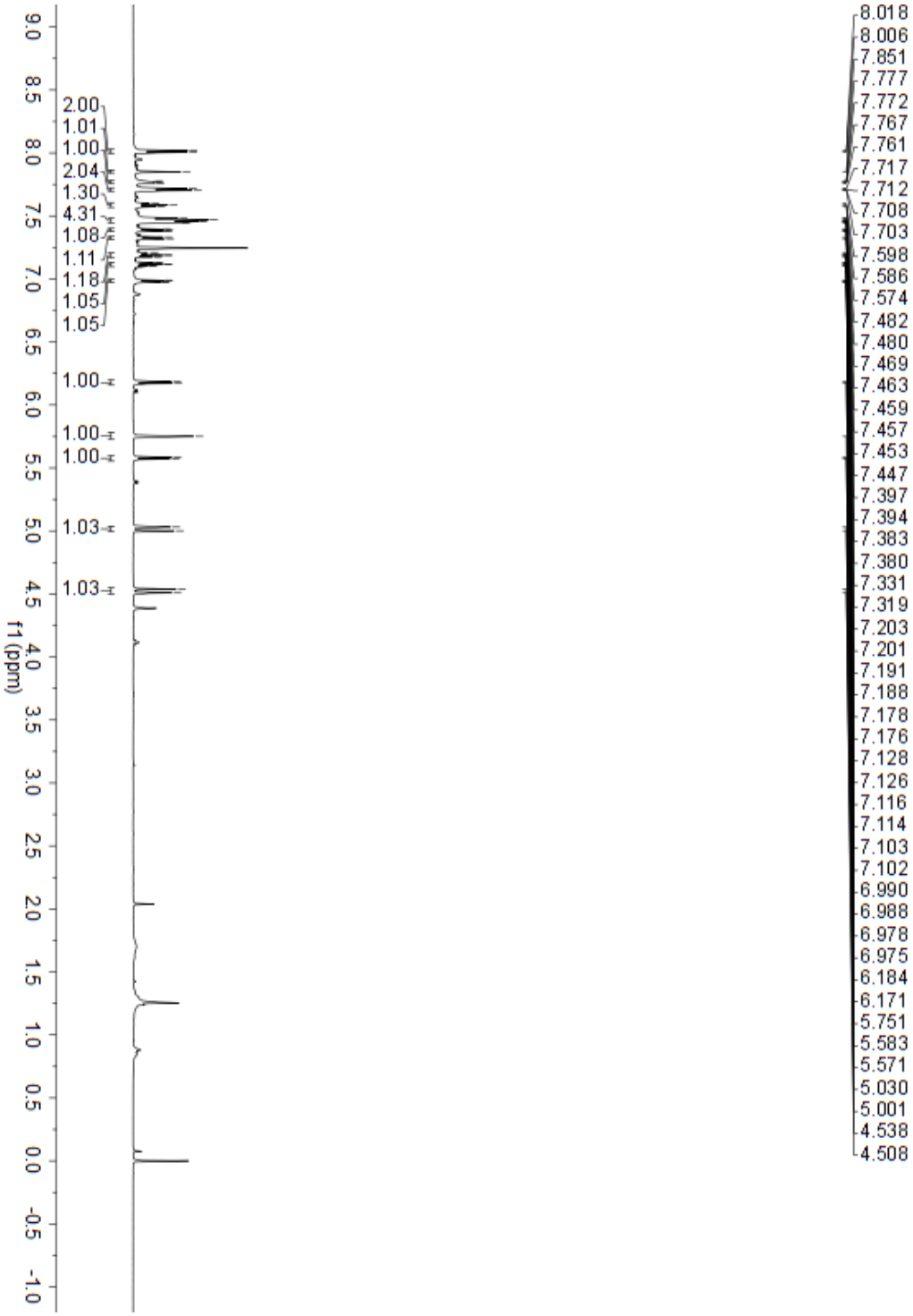

O
N
Ph
H
Br

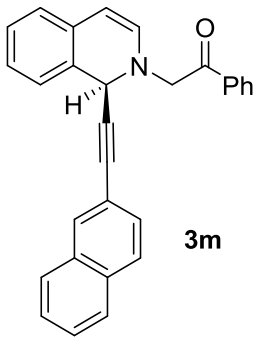
3l


f1 (ppm)
195.226
136.634
135.205
134.478
133.694
131.994
131.498
130.323
129.591
128.820
128.142
127.913
127.155
125.829
125.565
124.432
123.485
121.927
100.431
88.017
84.751
58.224
52.885

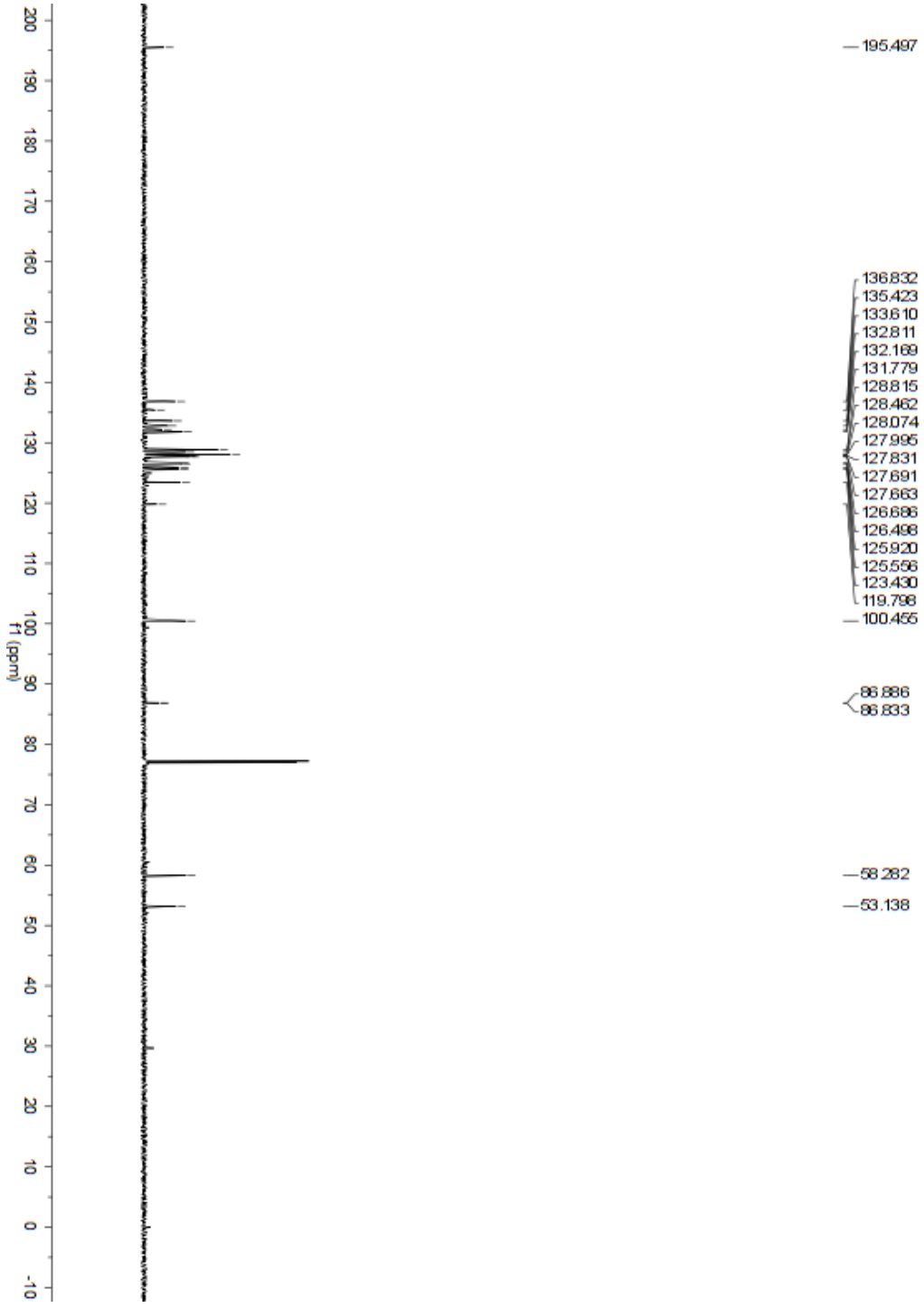

O
N
Ph
H

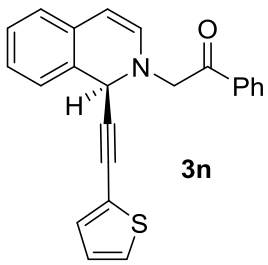
3m


f1 (ppm)
2.00
1.01
1.00
2.04
1.30
4.31
1.08
1.11
1.18
1.05
1.05
1.00
1.00
1.00
1.03
1.03
8.018
8.006
7.851
7.777
7.772
7.767
7.761
7.717
7.712
7.708
7.703
7.598
7.586
7.574
7.482
7.480
7.469
7.463
7.459
7.457
7.453
7.447
7.397
7.394
7.383
7.380
7.331
7.319
7.203
7.201
7.191
7.188
7.178
7.176
7.128
7.126
7.116
7.114
7.103
7.102
6.990
6.988
6.978
6.975
6.184
6.171
5.751
5.583
5.571
5.030
5.001
4.538
4.508

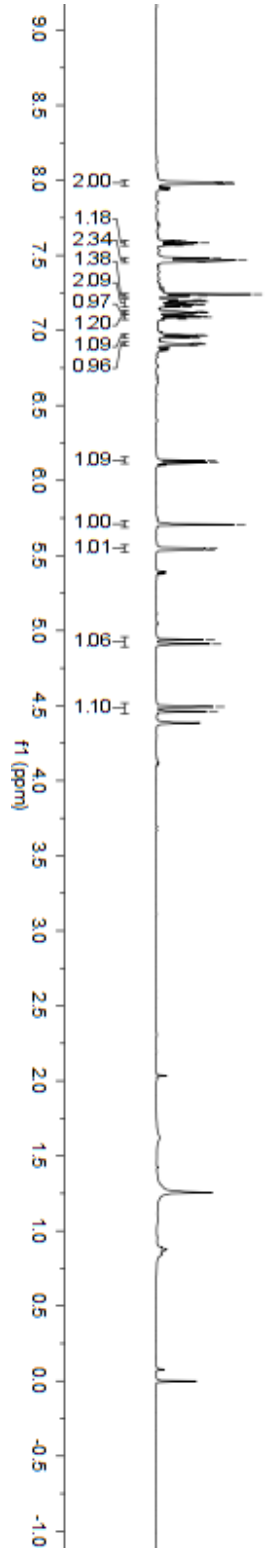

O
N
Ph
H

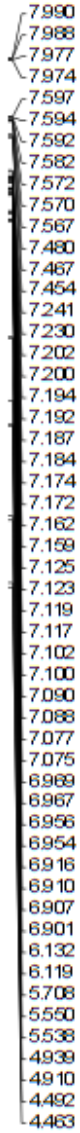
3m

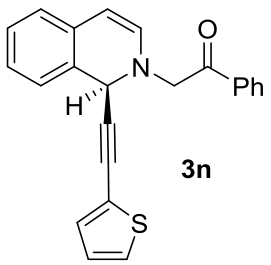

195.497
136.832
135.423
133.610
132.811
132.169
131.779
128.815
128.462
128.074
127.995
127.831
127.691
127.663
126.686
126.498
125.920
125.556
123.430
119.798
100.455
86.886
86.833
58.282
53.138
f1 (ppm)


O
N
Ph
H
S

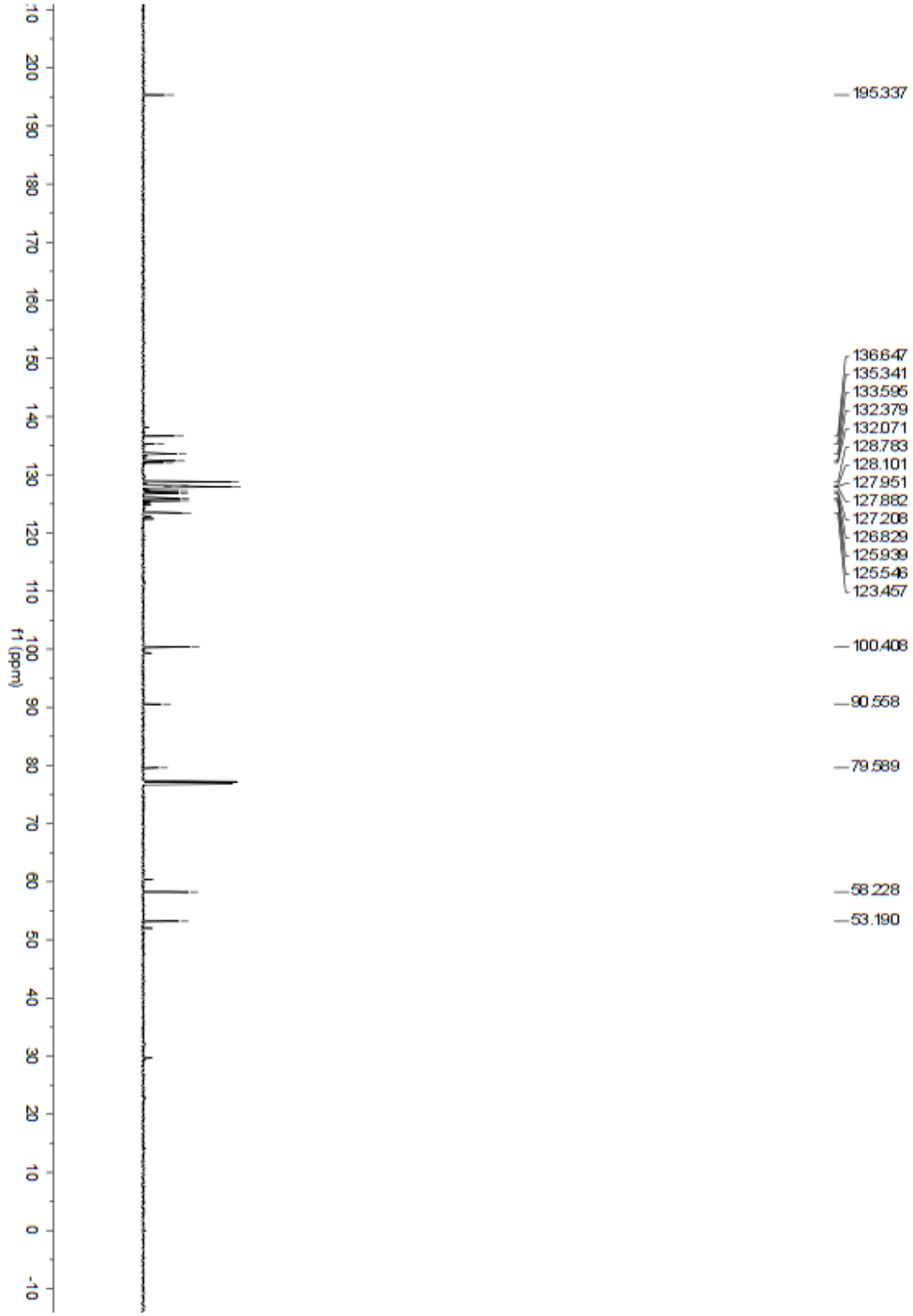
3n

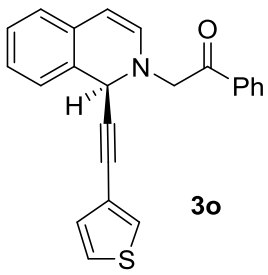

2.00
1.18
2.34
1.38
2.09
0.97
1.20
1.09
0.96
1.09
1.00
1.01
1.06
1.10
f1 (ppm)


