Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

New insights into copper-catalyzed cross-dehydrogenative-coupling of secondary amides and terminal alkynes: facile synthesis of ynamides

Shuang-Yan Zhuo, Jian-Liang Ye* and Xiao Zheng*

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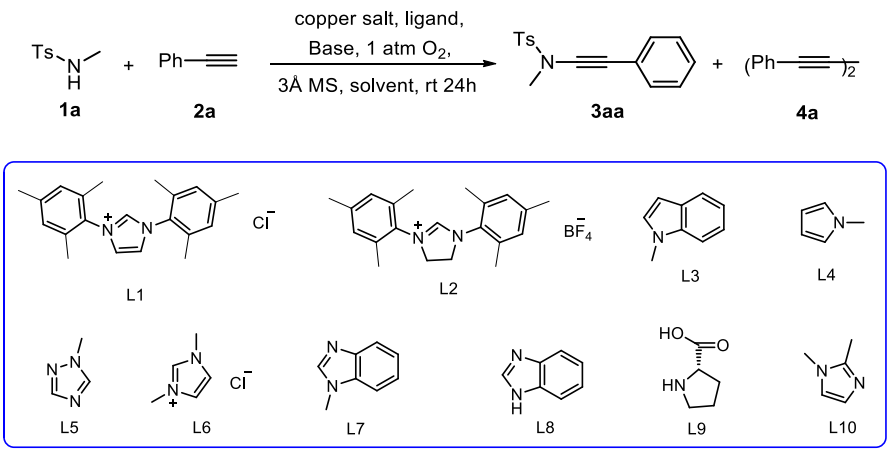
1. The Optimization of the Cross-dehydrogenative-coupling (CDC) Reaction Conditions

The optimization of reactions were conducted with the following procedure: In a 25 mL round bottom flask, the amide **1a** (1.5 mmol, 3.0 eq), ligand (0.25 mmol, 0.5 eq), copper salt (0.1 mmol, 0.2 eq), base (1.5 mmol, 3.0 eq), 3Å molecular sieves (160mg) were dissolved in dry solvent (2 mL) and the terminal alkyne **2a** (0.5 mmol, 1.0 eq) was successively added. The mixture was degassed three times by applying vacuum, and backfilling with oxygen while stirring vigorously. The mixture was stirred at room temperature for 24 h, filtered by diatomaceous earth over a plug of silica gel (washed with EtOAc), and the solvent was removed under reduced pressure. The crude residue was purified by flash chromatography on silica gel to afford ynamide **3aa** and homo-coupling dimer of alkyne **4a**.

Our investigation commenced with the cross-dehydrogenative-coupling (CDC) of amide **1a** with phenylacetylene **2a** (Table S1~ S3). Under a common copper-catalyzed aerobic oxidative CDC conditions, a desired ynamide **3aa** and an alkyne homo-coupling dimer **4a** were obtained while 3Å molecular sieve was added. For to get optimized conditions, a series of factors such as ligands, copper salt, bases and solvents were studied in the first (Table S1). To our delight, ynamide **3aa** was obtained in a yield of 56% by using 1-methylbenzimidazole as a ligand, while successfully avoiding the formation of **4a** (Table S1, entry 10). Noteworthily, bivalent copper salts have better catalysis than monovalent copper salts (Table S1, entry 15~19 vs 20~22), a relatively satisfactory results can be obtained in the presence of $Cu(OTf)_2$ (Table S1, entry 19). By using Na_2CO_3 as a base, the yield of ynamide **3aa** increased to 72%. Further, the utilization of toluene as a solvent resulted in an 88% yield of the desired ynamide **3aa** without observation of **4a** (Table S1, entry 10). On the basis of these, the optimization of amide **1a**, Na_2CO_3 base, $Cu(OTf)_2$ catalyst, 1-methylbenzimidazole ligand and reaction time was carried out one by one (Table S2). Finally, considering the indispensable role of molecular sieve, the dosage of molecular sieve in the reaction was further optimized, and the optimal reaction conditions were determined (Table S3). The effect of amide loadings in the CDC reaction also was investigated (Table S4)..

Table *S1.* Optimization of ligand, copper salt, base, and solvent



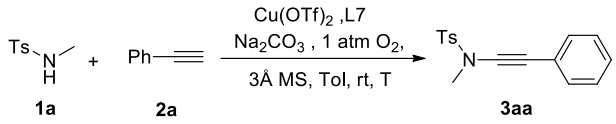
Entry	Ligand	Copper Salt	Base	Solvent (dry)	Yield (%)	
					3aa[a]	4a[a]
1	L1	$CuCl_2 \cdot 2H_2O$	t-BuOK	DCM	4	trace
2	L1	$CuCl_2 \cdot 2H_2O$	K_2CO_3	DCM	NR	
3	L2	$CuCl_2 \cdot 2H_2O$	K_2CO_3	DCM	nd	56

4	L2	$CuCl_2·2H_2O$	t-BuOK	DCM	20	73
5	L3	$CuCl_2·2H_2O$	K_2CO_3	DCM	nd	44
6	L4	$CuCl_2·2H_2O$	K_2CO_3	DCM	nd	53
7	L5	$CuCl_2·2H_2O$	K_2CO_3	DCM	5	60
8	L6	$CuCl_2·2H_2O$	K_2CO_3	DCM	8	59
9	L6	$CuCl_2·2H_2O$	t-BuOK	DCM	8	50
10	L7	$CuCl_2·2H_2O$	K_2CO_3	DCM	56	-
11	L8	$CuCl_2·2H_2O$	K_2CO_3	DCM	NR	
12	L9	$CuCl_2·2H_2O$	K_2CO_3	DCM	trace	trace
13	L10	$CuCl_2·2H_2O$	K_2CO_3	DCM	46	49
14	BK	$CuCl_2·2H_2O$	K_2CO_3	DCM	nd	trace
15	L7	$CuSO_4$	K_2CO_3	DCM	39	52
16	L7	$CuBr_2$	K_2CO_3	DCM	33	35
17	L7	$(AcO)_2Cu$	K_2CO_3	DCM	32	37
18	L7	$Cu(NO_3)_2$	K_2CO_3	DCM	65	34
19	L7	$Cu(OTf)_2$	K_2CO_3	DCM	67	30
20	L7	CuCl	K_2CO_3	DCM	23	52
21	L7	CuBr	K_2CO_3	DCM	18	50
22	L7	CuI	K_2CO_3	DCM	trace	47
23	L7	$Cu(OTf)_2$	Na_2CO_3	DCM	72	24
24	L7	$Cu(OTf)_2$	Li_2CO_3	DCM	18	trace
25	L7	$Cu(OTf)_2$	AcOLi	DCM	21	55
26	L7	$Cu(OTf)_2$	Cs_2CO_3	DCM	19	63
27	L7	$Cu(OTf)_2$	Na_2HPO_4	DCM	51	trace

28	L7	$Cu(OTf)_2$	NaOH	DCM	22	61
29	L7	$Cu(OTf)_2$	Na_2CO_3	THF	80	trace
30	L7	$Cu(OTf)_2$	Na_2CO_3	Toluene	88	trace
31	L7	$Cu(OTf)_2$	Na_2CO_3	DMF	18	71
32	L7	$Cu(OTf)_2$	Na_2CO_3	CH_3CN	45	42
33	L7	$Cu(OTf)_2$	Na_2CO_3	MTBE	45	53

[a] Isolated yield.

Table *S2*. Optimization of the quantities of amide, base, copper salt, ligand and reaction time

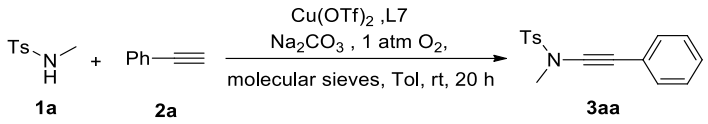


1a **2a** **3aa**

Entry	1a (eq)	Na_2CO_3 (eq)	$Cu(OTf)_2$ (eq)	L7 (eq)	Time (h)	Yield (%)[a]
1	3	3	0.2	0.5	24	88
2	2.5	3	0.2	0.5	24	79
3	3	3	0.2	0.4	24	89
4	3	3	0.2	0.2	24	75
5	3	3	0.15	0.3	24	64
6	3	3	0.1	0.2	24	61
7	3	2	0.2	0.4	24	84
8	3	1	0.2	0.4	24	26
9	3	3	0.2	0.4	16	72
10	3	3	0.2	0.4	18	83
11	3	3	0.2	0.4	20	89
12	3	3	0.2	0.4	22	89

[a] Isolated yield.

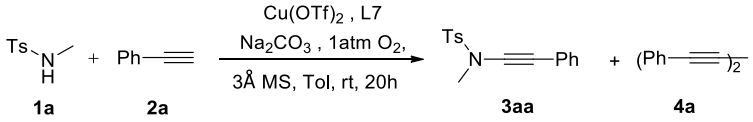
Table *S3*. The effects of molecular sieves



Entry	Molecular sieves	Weight (mg)	Yield (%)[a]
1	BK	0	trace
2	3Å	60	33
3	3Å	120	39
4	3Å	150	86
5	3Å	180	93
6	3Å	210	81
7	4Å	120	51
8	4Å	150	58
9	4Å	180	56

[a] Isolated yield.