7.990
7.988
7.977
7.974
7.597
7.594
7.592
7.582
7.572
7.570
7.567
7.480
7.467
7.454
7.241
7.230
7.202
7.200
7.194
7.192
7.187
7.184
7.174
7.172
7.162
7.159
7.125
7.123
7.119
7.117
7.102
7.100
7.090
7.088
7.077
7.075
6.969
6.967
6.956
6.954
6.916
6.910
6.907
6.901
6.132
6.119
5.708
5.550
5.538
4.939
4.910
4.492
4.463

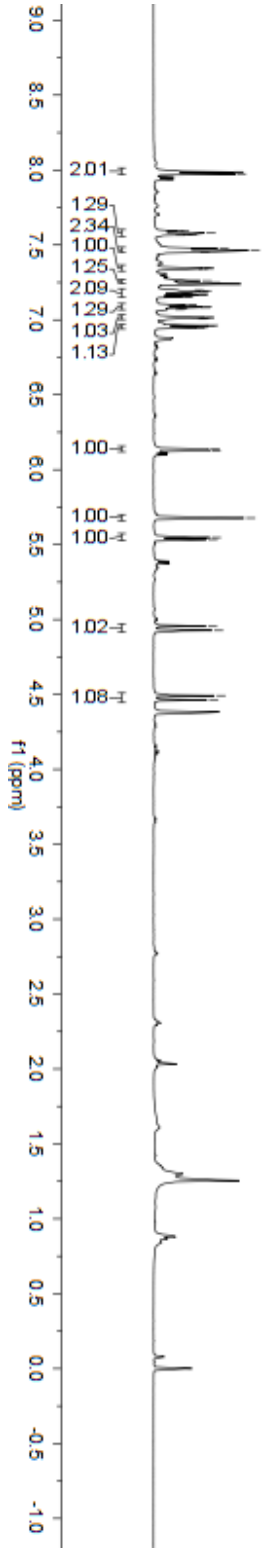

O
N
Ph
H
S

3n

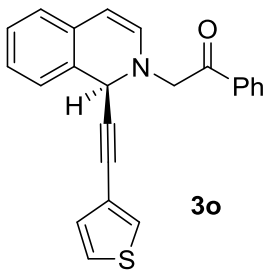

195.337
136.647
135.341
133.595
132.379
132.071
128.783
128.101
127.951
127.882
127.208
126.829
125.939
125.546
123.457
100.408
90.558
79.589
58.228
53.190
f1 (ppm)


O
N
Ph
H
S

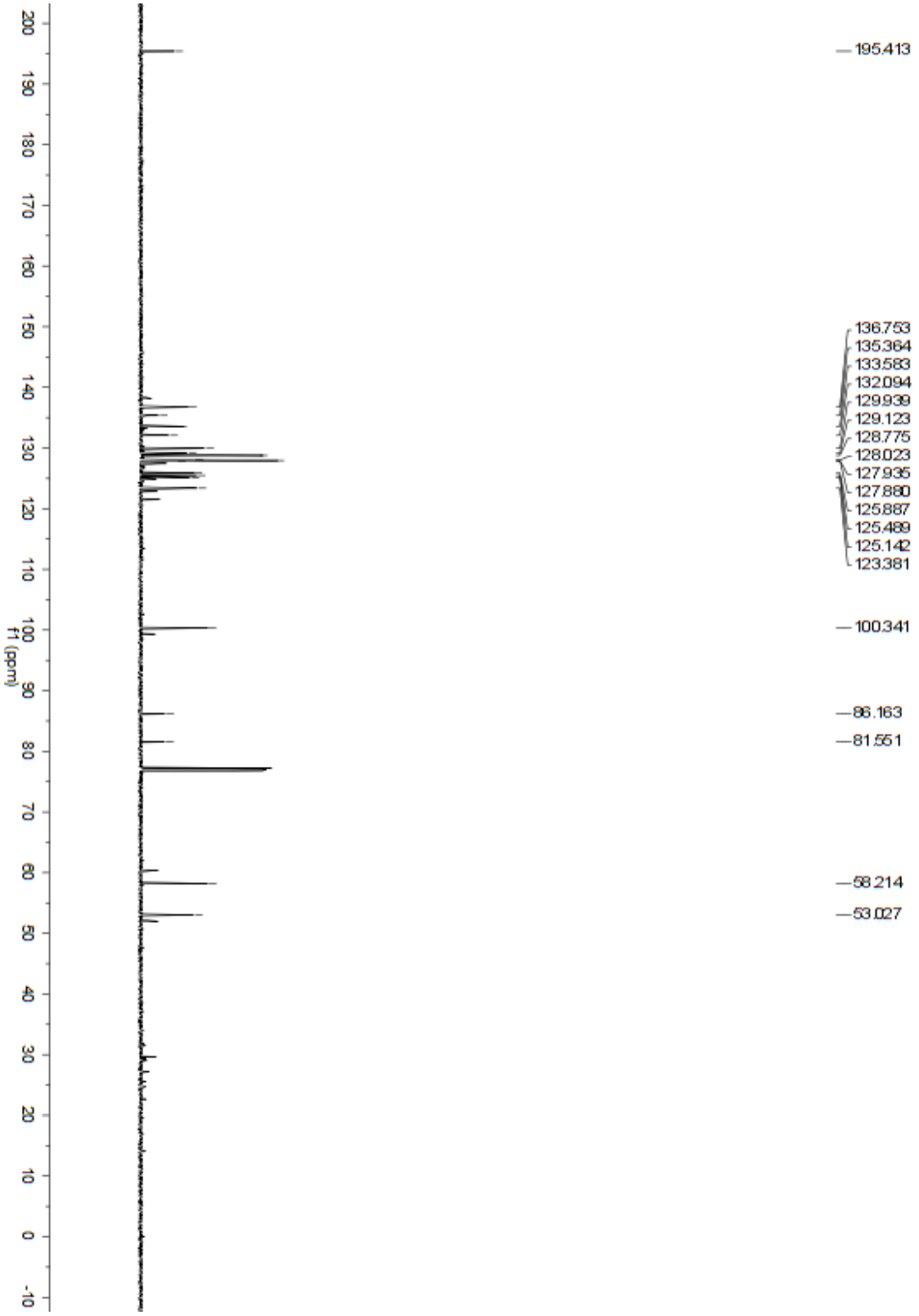
3o

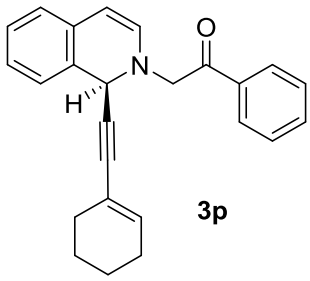

2.01
1.29
2.34
1.00
1.25
2.09
1.29
1.03
1.13
1.00
1.00
1.00
1.02
1.08
f1 (ppm)


7.987
7.986
7.975
7.972
7.594
7.592
7.579
7.569
7.567
7.564
7.475
7.463
7.460
7.347
7.345
7.342
7.340
7.261
7.249
7.197
7.192
7.189
7.184
7.180
7.178
7.168
7.165
7.155
7.153
7.097
7.095
7.085
7.082
7.072
7.070
7.017
7.015
7.008
7.006
6.963
6.961
6.950
6.948
6.139
6.126
5.677
5.547
5.534
4.956
4.927
4.492
4.463

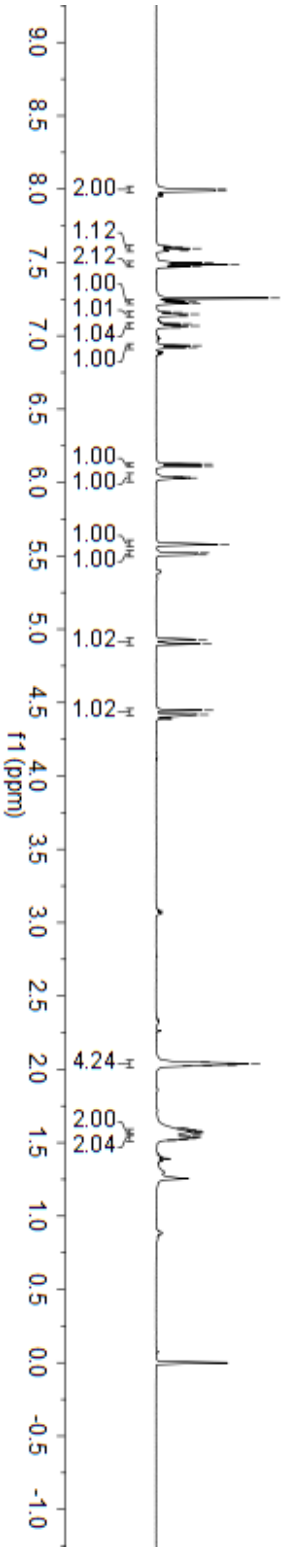

O
N
Ph
H
S

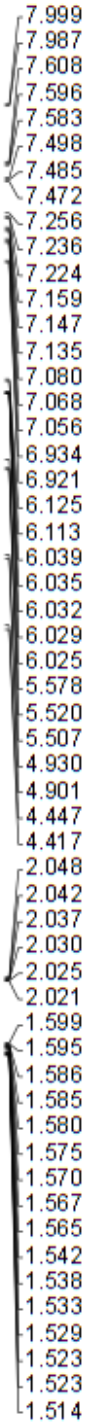
3o

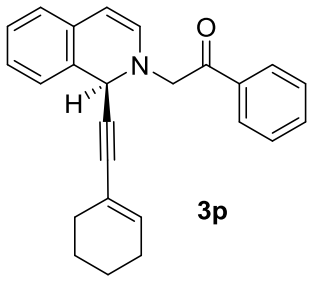

195.413
136.753
135.364
133.583
132.094
129.939
129.123
128.775
128.023
127.935
127.880
125.887
125.489
125.142
123.381
100.341
86.163
81.551
58.214
53.027
f1 (ppm)


O
N
H

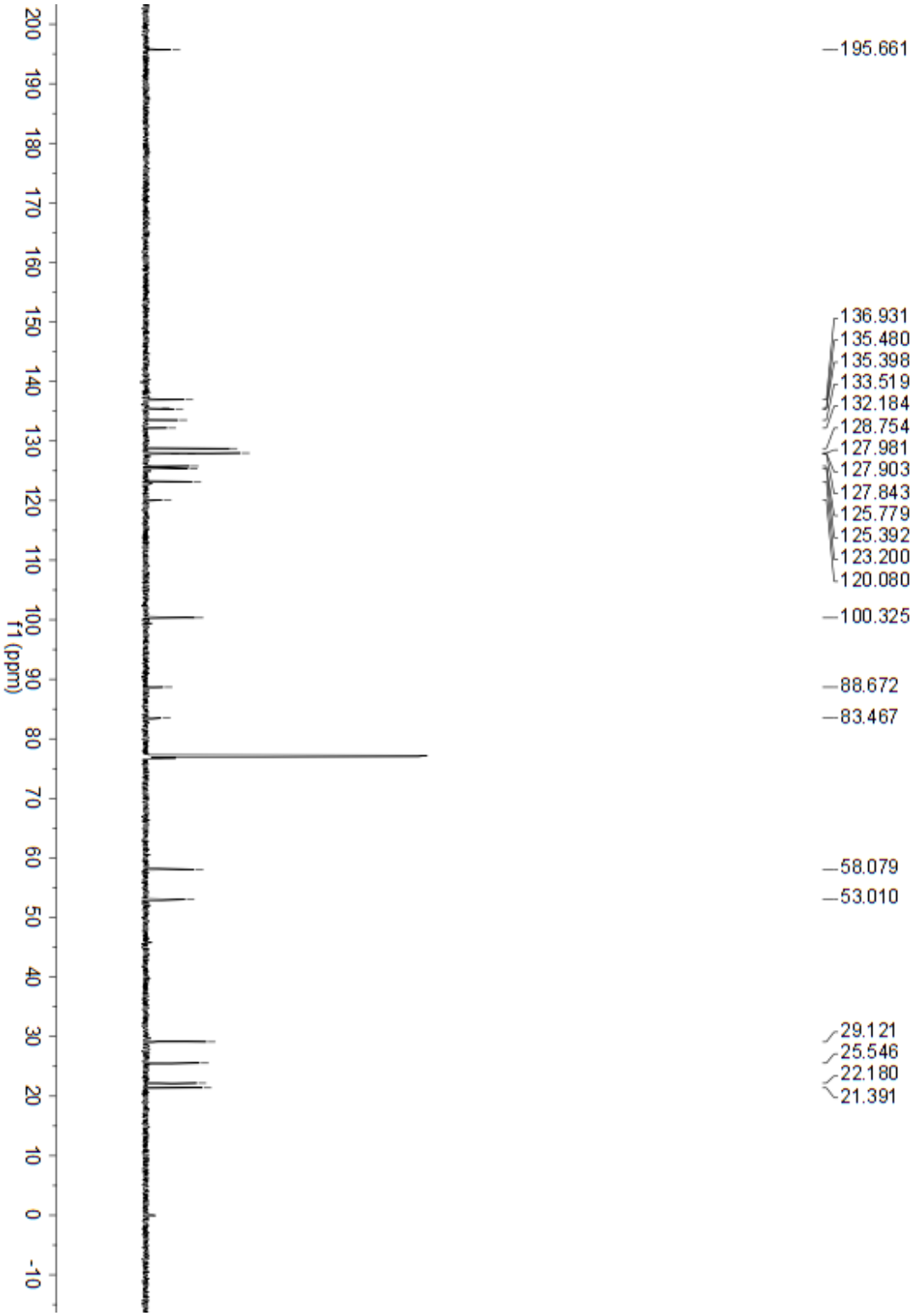
3p

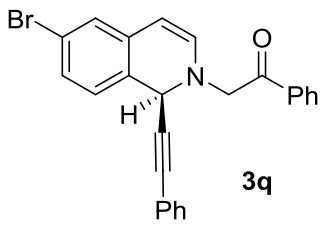

2.00
1.12
2.12
1.00
1.01
1.04
1.00
1.00
1.00
1.00
1.00
1.00
1.02
1.02
4.24
2.00
2.04
f1 (ppm)


7.999
7.987
7.608
7.596
7.583
7.498
7.485
7.472
7.256
7.236
7.224
7.159
7.147
7.135
7.080
7.068
7.056
6.934
6.921
6.125
6.113
6.039
6.035
6.032
6.029
6.025
5.578
5.520
5.507
4.930
4.901
4.447
4.417
2.048
2.042
2.037
2.030
2.025
2.021
1.599
1.595
1.586
1.585
1.580
1.575
1.570
1.567
1.565
1.542
1.538
1.533
1.529
1.523
1.523
1.514

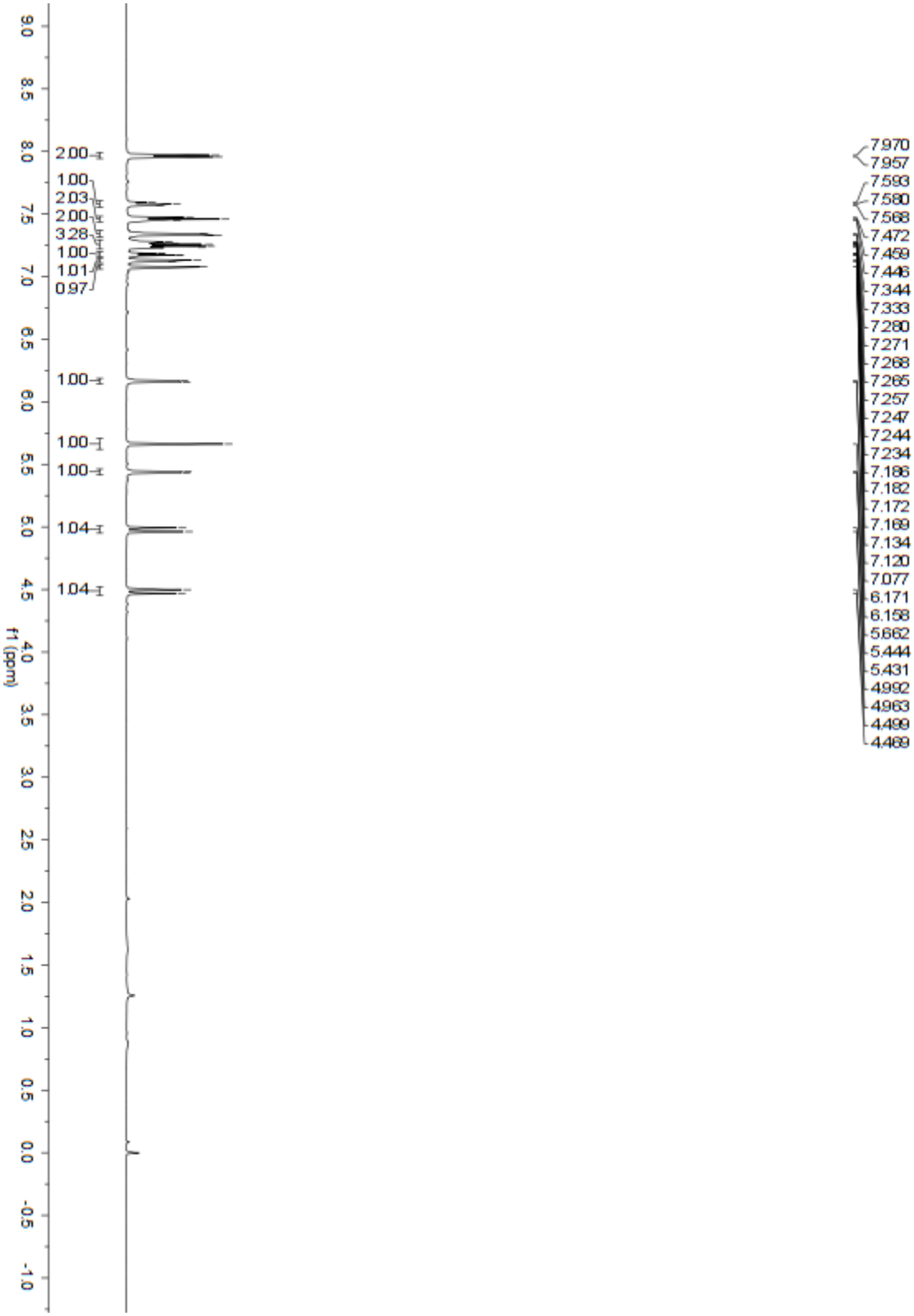

O
N
H

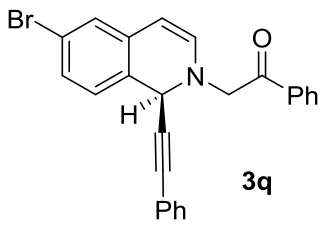
3p


f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
195.661
136.931
135.480
135.398
133.519
132.184
128.754
127.981
127.903
127.843
125.779
125.392
123.200
120.080
100.325
88.672
83.467
58.079
53.010
29.121
25.546
22.180
21.391

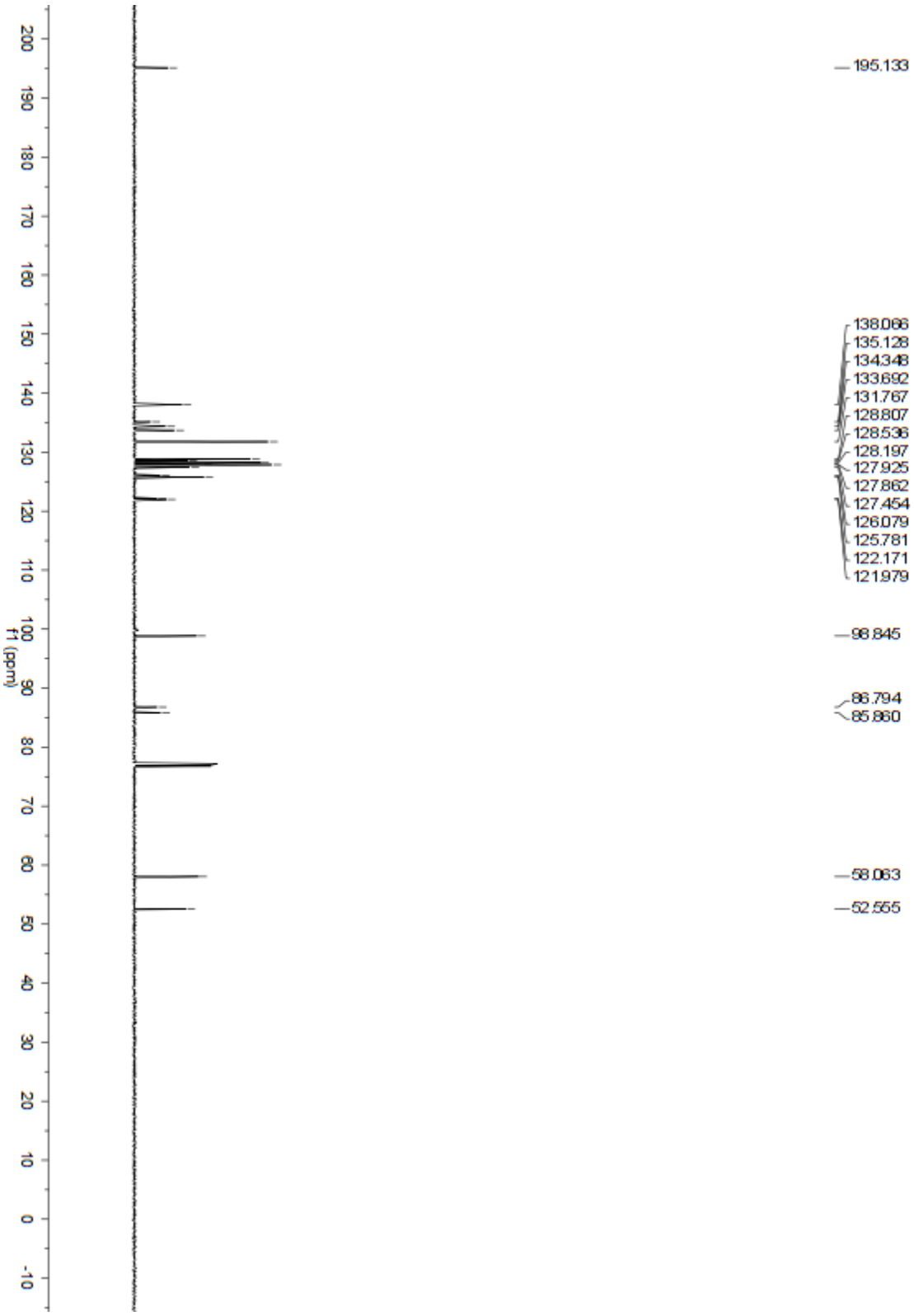

Br
O
N
Ph
H
Ph

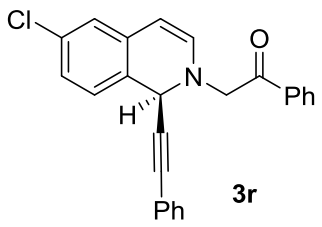
3q


2.00
1.00
2.03
2.00
3.28
1.00
1.01
0.97
1.00
1.00
1.00
1.04
1.04
f1 (ppm)
7.970
7.957
7.593
7.580
7.568
7.472
7.459
7.446
7.344
7.333
7.280
7.271
7.268
7.265
7.257
7.247
7.244
7.234
7.186
7.182
7.172
7.169
7.134
7.120
7.077
6.171
6.158
5.662
5.444
5.431
4.992
4.963
4.499
4.469

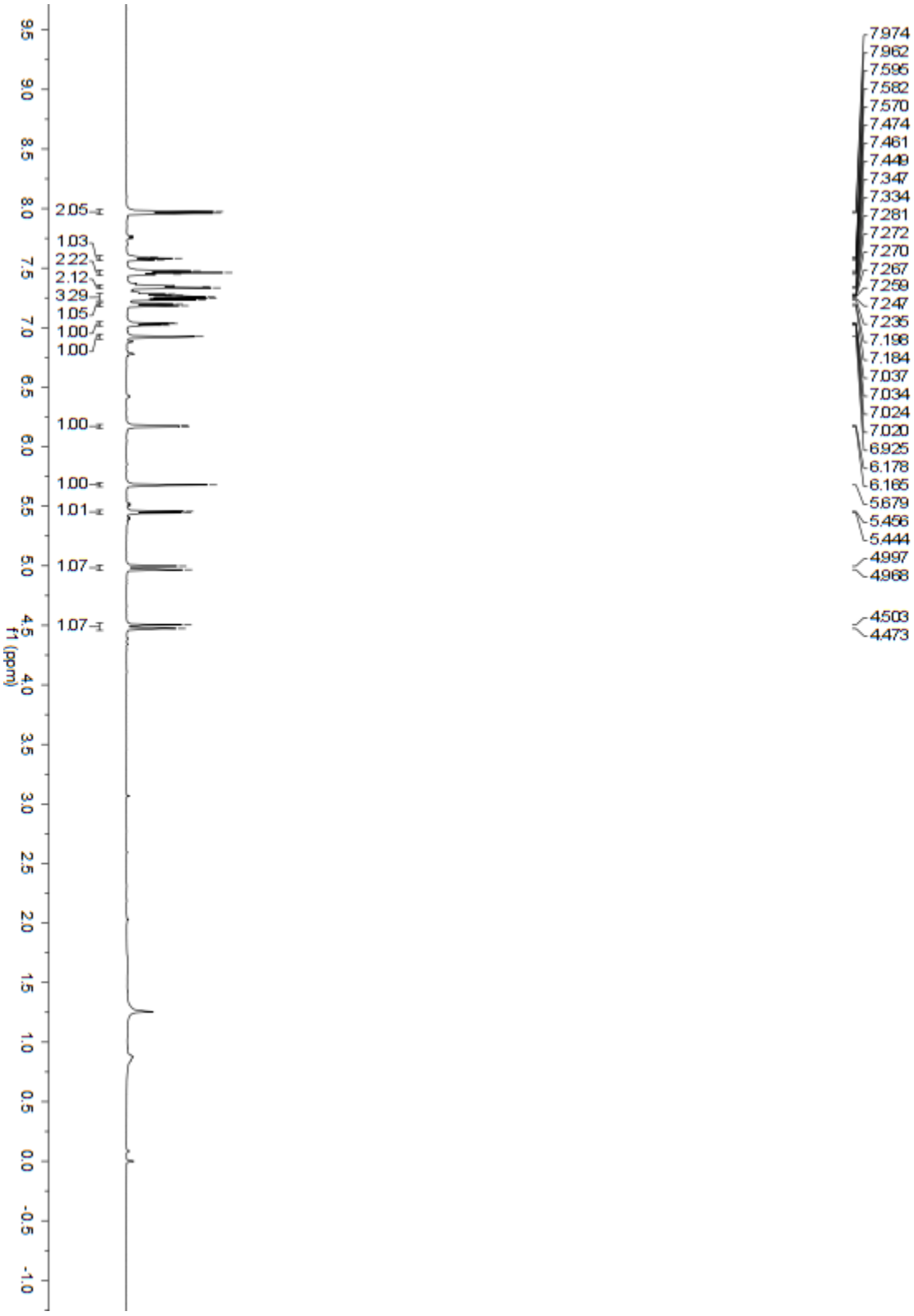

Br
O
N
Ph
H
Ph

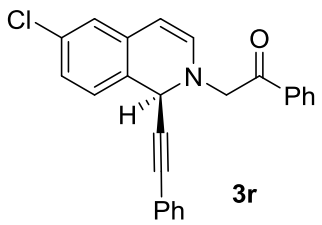
3q


195.133
138.066
135.128
134.348
133.692
131.767
128.807
128.536
128.197
127.925
127.862
127.454
126.079
125.781
122.171
121.979
98.845
86.794
85.860
58.063
52.555
f1 (ppm)