Table *S4*. The effect of amide loadings in the CDC reaction[a]



Entry	Amide 1a (eq)	3aa (%)[b]	4a (%)[b]
1	0	0	6
2	0.5	18	23
3	1	49	40
4	1.5	58	43
5	2	69	31
6	2.5	80	19
7	3	93	trace

[a] Reaction conditions: **1a** (x eq), 1-methylbenzimidazole (0.2 mmol, 0.4 eq), $Cu(OTf)_2$ (0.1 mmol, 0.2 eq), Na_2CO_3 (1.5 mmol, 3.0 eq), 3Å molecular sieves were dissolved in Tol (2 mL) and **2a** (0.5 mmol, 1.0 eq) was successively added.

The mixture was stirred at room temperature for 24 h in oxygen atmosphere. [b] Isolated yield.

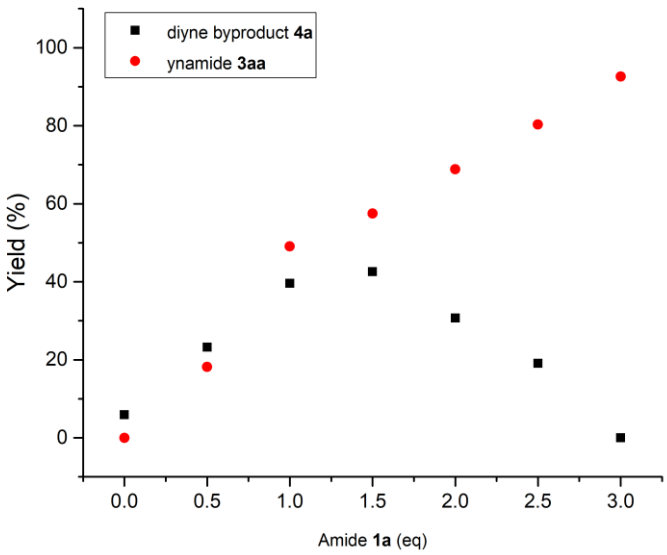
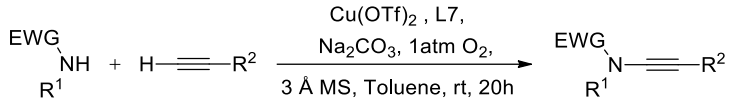


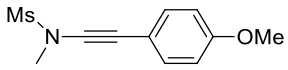
Figure *S1*. The effects of amide equivalent

2. Copper-catalyzed CDC Reaction of Amides with terminal alkynes:



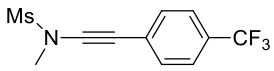
General procedure: In a 25 mL round bottom flask, the amide (1.5 mmol, 3.0 eq), 1-methylbenzimidazole (0.2 mmol, 0.4 eq), $Cu(OTf)_2$ (0.1 mmol, 0.2 eq), Na_2CO_3 (1.5 mmol, 3.0 eq), 3Å molecular sieves (180mg) were dissolved in dry solvent (2 mL) and the terminal alkynes (0.5 mmol, 1.0 eq) was successively added. The mixture was degassed three times by applying vacuum, and backfilling with oxygen while stirring vigorously. The mixture was stirred at room temperature for 20 h, filtered by diatomaceous earth over a plug of silica gel (washed with EtOAc), and the solvent was removed under reduced pressure. The crude residue was purified by flash chromatography over silica gel.

***N*-((4-methoxyphenyl)ethynyl)-*N*-methylmethanesulfonamide (3bb)**



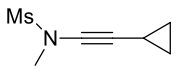
Following the **general procedure**, the reaction of **1b** and **2b** afforded **3bb** as a white solid (eluent: EtOAc/PE = 1/6; 93% yield): mp 92.3-96.0 ℃; IR (film) ν_{max}: 2232, 1595, 1366, 1273, 1261, 1191, 1167, 1091 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.39–7.34 (m, 2H), 6.86–6.81 (m, 3H), 3.81 (d, *J* = 3.96 Hz, 3H), 3.28 (d, *J* = 4.02 Hz, 3H), 3.12 (d, *J* = 3.96 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.6, 133.5, 114.2, 113.9, 81.6, 69.1, 55.3, 39.2 36.6; HRMS (ESI) calcd for $[C_{11}H_{13}NO_3SNa]^+$ (M + Na^+): 262.0508, Found: 262.0497. All spectral data are in accordance with the literature.[12]

***N*-methyl-*N*-((4-(trifluoromethyl)phenyl)ethynyl)methanesulfonamide (3bc)**



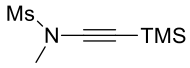
Following the **general procedure**, the reaction of **1b** and **2c** afforded **3bc** as a colorless oil (eluent: EtOAc/PE = 1/6; 91% yield): mp 82.1-84.3 ℃;IR (film) ν_{max}: 2236, 1595, 1365, 1275, 1259, 1189, 1167, 1087 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.34 Hz, 2H), 7.48 (d, *J* = 8.34 Hz, 2H), 3.32 (s, 3H), 3.14 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 131.0, 129.2 (q, *J* = 32.6 Hz), 126.4, 125.1 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.1 Hz), 85.4, 68.6, 39.0, 37.0; HRMS (ESI) calcd for $[C_{12}H_{15}F_3NO_3S]^+$ (M + MeOH + H^+): 310.0719, Found: 310.0721. All spectral data are in accordance with the literature.[15]

***N*-(cyclopropylethynyl)-*N*-methylmethanesulfonamide (3bm)**



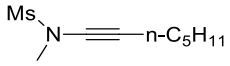
Following the **general procedure**, the reaction of **1b** and **2m** afforded **3bm** as a white solid (eluent: EtOAc/PE = 1/5; 86% yield): mp 43.2-45.8 ℃; IR (film) ν_{max}: 2926, 2216, 1748, 1697, 1451, 1367, 1283, 1259, 1228 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 3.08 (s, 3H), 2.96 (s, 3H), 1.25 (m, 1H), 0.74 (m, 2H), 0.62 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 73.3, 69.7, 39.1, 35.9, 8.6, -1.1; HRMS (ESI) calcd for $[C_7H_{11}NO_2SNa]^+$ (M + Na^+): 196.0403, Found: 196.0402. All spectral data are in accordance with the literature.[8]

***N*-methyl-*N*-((trimethylsilyl)ethynyl)methanesulfonamide (3bn)**



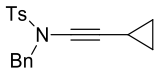
Following the **general procedure**, the reaction of **1b** and **2n** afforded **3bn** as a white solid (eluent: EtOAc/PE = 1/5; 99% yield): mp 41.2-44.3 °C; IR (film) ν_{max}: 2926, 2216, 1757, 1695, 1455, 1355, 1277, 1259, 1230 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 3.20 (d, *J* = 2.10 Hz, 3H), 3.07 (d, *J* = 2.10 Hz, 3H), 0.18 (d, *J* = 2.13 Hz, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 95.6, 71.8, 38.9, 36.6, 0.1; HRMS (ESI) calcd for $[C_7H_{15}NO_2SSiNa]^+$ (M + Na^+): 228.0485, Found: 228.0483. All spectral data are in accordance with the literature.[16]

***N*-(hept-1-yn-1-yl)-*N*-methylmethanesulfonamide (3br)**



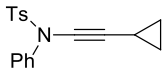
Following the **general procedure**, the reaction of **1b** and **2r** afforded **3br** as a colorless oil (eluent: EtOAc/PE = 1/6; 32% yield): IR (film) ν_{max}: 2928, 2214, 1753, 1691, 1357, 1281, 1261, 1232 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 3.16 (s, 3H), 3.03 (d, 3H), 2.27 (t, *J* = 7.20 Hz, 2H), 1.51 (m, 2H), 1.39–1.28 (m, 4H), 0.90 (t, *J* = 6.96 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 74.1, 69.2, 39.1, 35.8, 30.9, 28.5, 22.1, 18.2, 13.9; HRMS (ESI) calcd for $[C_9H_{18}NO_2S]^+$ (M + H^+): 204.1053, Found: 204.1059. All spectral data are in accordance with the literature.[17]

***N*-benzyl-*N*-(cyclopropylethynyl)-4-methylbenzenesulfonamide (3em)**



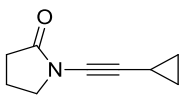
Following the **general procedure**, the reaction of **1e** and **2m** afforded **3em** as a white solid (eluent: EtOAc/PE = 1/7; 50% yield): mp 76.5-79.1 ℃; IR (film) ν_{max}: 2924, 2210, 1757, 1695, 1451, 1355, 1275, 1261, 1232 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.28 Hz, 2H), 7.30–7.24 (m, 7H), 4.42 (s, 2H), 2.43 (s, 3H), 1.20 (m, 1H), 0.69 (m, 2H), 0.49 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.3, 134.7, 134.6, 129.5, 128.7, 128.3, 128.0, 127.6, 75.3, 68.8, 55.5, 21.6, 8.6, -0.9; HRMS (ESI) calcd for $[C_{19}H_{19}NO_2SNa]^+$ (M + Na^+): 348.1029, Found: 348.1025. All spectral data are in accordance with the literature.[18]

***N*-(cyclopropylethynyl)-4-methyl-*N*-phenylbenzenesulfonamide (3fm)**



Following the **general procedure**, the reaction of **1f** and **2m** afforded **3fm** as a white solid (eluent: EtOAc/PE = 1/7; 66% yield): mp 81.2-84.3 ℃; IR (film) ν_{max}: 2920, 2216, 1751, 1693, 1451, 1363, 1275, 1259, 1232 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.22 Hz, 2H), 7.31–7.24 (m, 5H), 7.21 (d, *J* = 6.78 Hz, 2H), 2.42 (s, 3H), 1.32 (m, 1H), 0.78 (m, 2H), 0.65 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.6, 139.2, 132.8, 129.2, 128.8, 128.1, 127.8, 126.0, 74.5, 69.2, 21.6, 8.7, -0.8; HRMS (ESI) calcd for $[C_{18}H_{17}NO_2SNa]^+$ (M + Na^+): 334.0872, Found: 334.0879. All spectral data are in accordance with the literature.[19]