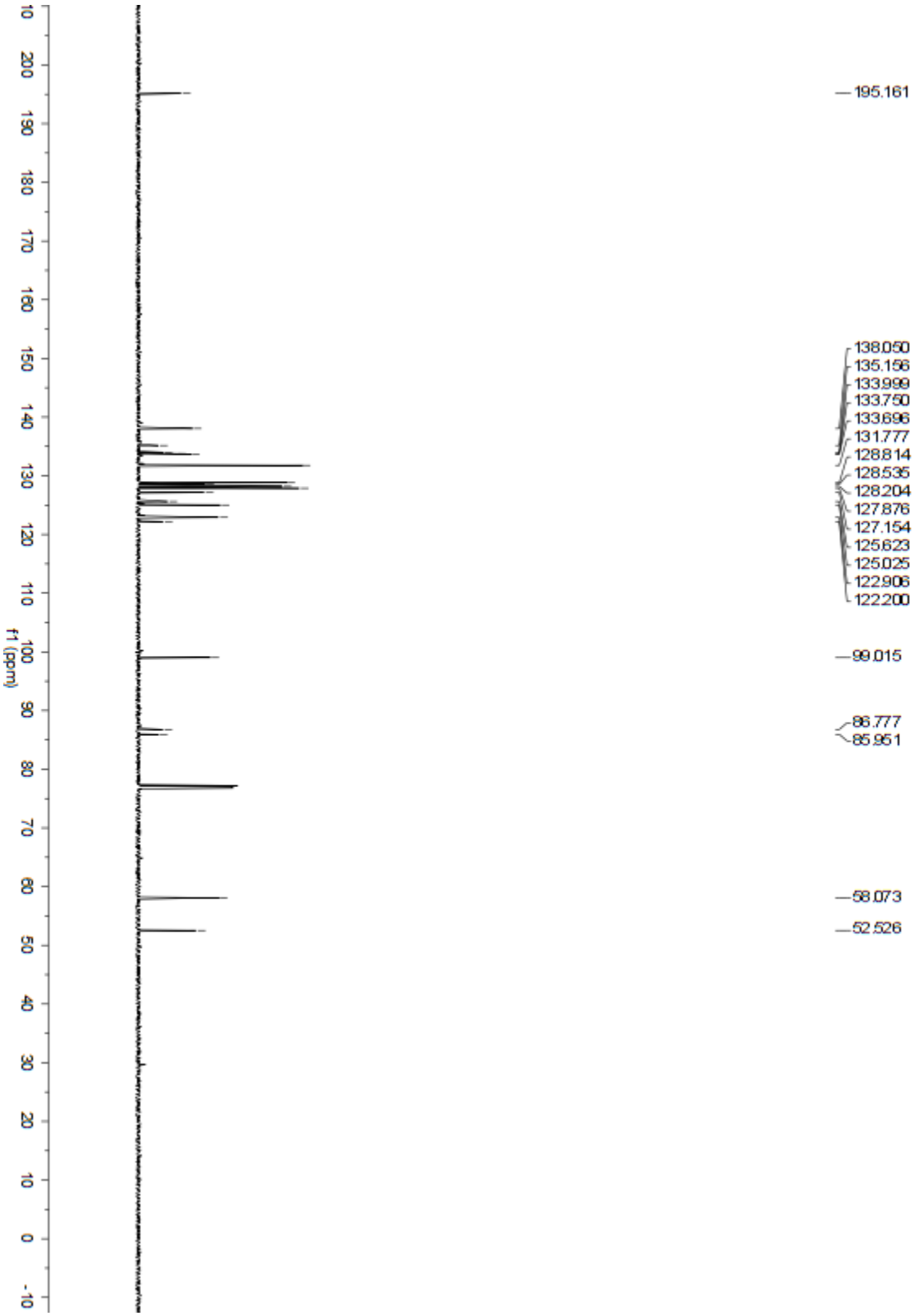

Cl
O
N
Ph
H
Ph

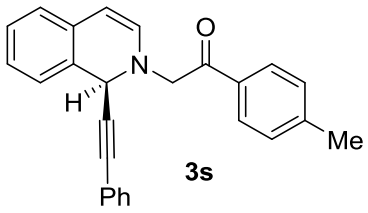
3r


2.05
1.03
2.22
2.12
3.29
1.05
1.00
1.00
1.00
1.00
1.01
1.07
1.07
f1 (ppm)
7.974
7.962
7.595
7.582
7.570
7.474
7.461
7.449
7.347
7.334
7.281
7.272
7.270
7.267
7.259
7.247
7.235
7.198
7.184
7.037
7.034
7.024
7.020
6.925
6.178
6.165
5.679
5.456
5.444
4.997
4.968
4.503
4.473

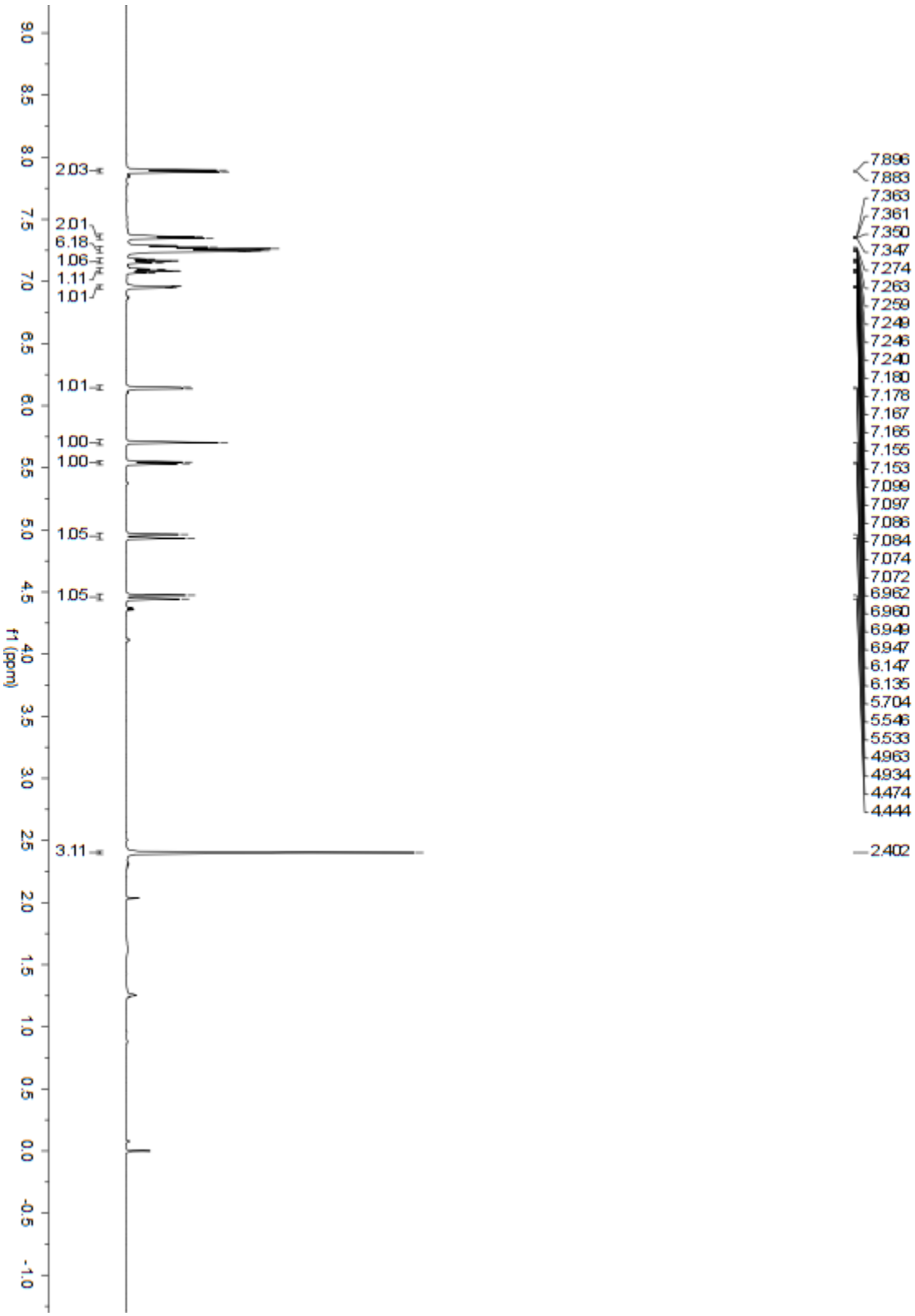

Cl
O
N
Ph
H
Ph

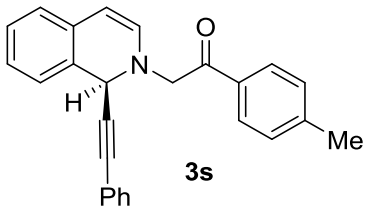
3r


f1 (ppm)
195.161
138.050
135.156
133.999
133.750
133.696
131.777
128.814
128.535
128.204
127.876
127.154
125.623
125.025
122.906
122.200
99.015
86.777
85.951
58.073
52.526

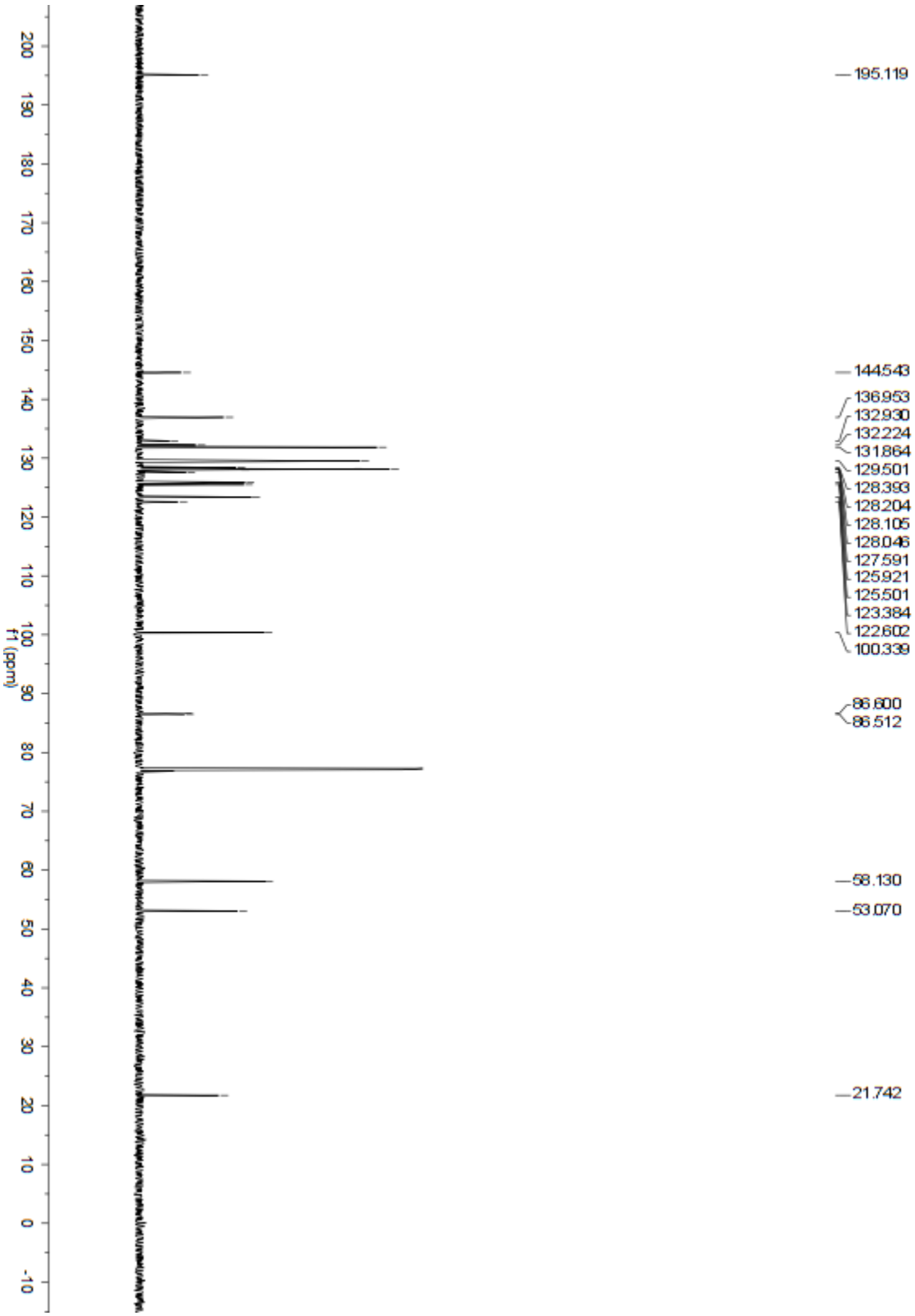

O
N
H
Me
Ph

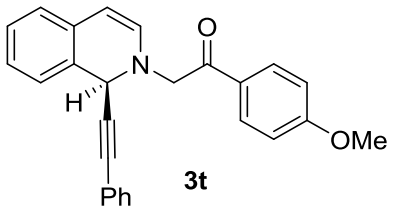
3s


2.03
2.01
6.18
1.06
1.11
1.01
1.01
1.00
1.00
1.05
1.05
3.11
f1 (ppm)
7.896
7.883
7.363
7.361
7.350
7.347
7.274
7.263
7.259
7.249
7.246
7.240
7.180
7.178
7.167
7.165
7.155
7.153
7.099
7.097
7.086
7.084
7.074
7.072
6.962
6.960
6.949
6.947
6.147
6.135
5.704
5.546
5.533
4.963
4.934
4.474
4.444
2.402