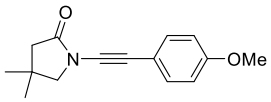
1-(cyclopropylethynyl)pyrrolidin-2-one (3hm)



Following the **general procedure**, the reaction of **1h** and **2m** afforded **3hm** as a colorless oil (eluent: EtOAc/PE = 1/4; 31% yield): IR (film) ν_{max}: 2922, 2214, 1753, 1700, 1357, 1279, 1261, 1228 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 3.57 (t, *J* = 7.14 Hz,

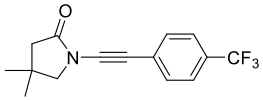
2H), 2.34 (t, *J* = 7.92 Hz, 2H), 2.03(m, *J* = 7.92, 7.14 Hz, 2H), 1.30 (m, 1H), 0.74 (m, 2H), 0.64 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.2, 76.0, 66.6, 49.9, 29.4, 18.5, 8.5, -0.9; HRMS (ESI) calcd for $[C_9H_{11}NONa]^+$ (M + Na^+): 172.0733, Found: 172.0731.

1-((4-methoxyphenyl)ethynyl)-4,4-dimethylpyrrolidin-2-one (3ib)



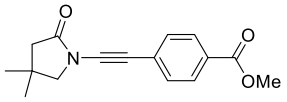
Following the **general procedure**, the reaction of **1i** and **2b** afforded **3ib** as a colorless oil (eluent: EtOAc/PE = 1/5; 47% yield): IR (film) ν_{max}: 3008, 2986, 2362, 2249, 1717, 1276, 1261 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.38 Hz, 2H), 6.36 (d, *J* = 8.38 Hz, 2H), 3.73 (s, 3H), 3.40 (s, 2H), 2.23 (s, 2H), 1.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 175.2, 159.4, 133.2, 114.5, 113.8, 79.1, 71.8, 63.0, 55.2, 44.9, 33.8, 27.4; HRMS (ESI) calcd for $[C_{15}H_{17}NO_2Na]^+$ (M + Na^+): 266.1151, Found: 266.1142.

4,4-dimethyl-1-((4-(trifluoromethyl)phenyl)ethynyl)pyrrolidin-2-one (3ic)



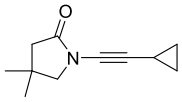
Following the **general procedure**, the reaction of **1i** and **2c** afforded **3ic** as a colorless oil (eluent: EtOAc/PE = 1/5; 51% yield): IR (film) ν_{max}: 2962, 2249, 1730, 1406, 1323, 1276, 1168, 1126, 1068 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (q, 4H), 3.44(s, 2H), 2.25 (s, 2H), 1.16 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 175.2, 131.3, 129.3 (q, *J* = 32.5 Hz), 126.6, 125.1 (q, *J* = 4.3 Hz), 123.9 (q, *J* = 272.0 Hz), 83.0, 71.3, 62.7, 44.8, 34.0, 27.3; HRMS (ESI) calcd for $[C_{15}H_{14}NOF_3Na]^+$ (M + Na^+): 304.0920, Found: 304.0911.

methyl 4-((4,4-dimethyl-2-oxopyrrolidin-1-yl)ethynyl)benzoate (3ig)



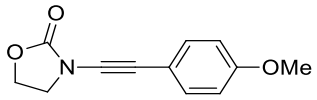
Following the **general procedure**, the reaction of **1i** and **2g** afforded **3ig** as a white solid (eluent: EtOAc/PE = 1/5; 66% yield): mp 117.8-119.3 ℃; IR (film) ν_{max}: 3004, 2960, 2363, 2245, 11719, 1403, 1276, 1170 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.56 Hz, 2H), 7.48 (d, *J* = 8.56 Hz, 2H), 3.91 (s, 3H), 3.51 (s, 2H), 2.32 (s, 2H), 1.23 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 175.2, 166.5, 130.9, 129.4, 128.9, 127.6, 83.6, 71.9, 62.7, 52.1, 44.8, 33.9, 27.3; HRMS (ESI) calcd for $[C_{16}H_{17}NO_3Na]^+$ (M + Na^+): 294.1101, Found: 294.1089.

1-(cyclopropylethynyl)-4,4-dimethylpyrrolidin-2-one (3im)



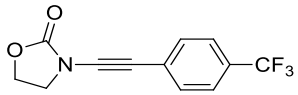
Following the **general procedure**, the reaction of **1i** and **2m** afforded **3im** as a colorless oil (eluent: EtOAc/PE = 1/4; 27% yield): IR (film) ν_{max}: 3006, 2960, 2873, 2358, 2260, 1717, 1412, 1312, 1276, 1261 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.26 (s, 2H), 2.15(s, 2H), 1.32-1.26 (m, 1H), 1.10(s, 6H), 0.74-0.71 (m, 2H), 0.66-0.63 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 175.7, 75.7, 68.0, 63.0, 44.7, 33.5, 27.4, 8.6, -0.8; HRMS (ESI) calcd for $[C_{11}H_{15}NONa]^+$ (M + Na^+): 200.1046, Found: 200.1040.

3-((4-methoxyphenyl)ethynyl)oxazolidin-2-one (3lb)



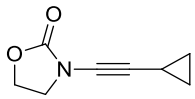
Following the **general procedure**, the reaction of **1l** and **2b** afforded **3lb** as a white solid (eluent: EtOAc/PE = 1/6; 96% yield): mp 99.5-102.6 ℃; IR (film) ν_{max}: 2242, 1608, 1366, 1277, 1257, 1189, 1167, 1089 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.76 Hz, 2H), 6.83 (d, *J* = 8.76 Hz, 2H), 4.45 (t, *J* = 7.74 Hz, 2H), 3.96 (t, *J* = 7.74 Hz, 2H), 3.79 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.6, 156.0, 133.3, 113.8, 77.5, 70.7, 63.0, 55.2, 47.0; HRMS (ESI) calcd for $[C_{12}H_{11}NO_3Na]^+$ (M + Na^+): 240.0631, Found: 240.0619. All spectral data are in accordance with the literature.[1]

3-((4-(trifluoromethyl)phenyl)ethynyl)oxazolidin-2-one (3lc)



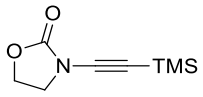
Following the **general procedure**, the reaction of **1l** and **1c** afforded **3lc** as a white solid (eluent: EtOAc/PE = 1/6; 68% yield): mp 100.9-103.0 ℃; IR (film) ν_{max}: 2236, 1597, 1367, 1273, 1263, 1189, 1165, 1091 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.28 Hz, 2H), 7.52 (d, *J* = 8.28 Hz, 2H), 4.52 (t, *J* = 7.41 Hz, 2H), 4.04 (t, *J* = 7.41 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.6, 131.3, 129.6 (q, *J* = 33.0 Hz), 126.1, 125.2 (q, *J* = 4.2 Hz), 123.9 (q, *J* = 272.0 Hz), 81.3, 70.4, 63.1, 46.8; HRMS (ESI) calcd for $[C_{12}H_8F_3NO_2Na]^+$ (M + Na^+): 278.0399, Found: 278.0400. All spectral data are in accordance with the literature.[20]

3-(cyclopropylethynyl)oxazolidin-2-one (3lm)



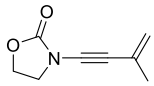
Following the **general procedure**, the reaction of **1l** and **2m** afforded **3lm** as a white solid (eluent: EtOAc/PE = 1/4; 91% yield): mp 50.6-52.5 ℃; IR (film) ν_{max}: 2924, 2212, 1757, 1695, 1453, 1369, 1283, 1257, 1226 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 4.42 (t, *J* = 8.22 Hz, 2H), 3.87 (t, *J* = 8.22 Hz, 2H), 1.35 (m, 1H), 0.82 (m, 2H), 0.71 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.7, 74.8, 65.4, 62.8, 46.9, 8.5, -1.1; HRMS (ESI) calcd for $[C_8H_9NO_2Na]^+$ (M + Na^+): 174.0526, Found: 174.0525. All spectral data are in accordance with the literature.[14]

3-((trimethylsilyl)ethynyl)oxazolidin-2-one (3ln)



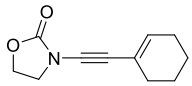
Following the **general procedure**, the reaction of **1l** and **2n** afforded **3ln** as a white solid (eluent: EtOAc/PE = 1/4; 84% yield): mp 78.0-81.3 ℃; IR (film) ν_{max}: 2926, 2222, 1755, 1697, 1453, 1359, 1279, 1261, 1232 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 4.42 (t, *J* = 7.99 Hz, 2H), 3.93 (t, *J* = 7.99 Hz, 2H), 0.20 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.8, 91.3, 73.7, 62.9, 46.8, 0.0; HRMS (ESI) calcd for $[C_8H_{14}NO_2]^+$ (M + H^+): 184.0788, Found: 184.0791. All spectral data are in accordance with the literature.[16]

3-(3-methylbut-3-en-1-yn-1-yl)oxazolidin-2-one (3lp)