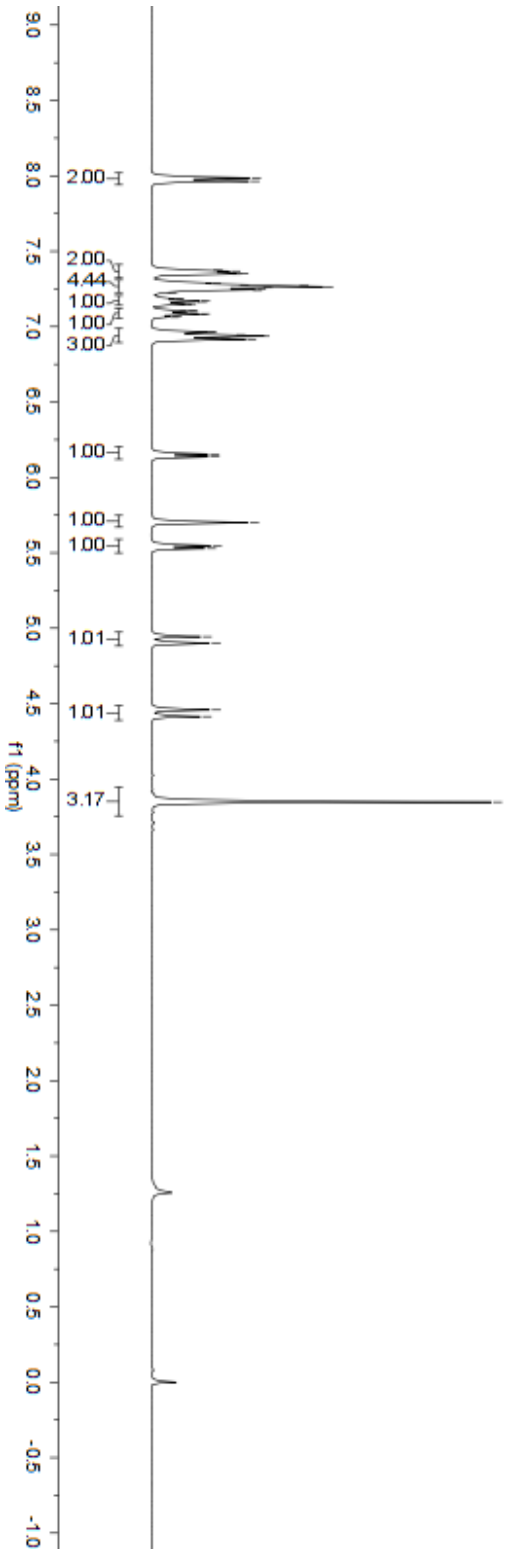

O
N
H
Me
Ph

3s

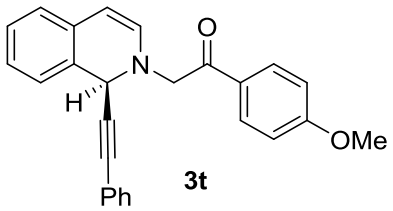

195.119
144.543
136.953
132.930
132.224
131.864
129.501
128.393
128.204
128.105
128.046
127.591
125.921
125.501
123.384
122.602
100.339
86.600
86.512
58.130
53.070
21.742
f1 (ppm)


O
N
H
OMe
Ph

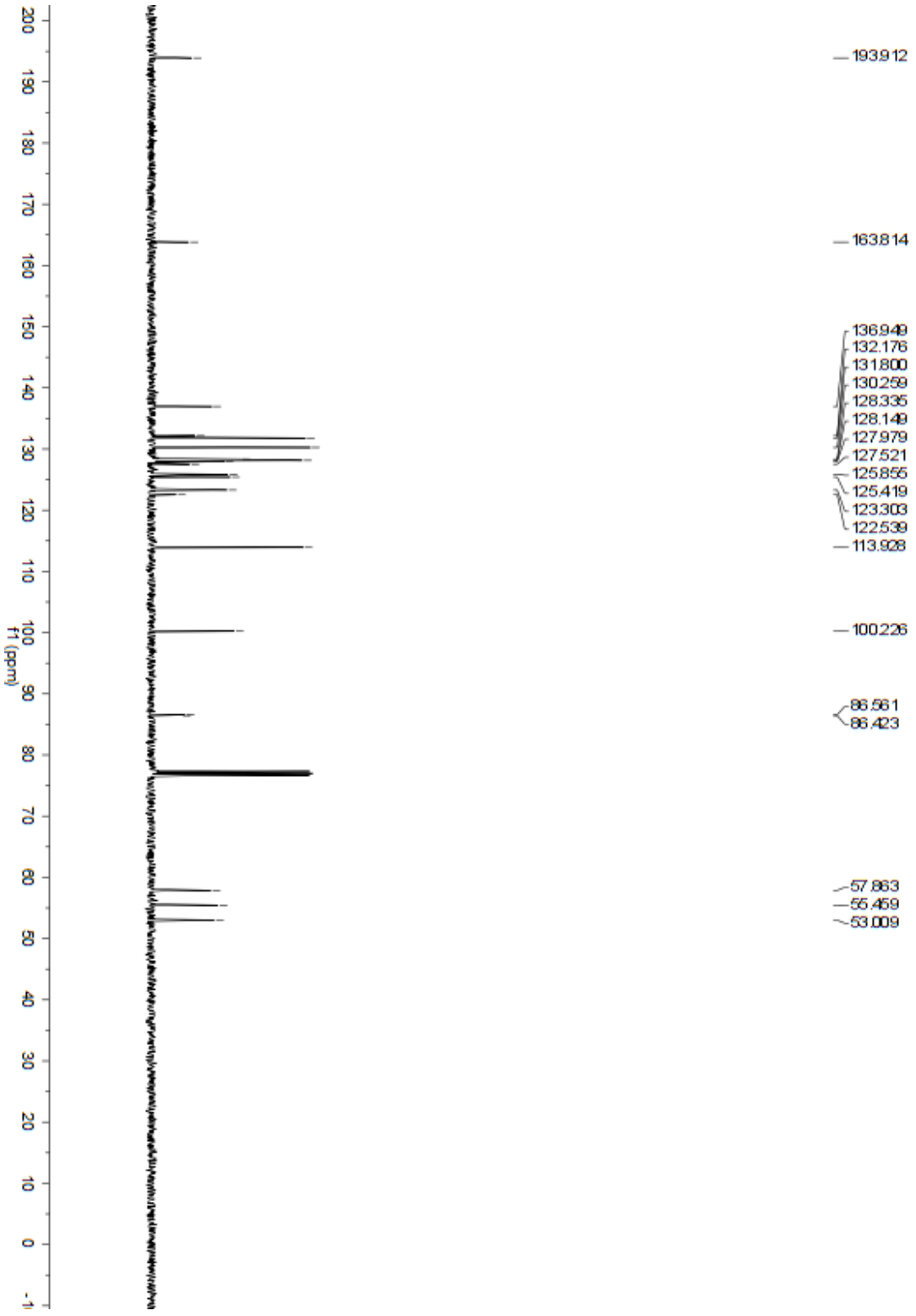
3t

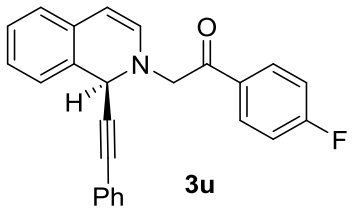

2.00
2.00
4.44
1.00
1.00
3.00
1.00
1.00
1.00
1.01
1.01
3.17
f1 (ppm)


7.986
7.964
7.373
7.368
7.363
7.354
7.348
7.290
7.278
7.270
7.264
7.259
7.246
7.242
7.225
7.186
7.182
7.169
7.165
7.150
7.146
7.104
7.100
7.085
7.082
7.067
7.063
6.965
6.961
6.945
6.936
6.919
6.914
6.155
6.136
5.701
5.547
5.529
4.944
4.900
4.458
4.414
3.847

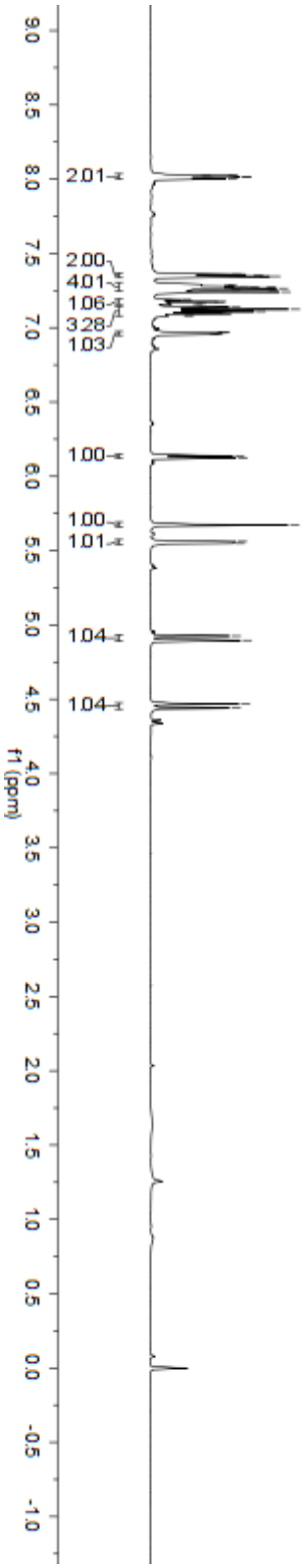

O
N
H
OMe
Ph

3t

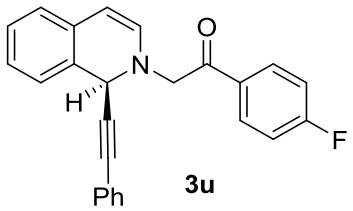

193.912
163.814
136.949
132.176
131.800
130.259
128.335
128.149
127.979
127.521
125.855
125.419
123.303
122.539
113.928
100.226
86.561
86.423
57.863
55.459
53.009
f1 (ppm)


O
N
H
F
Ph

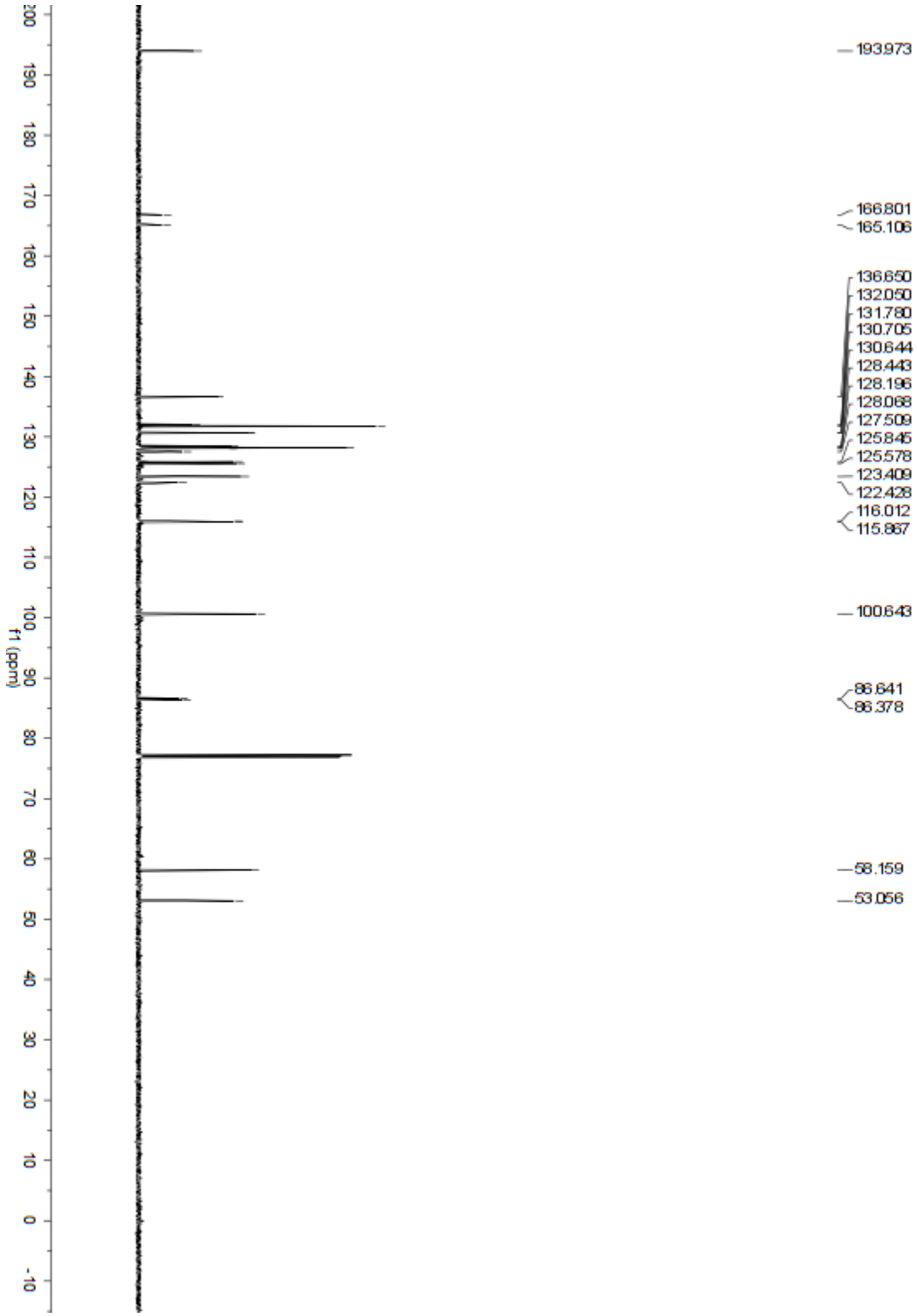
3u

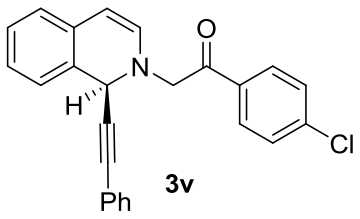

2.01
2.00
4.01
1.06
3.28
1.03
1.00
1.00
1.01
1.04
1.04
f1 (ppm)