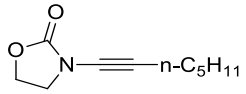
Following the **general procedure**, the reaction of **1l** and **2p** afforded **3lp** as a white solid (eluent: EtOAc/PE = 1/6; 79% yield): decompose at 95 ℃; IR (film) ν_{max}: 3004, 2988, 2360, 2242, 1757, 1276, 1261 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 5.25 (d, *J* = 42.93 Hz, 2H), 4.45 (t, *J* = 8.44 Hz, 2H), 3.94 (t, *J* = 8.44 Hz, 2H), 1.92 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.8, 125.7, 121.2, 78.1, 72.5, 62.9, 47.0, 23.5; HRMS (ESI) calcd for $[C_8H_9NO_2Na]$+ (M + Na+): 174.0531, Found: 174.0522. All spectral data are in accordance with the literature.[21]

3-(cyclohex-1-en-1-ylethynyl)oxazolidin-2-one (3lq)



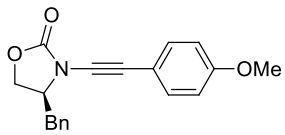
Following the **general procedure**, the reaction of **1l** and **2q** afforded **3lq** as a white solid (eluent: EtOAc/PE = 1/6; 42% yield): mp 71.6-74.5 ℃; IR (film) ν_{max}: 3003, 2918, 2358, 2243, 1761, 1420, 1276, 1261 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 6.13 (m, 1H), 4.43 (t, *J* = 8.08 Hz, 2H), 3.91 (t, *J* = 8.08 Hz, 2H), 2.15-2.08 (m, 4H), 1.66-1.56 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.0, 135.4, 119.4, 76.4, 72.7, 62.8, 47.1, 29.4, 25.7, 22.3, 21.4; HRMS (ESI) calcd for $[C_{11}H_{13}NO_2Na]^+$ (M + Na^+): 214.0838, Found: 214.0832. All spectral data are in accordance with the literature.[22]

3-(hept-1-yn-1-yl)oxazolidin-2-one (3lr)



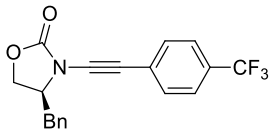
Following the **general procedure**, the reaction of **1l** and **2r** afforded **3lr** as a white solid (eluent: EtOAc/PE = 1/4; 51% yield): mp 53.4-56.2 ℃; IR (film) ν_{max}: 2928, 2212, 1751, 1695, 1448, 1363, 1277, 1265, 1230 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 4.35 (t, *J* = 7.98 Hz, 2H), 3.81 (t, *J* = 7.98 Hz, 2H), 2.23 (t, *J* = 7.20 Hz, 2H), 1.46 (m, 2H), 1.33-1.21 (m, 4H), 0.83 (t, *J* = 7.14 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.6, 71.1, 69.9, 62.8, 46.9, 30.8, 28.4, 22.1, 18.2, 13.8; HRMS (ESI) calcd for $[C_{10}H_{16}NO_2]^+$ (M + H^+): 182.1176, Found: 182.1182. All spectral data are in accordance with the literature.[23]

(*S*)-4-benzyl-3-((4-methoxyphenyl)ethynyl)oxazolidin-2-one (3mb)



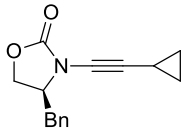
Following the **general procedure**, the reaction of **1m** and **2b** afforded **3mb** as a white solid (eluent: EtOAc/PE = 1/7; 94% yield): mp 92.9-95.3 ℃; $[\alpha]_D^{28}$ +168.1 (*c* 1.0, MeOH); IR (film) ν_{max}: 2234, 1595, 1366, 1279, 1269, 1187, 1167, 1087 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.70 Hz, 2H), 7.31 (t, *J* = 7.32, 7.37 Hz, 2H), 7.26 (t, *J* =7 .32 Hz, 1H), 7.21 (d, *J* = 7.37 Hz, 2H), 6.83 (d, *J* = 8.70 Hz, 2H), 4.33–4.27 (m, 2H), 4.13–4.07 (m, 1H), 3.77 (s, 3H), 3.21 (dd, *J* = 14.01, 3.26 Hz, 1H), 2.97 (dd, *J* = 14.80, 7.32 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 155.5, 134.1, 133.3, 129.2, 128.7, 127.2, 113.8, 113.7, 76.5, 72.7, 67.2, 58.2, 55.1, 37.6; HRMS (ESI) calcd for $[C_{19}H_{18}NO_3]^+$ (M + H^+): 308.1281, Found: 308.1281. All spectral data are in accordance with the literature.[1]

(*S*)-4-benzyl-3-((4-(trifluoromethyl)phenyl)ethynyl)oxazolidin-2-one (3mc)



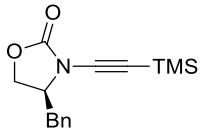
Following the **general procedure**, the reaction of **1m** and **2c** afforded **3mc** as a white solid (eluent: EtOAc/PE = 1/7; 48% yield): mp 118.0-121.4 ℃; $[\alpha]_D^{28}$ +127.4 (*c* 1.0, MeOH); IR (film) ν_{max}: 2232, 1593, 1363, 1277, 1267, 1185, 1161, 1093 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.25 Hz, 2H), 7.49 (d, *J* = 8.25 Hz, 2H), 7.35 (t, *J* = 7.32, 7.26 Hz, 2H), 7.29 (t, *J* = 7.32 Hz, 1H), 7.25 (d, *J* = 7.26 Hz, 2H), 4.43–4.36 (m, 2H), 4.20–4.15 (m, 1H), 3.77 (s, 3H), 3.21 (dd, *J* = 13.99, 3.18 Hz, 1H), 3.03 (dd, *J* = 14.55, 6.84 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.2, 134.0, 131.3, 129.5 (q, *J* = 32.2 Hz), 129.3, 129.0, 127.5, 126.1, 125.1 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 272.3 Hz), 80.4, 72.4, 67.6, 58.3, 38.1; HRMS (ESI) calcd for $[C_{19}H_{15}F_3NO_2]^+$ (M + H^+): 346.1049, Found: 346.1051.

(*S*)-4-benzyl-3-(cyclopropylethynyl)oxazolidin-2-one (3mm)



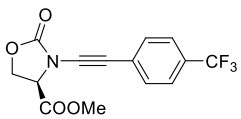
Following the **general procedure**, the reaction of **1m** and **2m** afforded **3mm** as a white solid (eluent: EtOAc/PE = 1/6; 54% yield): mp 51.5-57.6 ℃; $[\alpha]_D^{28}$ +143.4 (*c* 1.0, MeOH); IR (film) ν_{max}: 2924, 2216, 1753, 1693, 1453, 1355, 1281, 1263, 1232 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.22 (t, *J* = 7.38, 7.26 Hz, 2H), 7.16 (t, *J* = 7.38 Hz, 1H), 7.20 (d, *J* = 7.26 Hz, 2H), 4.27 (t, *J* = 8.52 Hz, 1H), 4.21-4.16 (m,1H), 4.06 (q, *J* = 9.32, 2.94 Hz, 1H), 3.17 (dd, *J* = 13.88, 4.02 Hz, 1H), 2.90 (dd, *J* = 14.68, 8.22 Hz, 1H), 1.39 (m, 1H), 0.84 (m, 2H), 0.73 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.2, 134.3, 129.3, 128.8, 127.3, 77.2, 67.1, 64.3, 58.2, 37.7, 8.8, 8.8, -0.9; HRMS (ESI) calcd for $[C_{15}H_{16}NO_2]^+$ (M + H^+): 242.1176, Found: 242.1171. All spectral data are in accordance with the literature.[24]

(*S*)-4-benzyl-3-((trimethylsilyl)ethynyl)oxazolidin-2-one (3mn)



Following the **general procedure**, the reaction of **1m** and **2n** afforded **3mn** as a white solid (eluent: EtOAc/PE = 1/6; 70% yield): mp 99.9-102.3 ℃; $[\alpha]_D^{28}$ +151.5 (*c* 1.0, MeOH); IR (film) ν_{max}: 2930, 2214, 1757, 1691, 1457, 1363, 1285, 1255, 1230 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.22 (t, *J* = 7.38, 7.20 Hz, 2H), 7.16 (t, *J* = 7.38 Hz, 1H), 7.09 (d, *J* = 7.20 Hz, 2H), 4.20–4.12 (m, 2H), 3.97 (q, *J* = 7.73, 2.88 Hz, 1H), 3.07 (dd, *J* = 13.86, 3.78 Hz, 1H), 2.82 (dd, *J* = 14.04, 7.86 Hz, 1H), 0.10 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.3, 134.1, 129.3, 128.9, 127.4, 90.3, 76.0, 67.3, 58.1, 37.6, 0.0; HRMS (ESI) calcd for $[C_{15}H_{20}NO_2]^+$ (M + H^+): 274.1258, Found: 274.1254. All spectral data are in accordance with the literature.[25]

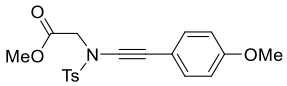
methyl (*R*)-2-oxo-3-((4-(trifluoromethyl)phenyl)ethynyl)oxazolidine-4-carboxylate (3nc)



Following the **general procedure**, the reaction of **1n** and **2c** afforded **3nc** as a white solid (eluent: EtOAc/PE = 1/5; 32% yield): mp 78.0-81.4 ℃; $[\alpha]_D^{27}$ +118.1 (*c* 1.0, MeOH); IR (film) ν_{max}: 3010, 2988, 2360, 2260, 1789, 1325, 1276, 1261 cm^{-1}; ^1H NMR (600