8.026
8.023
8.017
8.012
8.006
8.003
7.359
7.356
7.346
7.343
7.289
7.283
7.278
7.275
7.272
7.269
7.265
7.256
7.252
7.241
7.188
7.185
7.175
7.173
7.163
7.160
7.138
7.134
7.124
7.113
7.109
7.106
7.096
7.093
7.083
7.081
6.968
6.966
6.955
6.953
6.138
6.126
5.674
5.562
5.549
4.926
4.896
4.469
4.440

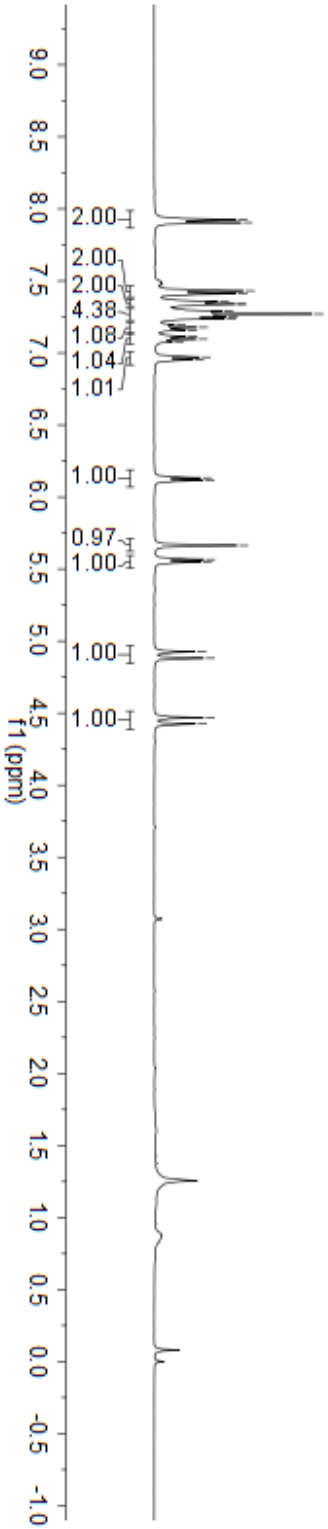

O
N
H
F
Ph

3u

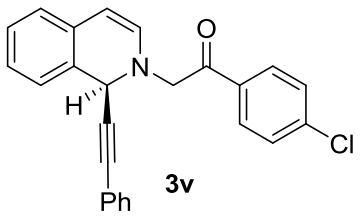

193.973
166.801
165.106
136.650
132.050
131.780
130.705
130.644
128.443
128.196
128.068
127.509
125.845
125.578
123.409
122.428
116.012
115.867
100.643
86.641
86.378
58.159
53.056
f1 (ppm)


O
N
H
Cl
Ph

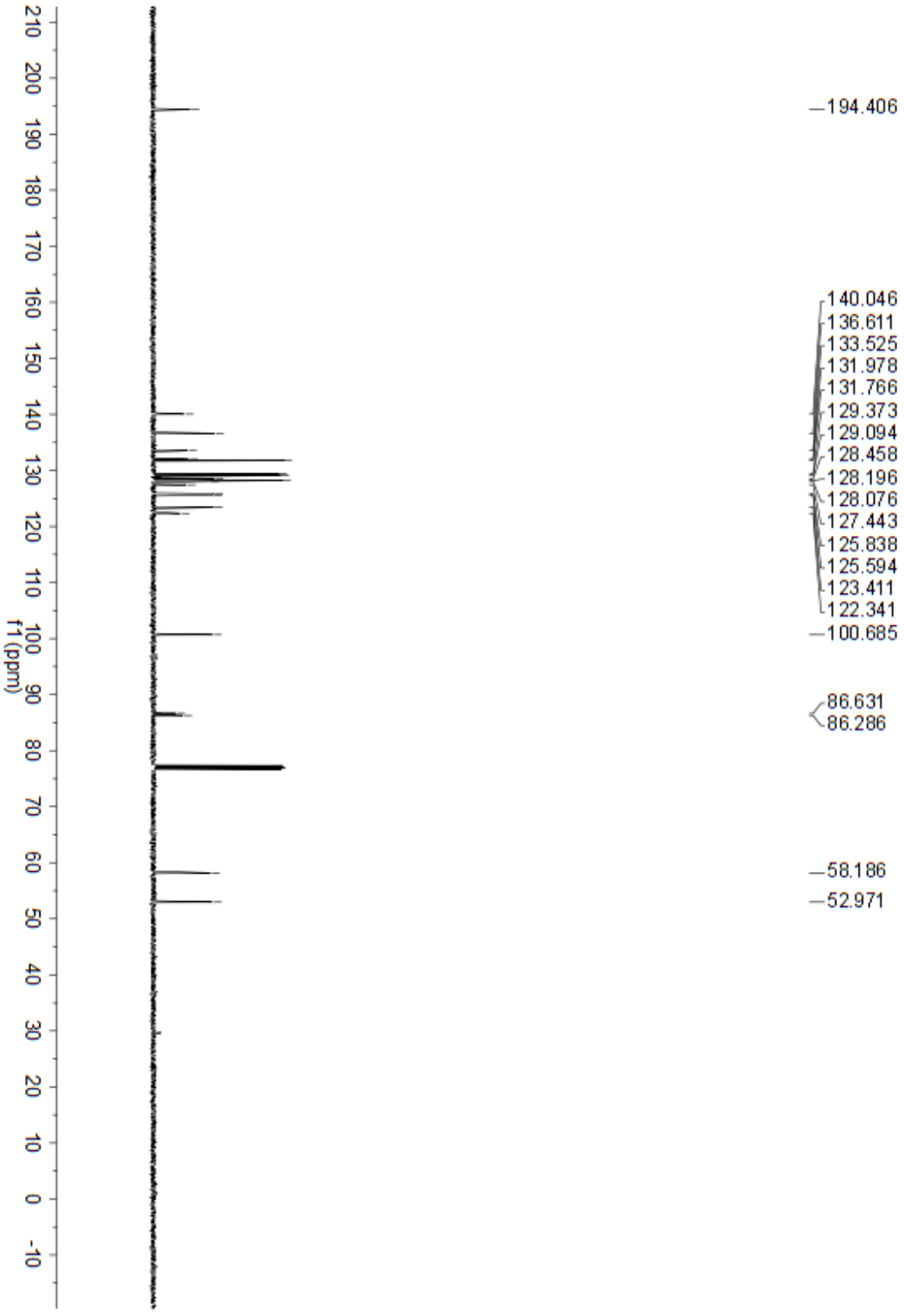
3v

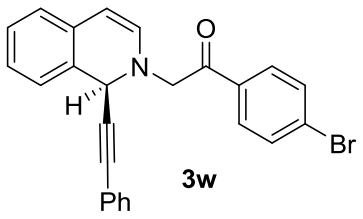

2.00
2.00
2.00
4.38
1.08
1.04
1.01
1.00
0.97
1.00
1.00
1.00
f1 (ppm)


7.926
7.905
7.432
7.411
7.356
7.340
7.337
7.289
7.271
7.252
7.239
7.195
7.177
7.159
7.114
7.096
7.078
6.971
6.952
6.133
6.115
5.664
5.567
5.548
4.926
4.882
4.469
4.425

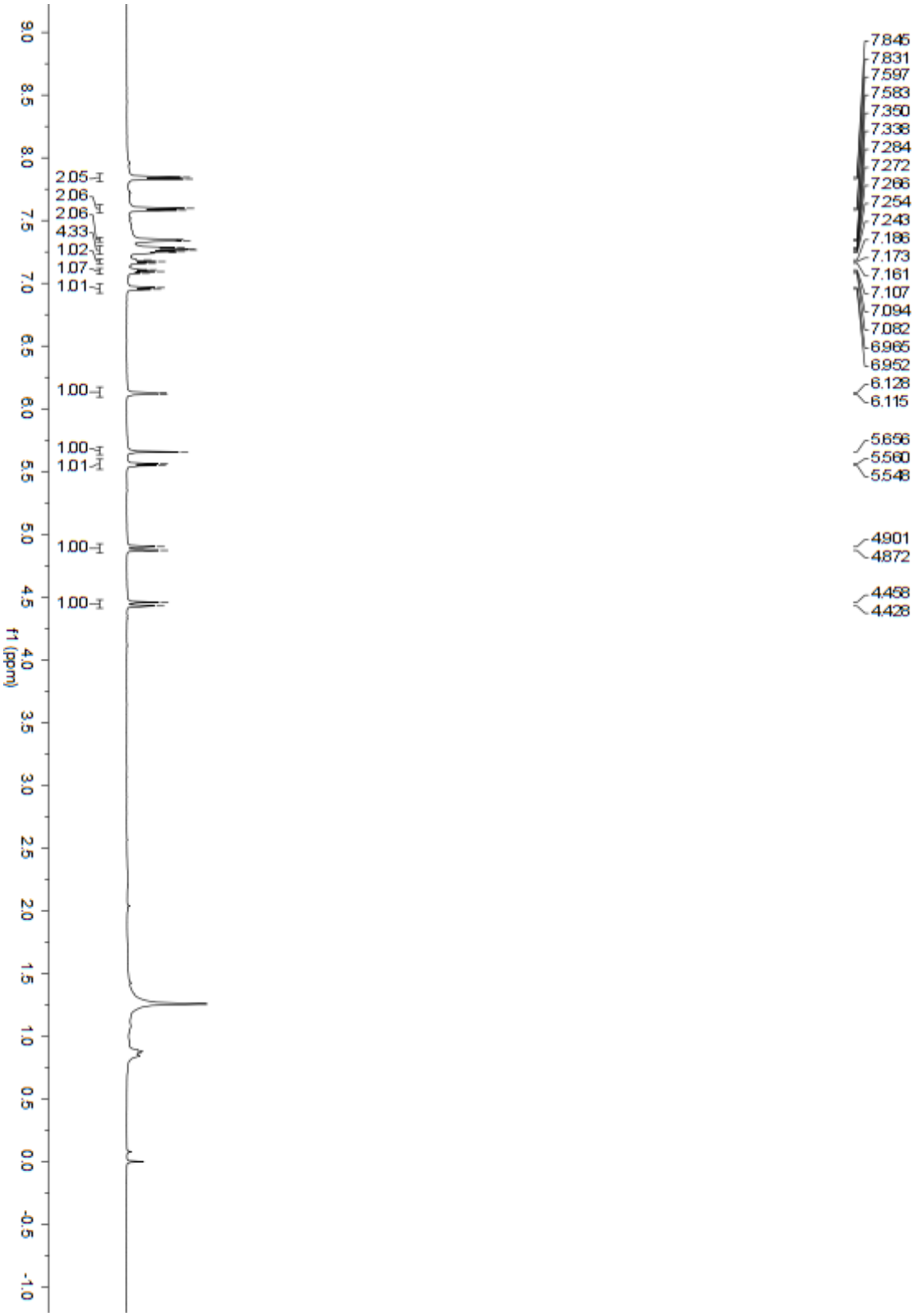

O
N
H
Cl
Ph

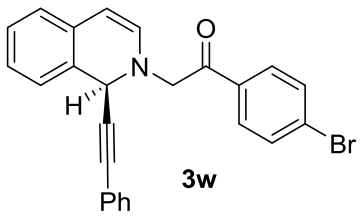
3v


f1 (ppm)
194.406
140.046
136.611
133.525
131.978
131.766
129.373
129.094
128.458
128.196
128.076
127.443
125.838
125.594
123.411
122.341
100.685
86.631
86.286
58.186
52.971

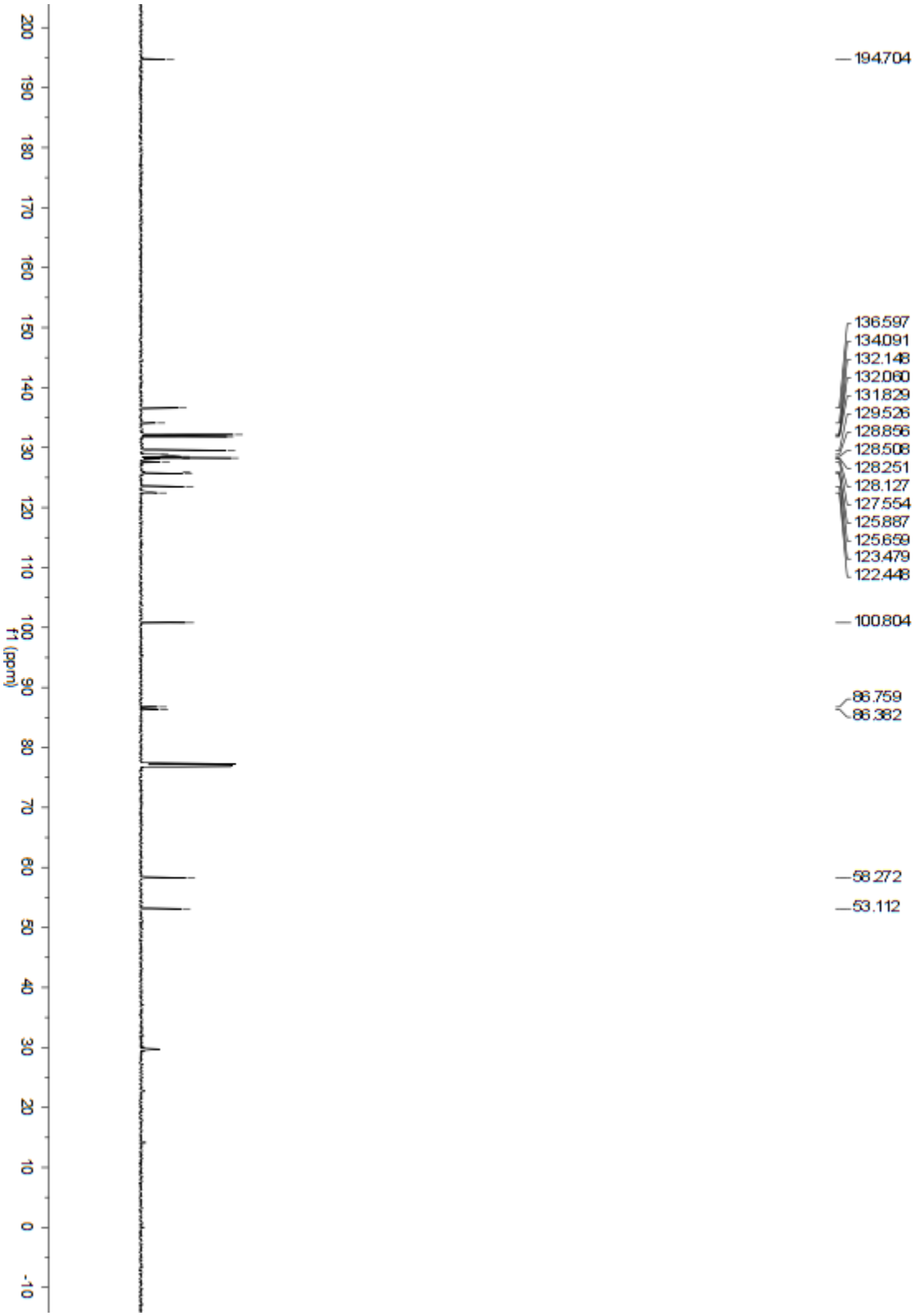

O
N
H
Br
Ph

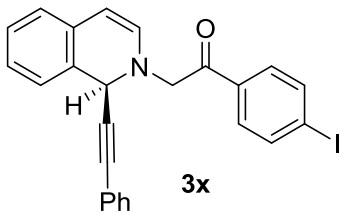
3w


2.05
2.06
2.06
4.33
1.02
1.07
1.01
1.00
1.00
1.01
1.00
1.00
f1 (ppm)
7.845
7.831
7.597
7.583
7.350
7.338
7.284
7.272
7.266
7.254
7.243
7.186
7.173
7.161
7.107
7.094
7.082
6.965
6.952
6.128
6.115
5.656
5.560
5.548
4.901
4.872
4.458
4.428

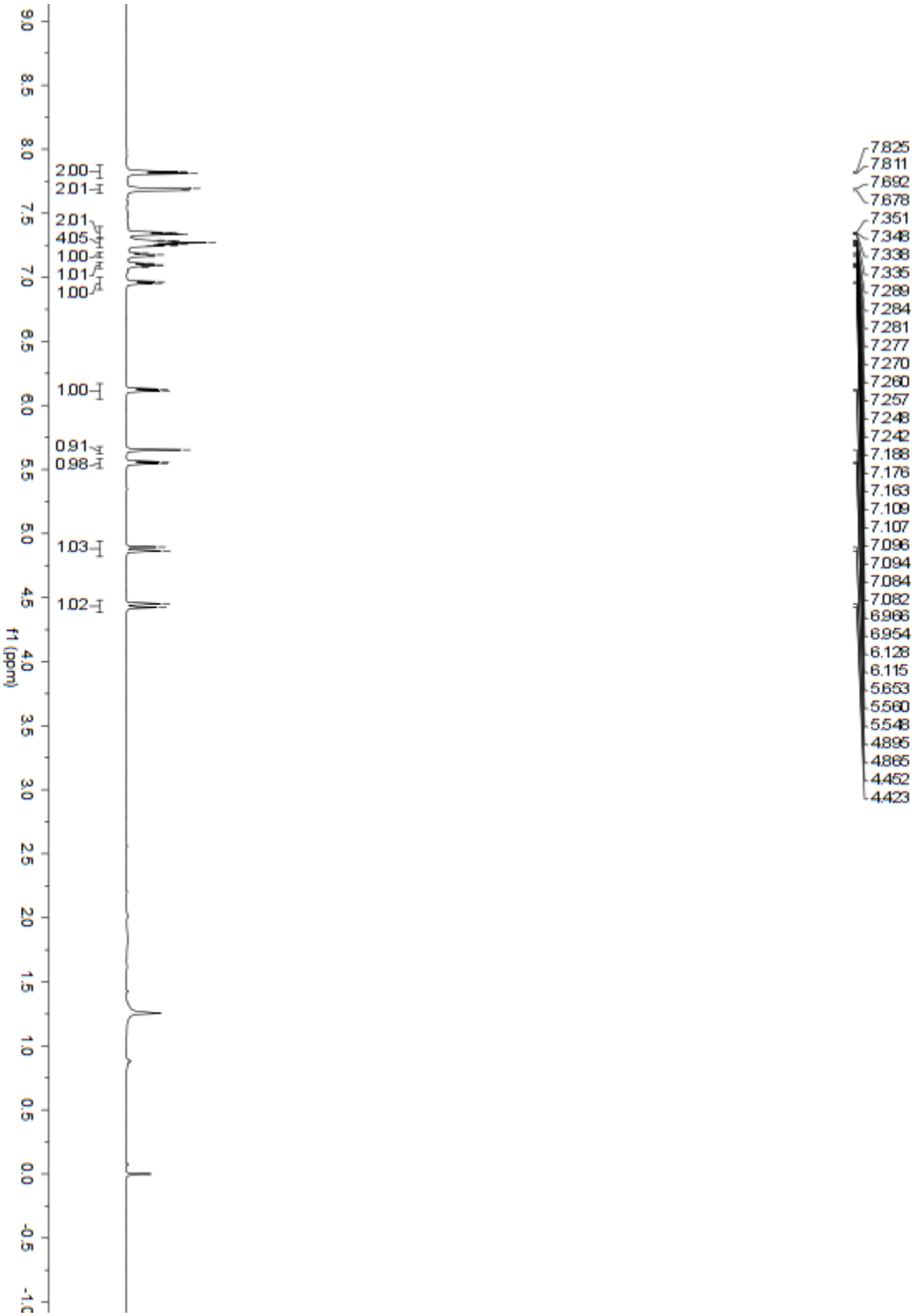

O
N
H
Br
Ph

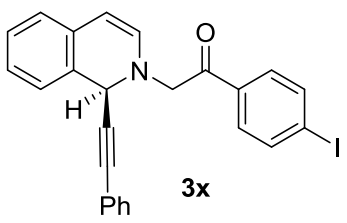
3w


194.704
136.597
134.091
132.148
132.060
131.829
129.526
128.856
128.508
128.251
128.127
127.554
125.887
125.659
123.479
122.448
100.804
86.759
86.382
58.272
53.112
f1 (ppm)

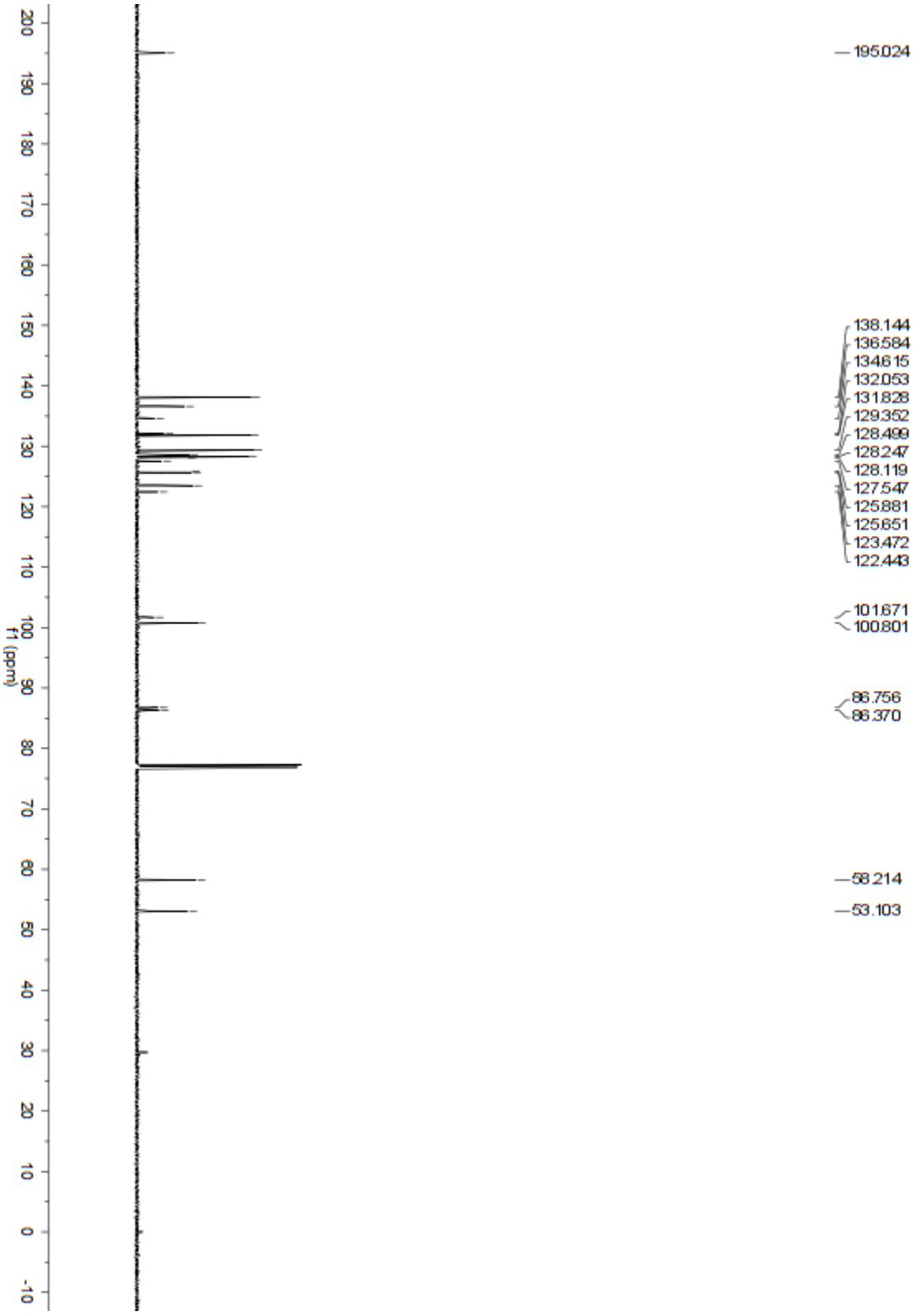

O
N
H
I
Ph

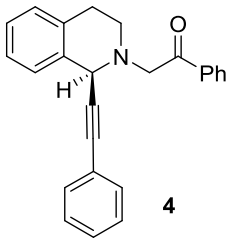
3x


2.00
2.01
2.01
4.05
1.00
1.01
1.00
1.00
0.91
0.98
1.03
1.02
f1 (ppm)
7.825
7.811
7.692
7.678
7.351
7.348
7.338
7.335
7.289
7.284
7.281
7.277
7.270
7.260
7.257
7.248
7.242
7.188
7.176
7.163
7.109
7.107
7.096
7.094
7.084
7.082
6.966
6.954
6.128
6.115
5.653
5.560
5.548
4.895
4.865
4.452
4.423

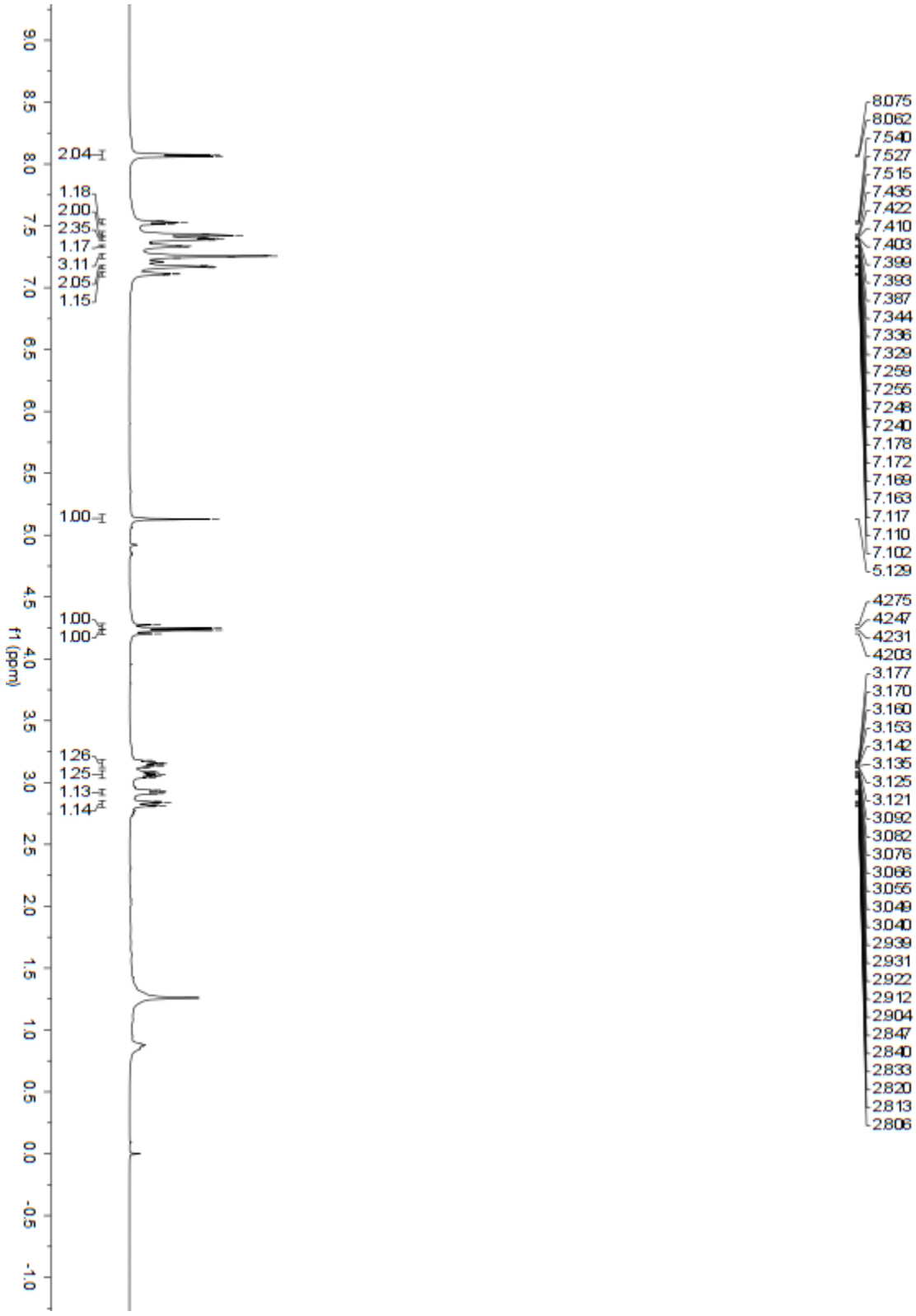

O
N
H
I
Ph

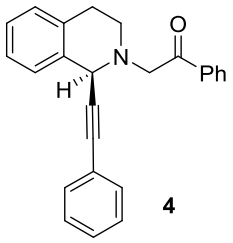
3x


195.024
138.144
136.584
134.615
132.053
131.828
129.352
128.499
128.247
128.119
127.547
125.881
125.651
123.472
122.443
101.671
100.801
86.756
86.370
58.214
53.103
f1 (ppm)