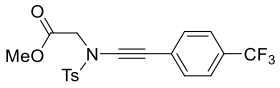
MHz, $CDCl_3$) δ 7.55 (q, 4H), 4.73-4.66 (m, 2H), 4.54 (dd, *J* = 8.58, 3.77 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.1, 154.4, 131.6, 129.9 (q, *J* = 32.3 Hz), 125.8, 125.4 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 272.0 Hz), 79.8, 71.2, 65.5, 58.6, 53.5; HRMS (ESI) calcd for $[C_{14}H_{10}NO_4F_3Na]^+$ (M + Na^+): 336.0454, Found: 336.0441.

methyl *N*-((4-methoxyphenyl)ethynyl)-*N*-tosylglycinate (3sb)



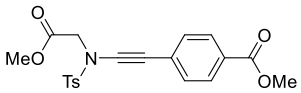
Following the **general procedure**, the reaction of **1s** and **2b** afforded **3sb** as a pale yellow oil (eluent: EtOAc/PE = 1/7; 46% yield): IR (film) ν_{max}: 3005, 2987, 2361, 2237, 1508, 1276, 1261, 1170 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.22 Hz, 2H), 7.28 (d, *J* = 8.22 Hz, 2H), 7.22 (d, *J* = 9.05 Hz, 2H), 7.74 (d, *J* = 9.05 Hz, 2H), , 4.23 (s, 2H), 3.73 (s, 3H), 3.63 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.7, 159.7, 144.8, 134.4, 133.7, 129.5, 128.1, 114.2, 113.8, 80.6, 70.0, 55.3, 52.5, 52.4, 21.7; HRMS (ESI) calcd for $[C_{19}H_{19}NO_5SNa]^+$ (M + Na^+): 396.0876, Found: 396.0865.

methyl *N*-tosyl-*N*-((4-(trifluoromethyl)phenyl)ethynyl)glycinate (3sc)



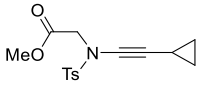
Following the **general procedure**, the reaction of **1s** and **2c** afforded **3sc** as a colorless oil (eluent: EtOAc/PE = 1/7; 80% yield): IR (film) ν_{max}: 2949, 2239, 1761, 1615, 1372, 1327, 1276, 1217, 1168, 1124, 1067 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.50 Hz, 2H), 7.42 (d, *J* = 8.50 Hz, 2H), 7.31 (d, *J* = 7.94 Hz, 2H), 7.28 (d, *J* = 7.94 Hz, 2H), 4.25 (s, 2H), 3.61 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.3, 145.2, 134.1, 131.1, 129.7, 129.2 (q, *J* = 32.2 Hz), 128.0, 126.4, 125.0 (q, *J* = 3.4 Hz), 123.8 (q, *J* = 274.0 Hz), 84.5, 69.7, 52.5, 52.0, 21.6; HRMS (ESI) calcd for $[C_{19}H_{16}NO_4SF_3Na]^+$ (M + Na^+): 434.0644, Found:434.0632.

methyl 4-(((*N*-(2-methoxy-2-oxoethyl)-4-methylphenyl)sulfonamido)ethynyl)benzoate (3sg)



Following the **general procedure**, the reaction of **1s** and **2g** afforded **3sg** as a colorless oil (eluent: EtOAc/PE = 1/7; 40% yield): IR (film) ν_{max}: 3006, 2988, 2360, 2234, 1715, 1276, 1261 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.32 Hz, 2H), 7.87 (d, *J* = 8.32 Hz, 2H), 7.38-7.36 (m, 4H), 4.34 (s, 2H), 3.91 (s, 3H), 3.72 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.4, 166.5, 145.2, 134.2, 130.7, 129.7, 129.4, 128.9, 128.1, 127.4, 85.1, 70.4, 52.6, 52.2, 52.1, 21.7; HRMS (ESI) calcd for $[C_{20}H_{19}NO_6SNa]^+$ (M + Na^+): 424.0825, Found: 424.0811.

methyl *N*-(cyclopropylethynyl)-*N*-tosylglycinate (3sm)



Following the **general procedure**, the reaction of **1s** and **2m** afforded **3sm** as a white solid (eluent: EtOAc/PE = 1/6; 23% yield): mp 71.9-73.0 ℃; IR (film) ν_{max}: 3010, 2988, 2360, 1748, 1276, 1261, 1165 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.96 Hz, 2H), 7.27 (d, *J* = 7.96 Hz, 2H), 4.11 (s, 2H), 3.61 (s, 3H), 2.38(s, 3H), 1.21-1.17 (m, 1H), 0.71-0.67 (m, 2H), 0.55-0.53 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.8, 144.6, 134.4, 129.4, 128.0, 74.8, 68.4, 52.4, 52.3, 21.7, 8.8, -0.9; HRMS (ESI) calcd for $[C_{15}H_{17}NO_4SNa]^+$ (M + Na^+): 330.0770, Found: 330.0760.

3. Computational Studies

3.1 Computational methods: All calculations were carried out with the Gaussian 09 programs[1]. The geometries of all the species were fully optimized by using DFT of the B3LYP method[2-4] with the def2-SVP basis set[5] in conjunction with the SMD implicit solvation model in toluene.[6] All stationary points were verified as either minima (zero imaginary frequencies) or transition states (a single imaginary frequency). Single point energies were conducted over the B3LYP-optimized geometries with M06 functional[7] and the def2-TZVP basis set[5] in conjunction with the SMD implicit solvation model in toluene.[6] The D3 dispersion correction developed by Grimme was added in all the optimization and single point calculations.[8] Minimum energy crossing points (MECP) between triplet and singlet states were located by using the sobMECP program.[9] Reported energies are Gibbs free energies determined by summing these single-point electronic energies and free energy corrections except for the estimation of the MECP energies. The final energies of the MECP are the M06-D3/def2-TZVP calculated single point energies in toluene. Molecular structure graphics were generated using *CYLview 1.0b*.[10]

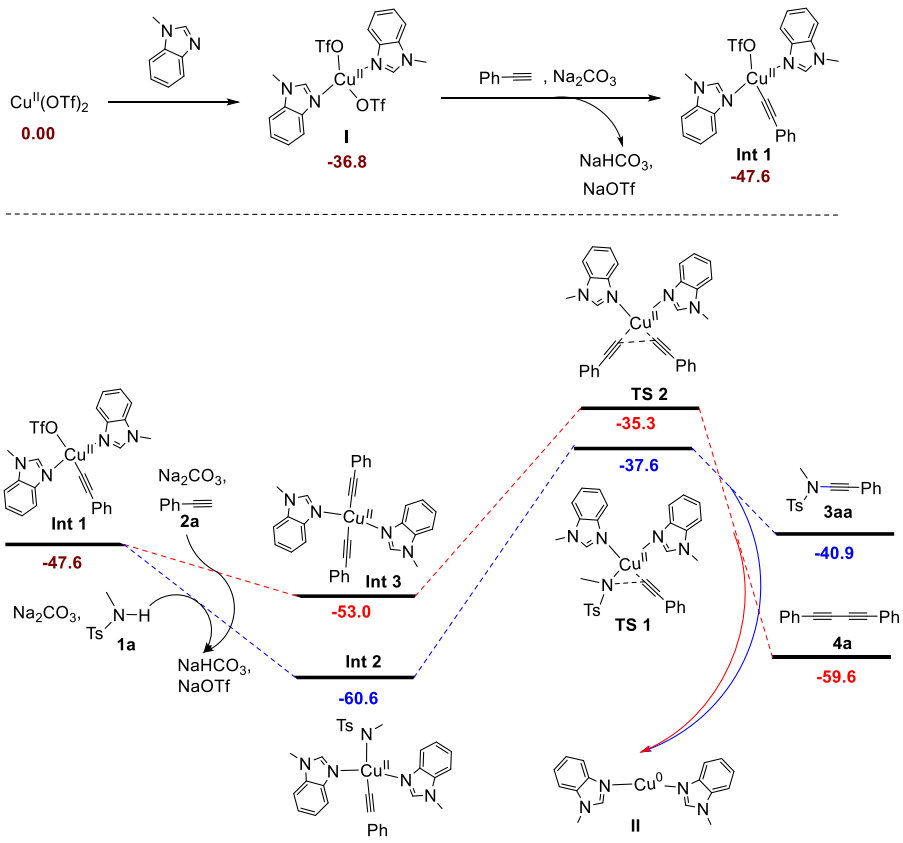


Figure *S2.* DFT calculations on the assumed Cu (II)-mediated cross-dehydrogenation-coupling (CDC) process. The values are relative free energies (ΔG, in kcal/mol) of the transition states and intermediates.