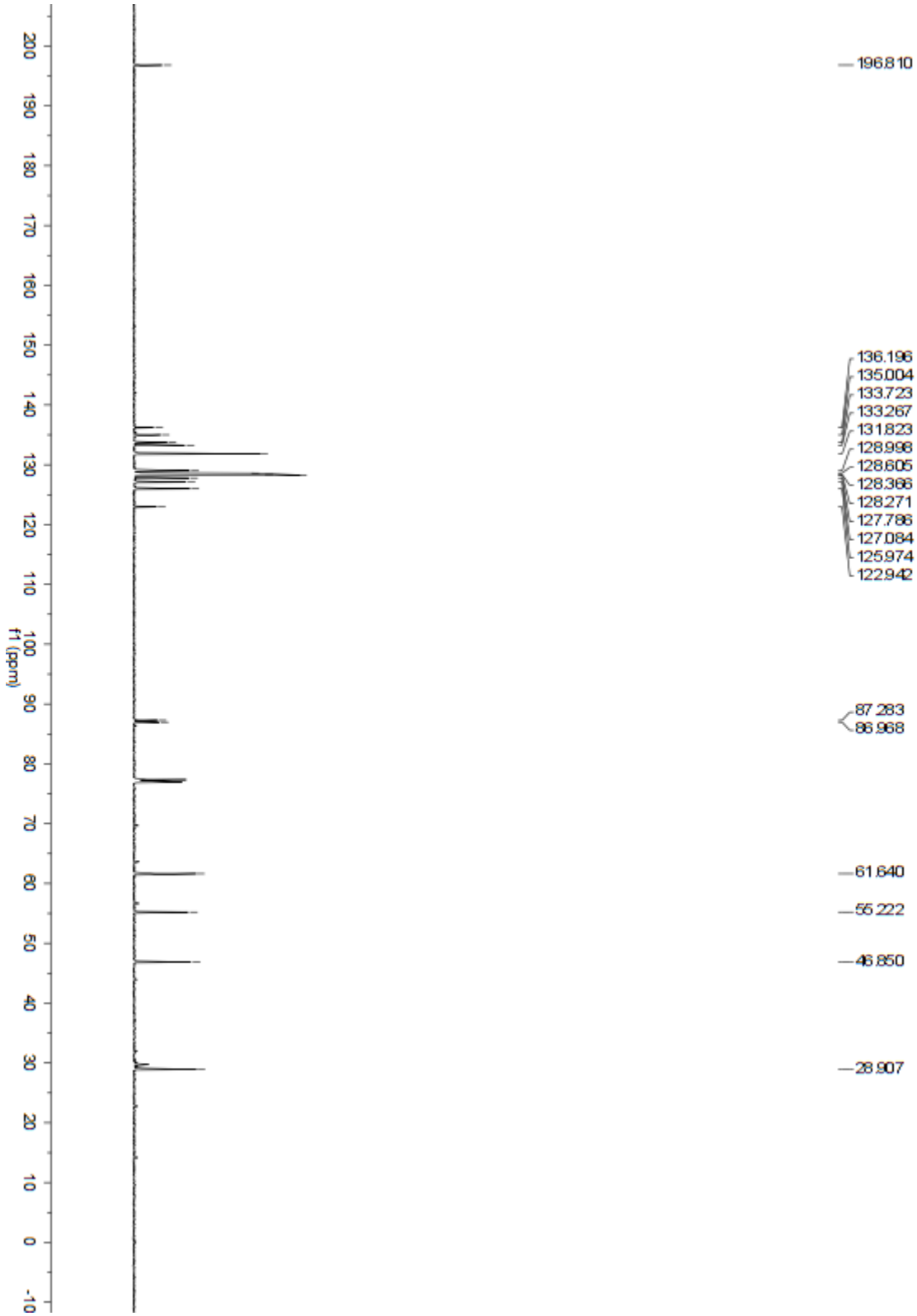

O
N
Ph
H

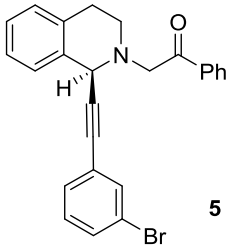
4


f1 (ppm)
2.04
1.18
2.00
2.35
1.17
3.11
2.05
1.15
1.00
1.00
1.00
1.26
1.25
1.13
1.14
8.075
8.062
7.540
7.527
7.515
7.435
7.422
7.410
7.403
7.399
7.393
7.387
7.344
7.336
7.329
7.259
7.255
7.248
7.240
7.178
7.172
7.169
7.163
7.117
7.110
7.102
5.129
4.275
4.247
4.231
4.203
3.177
3.170
3.160
3.153
3.142
3.135
3.125
3.121
3.092
3.082
3.076
3.066
3.055
3.049
3.040
2.939
2.931
2.922
2.912
2.904
2.847
2.840
2.833
2.820
2.813
2.806

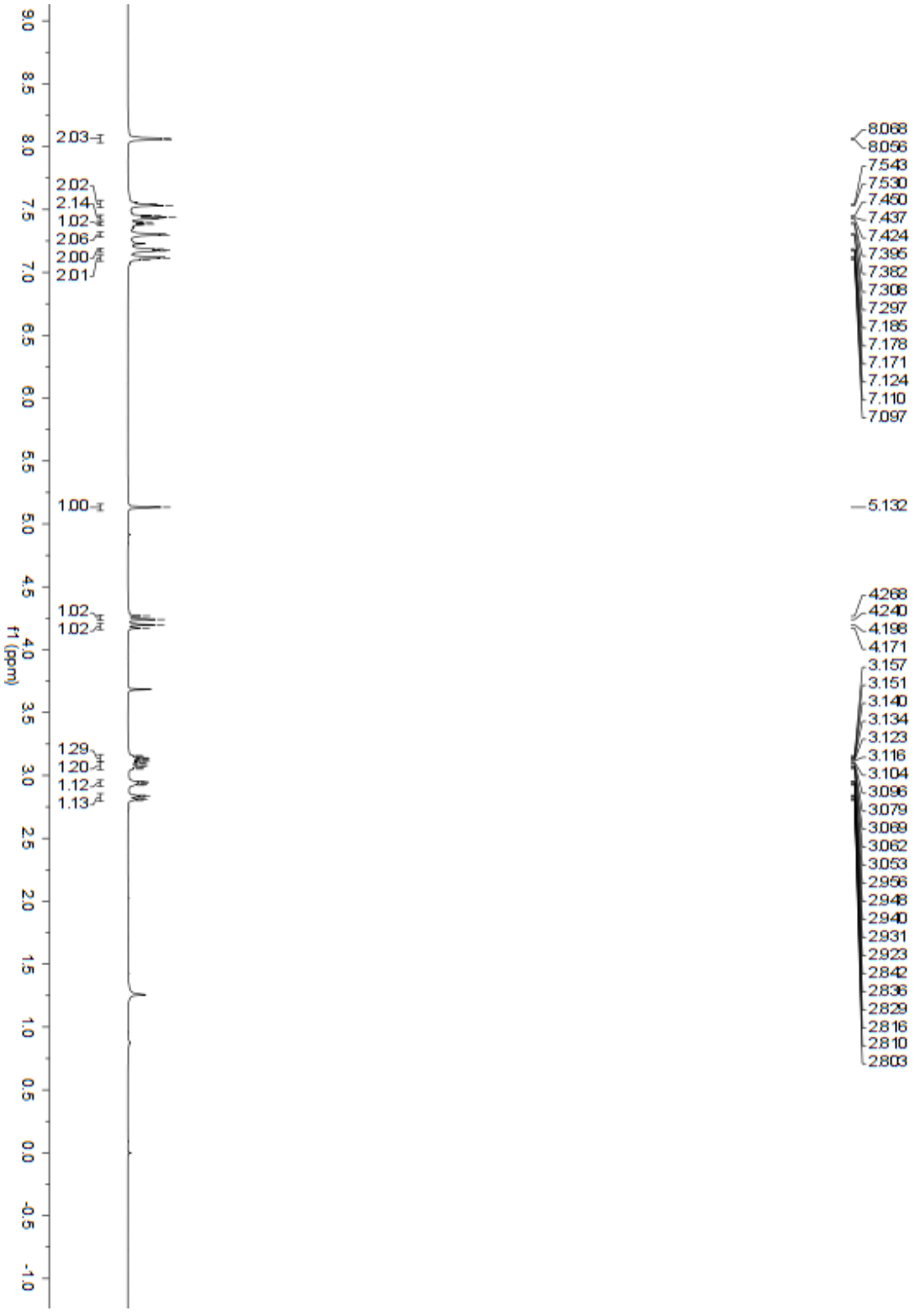

O
N
Ph
H

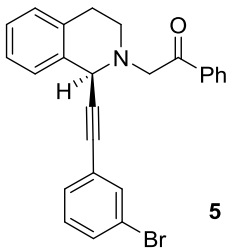
4


196.810
136.196
135.004
133.723
133.267
131.823
128.998
128.605
128.366
128.271
127.786
127.084
125.974
122.942
87.283
86.968
61.640
55.222
46.850
28.907
f1 (ppm)

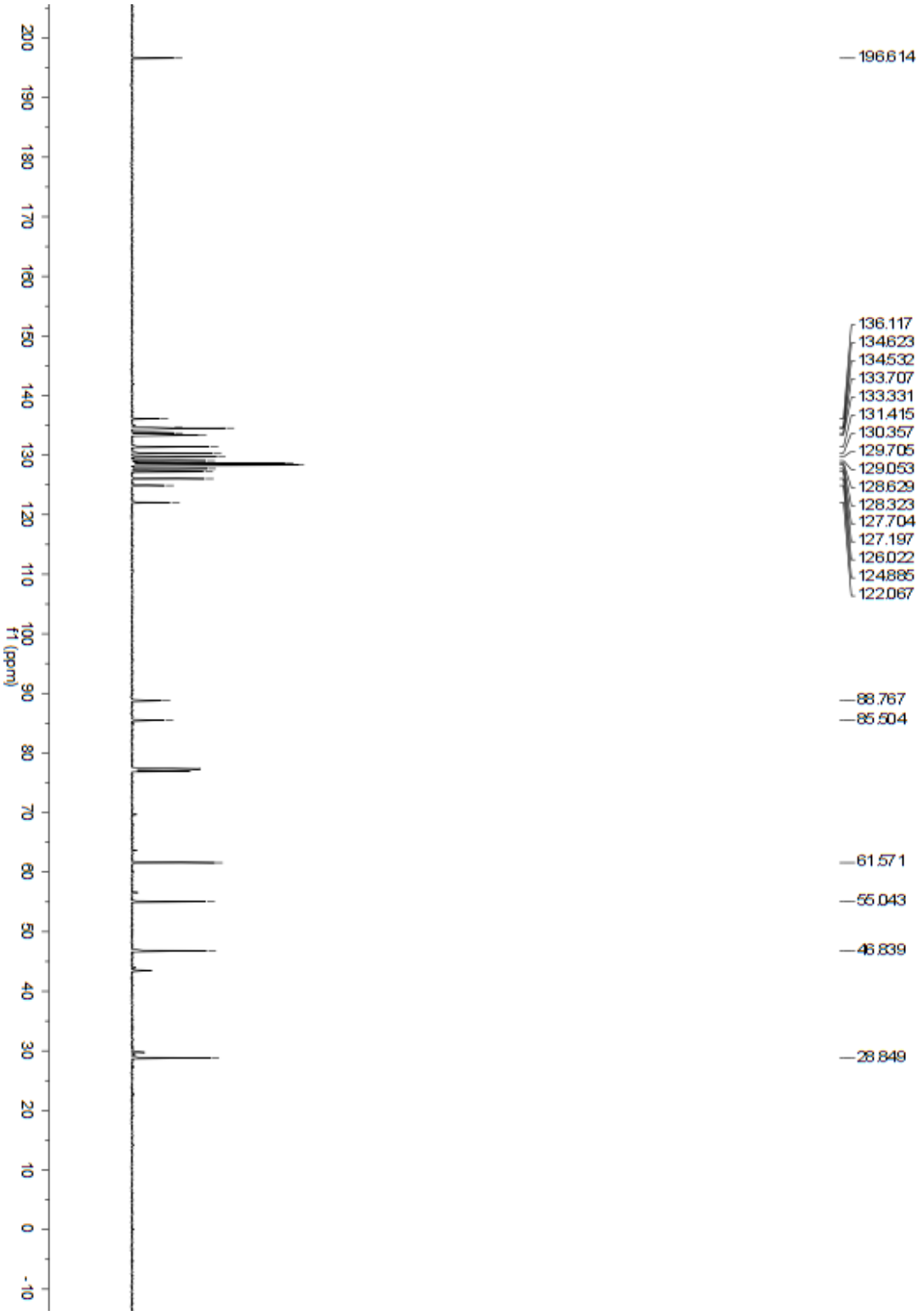

O
N
Ph
H
Br

5


f1 (ppm)
2.03
2.02
2.14
1.02
2.06
2.00
2.01
1.00
1.02
1.02
1.29
1.20
1.12
1.13
8.068
8.056
7.543
7.530
7.450
7.437
7.424
7.395
7.382
7.308
7.297
7.185
7.178
7.171
7.124
7.110
7.097
5.132
4.268
4.240
4.198
4.171
3.157
3.151
3.140
3.134
3.123
3.116
3.104
3.096
3.079
3.069
3.062
3.053
2.956
2.948
2.940
2.931
2.923
2.842
2.836
2.829
2.816
2.810
2.803


O
N
Ph
H
Br

5


196.614
136.117
134.623
134.532
133.707
133.331
131.415
130.357
129.705
129.053
128.629
128.323
127.704
127.197
126.022
124.885
122.067
88.767
85.504
61.571
55.043
46.839
28.849
f1 (ppm)