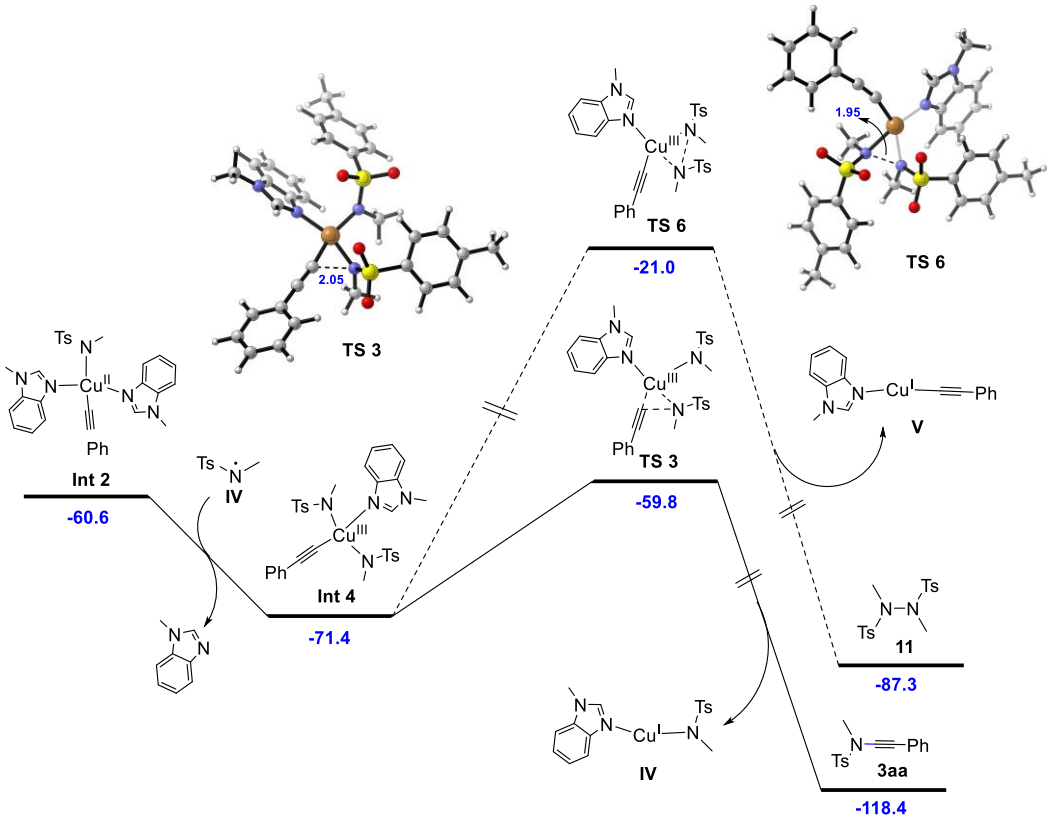


Figure *S3.* DFT calculations on the assumed Cu (III)-mediated cross-dehydrogenation-coupling (CDC) process leading to ynamide. The values are relative free energies (ΔG, in kcal/mol) of the transition states and intermediates.

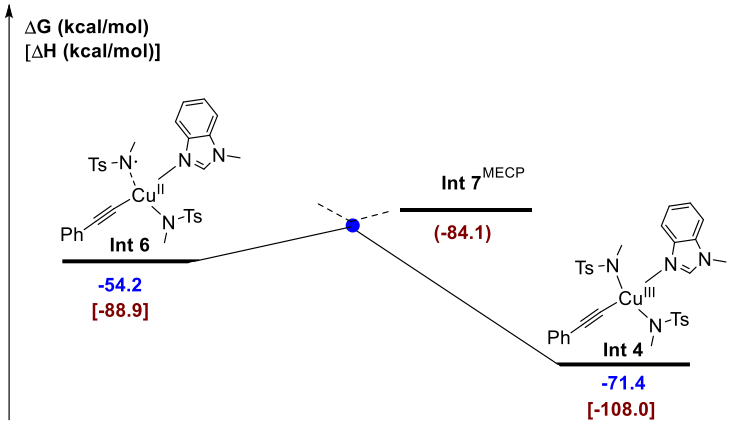


Figure *S4.* MECP between the triplet intermediate **Int6** and singlet intermediate **Int4** potential energy surfaces.

Comments on **Figure S4**: Nitrogen radical **IV** coordinate to Cu(II) intermediate **Int2** (Figure S3) along with the dissociation of ligand, generating a triplet Cu(II) complex **Int6** (ΔH = -88.9 kcal /mol). The corresponding singlet state intermediate **Int4**, which is more stable by 19.1 kcal/mol, afforded as Cu(III) complex through a minimum energy crossing point **Int7**^{MECP}. The relative energy of **Int7**^{MECP} is determined to be -84.1 kcal/mol, which is only 4.8 kcal/mol higher than Cu(II) intermediate **Int6**.

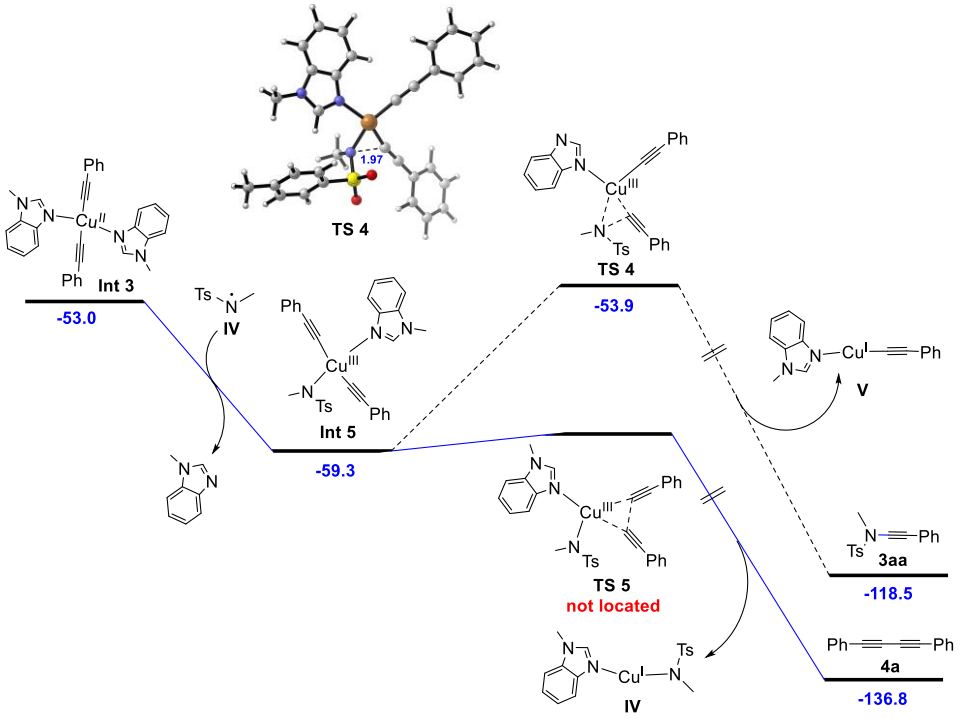


Figure *S5.* DFT calculations on the assumed Cu (III)-mediated cross-dehydrogenation-coupling (CDC) process leading to diyne **4a**. The values are relative free energies (ΔG, in kcal/mol) of the transition states and intermediates.

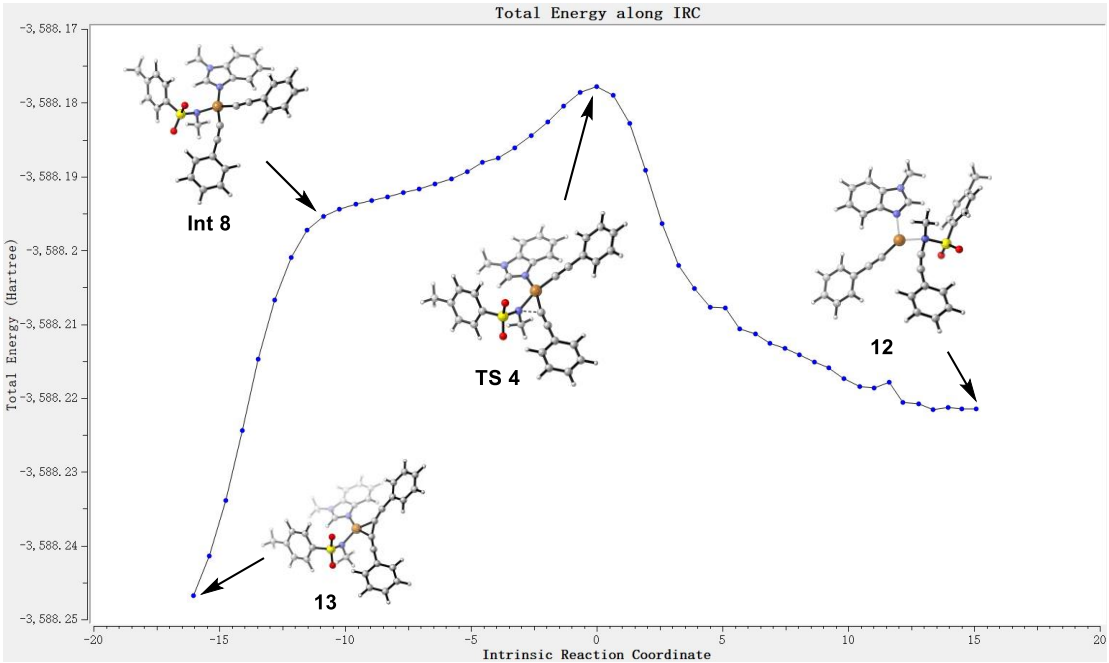


Figure *S6.* IRC analysis of **TS 4**

Comments on **Figure S5** and **S6**: Computational results indicated that the possible Cu(III) intermediate **Int5** (–59.3 kcal /mol) with the coordination of two alkyne anions and one amide anion is thermodynamically comparable to the Cu(II) intermediate **Int2** (–60.6 kcal /mol) (Figure S5). It is suggested that **Int5** may be formed while small amounts of secondary amides was used. When the **Int5** is generated, facile CDC process via **TS4** ($\Delta G^{\neq}$ = 5.4 kcal /mol) leads to ynamide **3aa**. However, the transition state **TS5**, which leads to diyne **4a**, can't be located. IRC analysis of **TS4** verified that the calculated transition state links reactant **Int8** and product ynamide **3aa**-**V** complex **12**. It is noteworthy that **Int8**

formation promptly produces diyne **4a**-**IV** complex **13** without any energy penalty (Figure S6). It is suggested that the **Int5** preferentially delivers to diyne **4a** instead of ynamide **3aa**. Indeed, as controlled experimental results shown (Figure S1), the formation of diyne **4a** was facilitated by the presence of small amounts (~ < 1.5 equiv.) of secondary amides, and gradually inhibited while the amount of amide increased from 1.5 to 3 equiv owing to Cu(III) intermediate **Int4** (–71.4 kcal /mol) being predominantly generated instead of the **Int5**.

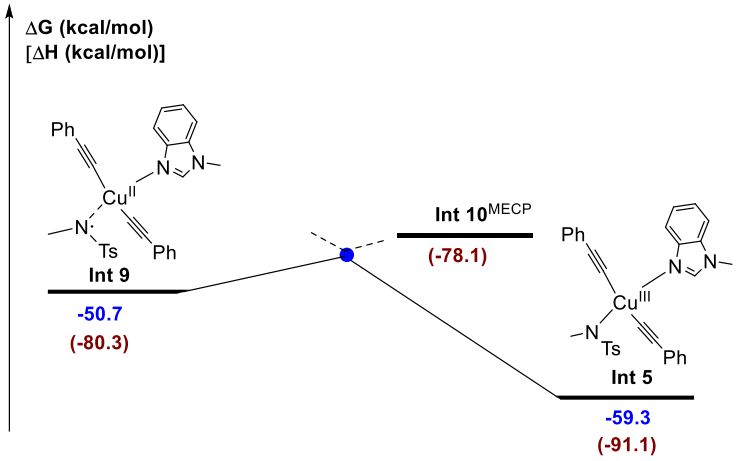


Figure *S7*. MECP between the triplet intermediate **Int9** and singlet intermediate **Int5** potential energy surfaces.

Comments on **Figure S7**: Nitrogen radical coordinate to Cu(II) intermediate **Int3** (Figure S5) along with the dissociation of ligand, forming a triplet Cu(II) complex **Int9** (ΔH = –80.3 kcal /mol). The corresponding singlet state intermediate **Int5**, which is more stable by 10.8 kcal/mol, afforded as Cu(III) complex through a minimum energy crossing point **Int10**^{MECP}. The relative energy of **Int10**^{MECP} is determined to be –78.1 kcal/mol, which is only 2.2 kcal/mol higher than Cu(II) intermediate **Int9**.

3.2 Molecular Geometries and Energies (in Hartree)：

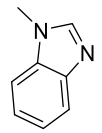
$Cu(OTf)_2$

Thermal correction to Gibbs Free Energy = 0.007624
Single-point electronic energies = -3563.547441
Free Energies (298K) = -3563.539817

Charge = 0 Multiplicity = 2

Cu	0.00001	0.00002	0.0245
O	1.48085	0.67179	-1.16964
S	2.42462	0.89035	0.01234
O	1.50499	0.64104	1.20691
O	3.26943	2.0627	0.01896
C	3.52144	-0.63383	-0.02308
F	4.31272	-0.63529	1.03605
F	4.244	-0.6291	-1.13036
F	2.73668	-1.70888	-0.00169
O	-1.48085	-0.67171	-1.16964
S	-2.42459	-0.89035	0.01234
O	-1.50502	-0.64096	1.20694
O	-3.26938	-2.06272	0.01895

C	-3.52146	0.63379	-0.02308
F	-2.73673	1.70887	-0.00167
F	-4.31276	0.63521	1.03604
F	-4.24401	0.62903	-1.13037



Ligand

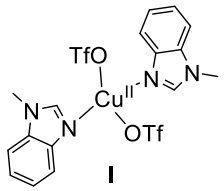
Thermal correction to Gibbs Free Energy = 0.114290

Single-point electronic energies = -419.032537

Free Energies (298K) = -418.918247

Charge = 0 Multiplicity = 1

C	1.757	-1.1634	0.00003
N	0.66427	-1.88366	-0.00008
C	-0.36911	-0.96294	0.00002
C	0.16051	0.35599	0.00006
N	1.53293	0.1931	0.00027
C	-1.76042	-1.15328	-0.00002
C	-2.57692	-0.02354	-0.00004
C	-2.03247	1.28044	-0.00001
C	-0.65386	1.49494	0.00004
C	2.52019	1.25055	-0.00016
H	-2.17682	-2.16308	-0.00007
H	-3.66335	-0.14439	-0.00009
H	-2.70755	2.14028	-0.00001
H	-0.23345	2.503	0.00011
H	2.41418	1.88479	0.89482
H	2.41388	1.88429	-0.89546
H	3.52664	0.81024	-0.00019
H	2.7765	-1.55379	0.00008



I

Thermal correction to Gibbs Free Energy = 0.282007

Single-point electronic energies = -4401.716980

Free Energies (298K) = -4401.434974

Charge = 0 Multiplicity = 2

C	-2.79496	1.56606	-1.03251
N	-2.29544	0.55439	-0.33947
C	-3.37348	-0.0985	0.24822

C	-4.55357	0.57847	-0.13621
N	-4.14149	1.62785	-0.94855
C	-3.43518	-1.20367	1.10765
C	-4.69573	-1.60504	1.5424
C	-5.86999	-0.92889	1.14419
C	-5.82135	0.17896	0.29996
C	-5.00702	2.61684	-1.56476
Cu	-0.3627	0.08815	-0.23285
O	0.11957	1.96578	-0.70005
S	-0.03939	3.10222	0.31919
O	-0.34474	2.60464	1.66485
O	-0.82031	4.21273	-0.23171
C	1.72148	3.73515	0.41547
F	1.75048	4.86867	1.11477
F	2.20524	3.96863	-0.8044
F	2.50135	2.83848	1.02263
C	1.86471	-0.95812	1.40763
N	1.50266	-0.27969	0.33165
C	2.66784	0.04427	-0.35189
C	3.75788	-0.48597	0.37433
N	3.20471	-1.11233	1.48416
C	2.87976	0.75977	-1.5377
C	4.19654	0.91352	-1.96372
C	5.28026	0.375	-1.23487
C	5.08204	-0.33329	-0.05079
C	3.93587	-1.84616	2.5
O	-0.71984	-1.78357	-0.79849
S	-0.68141	-3.11496	-0.05892
O	-1.76045	-4.01234	-0.46018
O	-0.40163	-2.95482	1.38175
C	0.8685	-3.90274	-0.76251
F	1.95639	-3.18041	-0.46415
F	0.77902	-4.00346	-2.08558
F	1.02068	-5.12034	-0.24361
H	-2.53374	-1.72226	1.43095
H	-4.77729	-2.467	2.20857
H	-6.83779	-1.28015	1.51009
H	-6.72524	0.71055	-0.00306
H	-4.39522	3.33917	-2.12021
H	-5.57749	3.1534	-0.79153
H	-5.70894	2.12899	-2.25812
H	2.04053	1.19659	-2.07814
H	4.39891	1.47066	-2.88157
H	6.2975	0.52041	-1.60637
H	5.91717	-0.74774	0.51678
H	4.45307	-2.70571	2.04664
H	3.23268	-2.21281	3.25875
H	4.6767	-1.19183	2.9837
H	-2.19622	2.2964	-1.57242
H	1.17233	-1.40984	2.11397

2a

Thermal correction to Gibbs Free Energy = 0.079376
Single-point electronic energies = -308.2658332
Free Energies (298K) = -308.1864572

Charge = 0 Multiplicity = 1

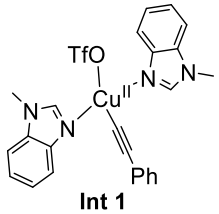
C	-1.51587	-1.21076	0.00001
C	-0.12079	-1.21581	-0.00002
C	0.59497	-0.00002	-0.00003
C	-0.12077	1.2158	-0.00002
C	-1.51584	1.21078	0.00001
C	-2.21737	0.00001	0.00003
H	-2.05989	-2.1588	0.00003
H	0.42848	-2.15982	-0.00003
H	0.42853	2.15979	-0.00003
H	-2.05986	2.15882	0.00002
H	-3.31043	0.00003	0.00006
C	2.02833	-0.00001	-0.00007
C	3.24307	0.	-0.00004
H	4.31875	0.00002	0.00063

Na_2CO_3

Thermal correction to Gibbs Free Energy = -0.013556
Single-point electronic energies = -588.4985647
Free Energies (298K) = -588.5121207

Charge = 0 Multiplicity = 1

O	-0.00025	-0.78056	-0.00002
C	-0.00004	0.56529	0.
O	1.12523	1.16679	-0.00026
O	-1.12505	1.16684	0.00026
Na	2.16616	-0.71897	0.00011
Na	-2.16609	-0.71888	-0.00009



Int 1

Thermal correction to Gibbs Free Energy = 0.353359
Single-point electronic energies = -3747.8340496
Free Energies (298K) = -3747.4806906

Charge = 0 Multiplicity = 2

Cu	-0.0878	0.19859	0.21872
O	-1.57978	1.58771	0.06867
S	-2.39905	2.19558	-1.05281
O	-3.72638	2.62422	-0.61213
O	-1.61012	3.11365	-1.8951
C	-2.70508	0.72227	-2.17216
F	-1.54135	0.12559	-2.4731
F	-3.49586	-0.17597	-1.58182
F	-3.28203	1.1179	-3.30513
C	1.32586	-1.07637	-0.20978
C	2.27935	-1.80347	-0.479
C	3.4205	-2.61728	-0.77523
C	3.29278	-3.8291	-1.48923
C	4.41334	-4.61223	-1.76971
C	5.68346	-4.20722	-1.34438
C	5.82473	-3.00817	-0.6362
C	4.70937	-2.21902	-0.35391
H	2.30277	-4.14595	-1.82607
H	4.29487	-5.54607	-2.32607
H	6.55971	-4.82221	-1.56559
H	6.81413	-2.68381	-0.30216
H	4.82067	-1.28182	0.19617
C	-1.32842	-2.4988	0.38625
N	-1.51142	-1.21876	0.66142
C	-2.76654	-1.12384	1.26427
C	-3.31838	-2.42571	1.33246
N	-2.375	-3.26887	0.76157
C	-3.49347	-0.02857	1.7554
C	-4.74712	-0.28352	2.30637
C	-5.28273	-1.58811	2.37365
C	-4.57719	-2.68579	1.88484
C	-2.50459	-4.70405	0.59961
H	-3.09789	0.98122	1.67468
H	-5.33745	0.55315	2.6877
H	-6.2725	-1.7387	2.81176
H	-4.98532	-3.69737	1.92705
H	-2.6354	-5.18851	1.57949
H	-1.59736	-5.0999	0.12502
H	-3.37258	-4.94044	-0.03512
C	1.10147	2.89993	-0.24336
N	1.21037	1.75433	0.40801
C	2.40622	1.81016	1.11223
C	3.01146	3.06286	0.85574
N	2.15297	3.72252	-0.01323
C	3.0229	0.8854	1.96613
C	4.23796	1.25262	2.54154
C	4.83325	2.507	2.27934
C	4.23094	3.43624	1.43204
C	2.34703	5.05135	-0.56189
H	2.56402	-0.08615	2.15186

H	4.74523	0.55342	3.21088
H	5.78707	2.754	2.75201
H	4.68765	4.40664	1.22826
H	2.39683	5.79614	0.24754
H	1.50398	5.29638	-1.22084
H	3.28048	5.09101	-1.14411
H	-0.43052	-2.89439	-0.08487
H	0.26518	3.16834	-0.89113

$NaHCO_3$

Thermal correction to Gibbs Free Energy = -0.000026
Single-point electronic energies = -426.7642204
Free Energies (298K) = -426.7642464

Charge = 0 Multiplicity = 1

O	-0.03927	-1.13645	-0.00005
C	0.56856	-0.03985	0.00012
O	1.92775	-0.09862	-0.00001
O	0.03504	1.10698	-0.00005
Na	-1.91209	0.0402	0.00001
H	2.2334	0.82164	-0.00001

NaOTf

Thermal correction to Gibbs Free Energy = -0.007099
Single-point electronic energies = -1123.8987516
Free Energies (298K) = -1123.9058506

Charge = 0 Multiplicity = 1

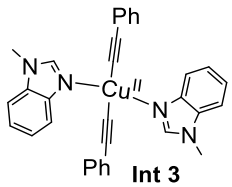
O	-1.0629	0.27198	1.22283
S	-0.31687	0.722	0.
O	0.21897	2.07859	-0.00006
O	-1.06295	0.27191	-1.22276
C	1.16535	-0.41943	0.
F	1.91556	-0.23186	1.08288
F	1.91558	-0.23182	-1.08286
F	0.73101	-1.69375	-0.00003
Na	-2.52058	-0.96349	-0.00001

1a

Thermal correction to Gibbs Free Energy = 0.142294
Single-point electronic energies = -914.7101794
Free Energies (298K) = -914.5678854

Charge = 0 Multiplicity = 1

N	-2.32824	0.33051	1.04379
C	-2.178	1.77101	1.2004
C	0.08222	-0.23567	-0.2153
C	0.70354	0.8735	-0.79354
C	2.08607	1.02638	-0.65822
C	2.85631	0.08505	0.04217
C	2.20311	-1.02786	0.60495
C	0.82583	-1.19623	0.48108
C	4.34815	0.23991	0.18692
S	-1.70219	-0.41154	-0.32054
O	-2.02278	-1.83336	-0.17465
O	-2.15855	0.37979	-1.46691
H	-2.13197	-0.22844	1.87395
H	-2.79244	2.09482	2.05369
H	-2.55743	2.27039	0.29813
H	-1.13327	2.0928	1.37434
H	0.11071	1.59641	-1.35664
H	2.57541	1.89168	-1.11339
H	2.78932	-1.77913	1.14198
H	0.32564	-2.07041	0.90292
H	4.71273	1.1631	-0.28694
H	4.87865	-0.61051	-0.27372
H	4.64271	0.26241	1.2496



Int 3

Thermal correction to Gibbs Free Energy = 0.422219

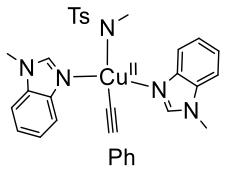
Single-point electronic energies = -3093.9400663

Free Energies (298K) = -3093.5178473

Charge = 0 Multiplicity = 2

Cu	0.00005	0.00005	-0.58913
C	1.88615	-0.37337	-0.99721
C	-1.88607	0.3733	-0.99741
C	-3.0801	0.57348	-1.22511
C	-4.47907	0.76551	-1.46267
C	-4.9492	1.81869	-2.27931
C	-6.31599	1.99907	-2.49641
C	-7.24685	1.13718	-1.90545
C	-6.79654	0.08839	-1.09506
C	-5.43158	-0.09934	-0.87558
C	3.08014	-0.57374	-1.22494
C	4.4791	-0.766	-1.46244
C	5.43171	0.09908	-0.87588
C	6.79665	-0.08889	-1.09535
C	7.24681	-1.13816	-1.9052

C	6.31584	-2.0003	-2.49563
C	4.94908	-1.81967	-2.27854
H	-4.22502	2.49161	-2.74486
H	-6.65828	2.81934	-3.13361
H	-8.31691	1.28071	-2.07719
H	-7.51645	-0.59166	-0.63104
H	-5.08201	-0.92037	-0.24533
H	5.08227	0.92049	-0.24605
H	7.51664	0.59134	-0.63174
H	8.31685	-1.28188	-2.07692
H	6.65801	-2.82094	-3.13241
H	4.22481	-2.49277	-2.74368
C	-0.3538	2.97928	-0.01403
N	0.35502	1.90023	0.24785
C	1.36407	2.29874	1.11329
C	1.2228	3.68595	1.35896
N	0.11808	4.08495	0.62041
C	2.39402	1.57144	1.72659
C	3.25874	2.26649	2.56984
C	3.11082	3.65222	2.80466
C	2.08931	4.38808	2.20509
C	-0.42253	5.42821	0.55297
H	2.50427	0.50527	1.52733
H	4.07332	1.72862	3.06136
H	3.81238	4.15809	3.47279
H	1.97092	5.45801	2.38761
H	-1.29878	5.43454	-0.10857
H	0.33036	6.12551	0.1535
H	-0.72981	5.76943	1.5539
C	0.35334	-2.97958	-0.01425
N	-0.35504	-1.90028	0.24769
C	-1.36388	-2.2983	1.1136
C	-1.22292	-3.68551	1.35951
N	-0.11863	-4.08499	0.62059
C	-2.39336	-1.57058	1.72718
C	-3.25794	-2.26519	2.57092
C	-3.11036	-3.65091	2.80595
C	-2.08932	-4.38721	2.20612
C	0.42158	-5.42842	0.55321
H	1.23237	-2.99041	-0.65723
H	-2.50336	-0.50441	1.52777
H	-4.07215	-1.72697	3.06267
H	-3.81182	-4.15644	3.47445
H	-1.97118	-5.45714	2.3888
H	-0.33159	-6.12557	0.154
H	0.72899	-5.76958	1.55412
H	1.29768	-5.43508	-0.10852
H	-1.23305	2.98971	-0.65671



Int 2

Thermal correction to Gibbs Free Energy = 0.488053

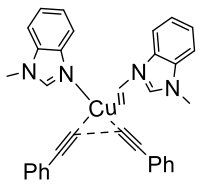
Single-point electronic energies = -3700.3994558

Free Energies (298K) = -3699.9114028

Charge = 0 Multiplicity = 2

Cu	0.15117	-0.62297	-0.08016
C	0.75745	1.09123	0.63372
C	1.14778	2.17707	1.06063
C	1.63261	3.42579	1.56478
C	0.74489	4.46671	1.91903
C	1.22731	5.68123	2.40842
C	2.60368	5.88894	2.55439
C	3.49561	4.86776	2.20634
C	3.02007	3.65008	1.71888
N	-0.78494	-2.41227	-0.15096
C	-1.44072	-2.81618	-1.38564
C	-2.69651	-1.64836	1.66463
C	-2.28219	-0.47793	2.31345
C	-3.20284	0.54466	2.53923
C	-4.54431	0.42178	2.12962
C	-4.9366	-0.76442	1.48794
C	-4.02376	-1.79944	1.25662
C	-5.52798	1.53313	2.39746
S	-1.46919	-2.90449	1.23223
O	-0.44005	-2.82882	2.29554
O	-2.21187	-4.16859	1.04872
H	-0.32988	4.30613	1.80519
H	0.52353	6.47352	2.67861
H	2.97924	6.8412	2.93819
H	4.57262	5.02134	2.31801
H	3.71648	2.85266	1.4491
H	-0.76137	-2.58579	-2.2211
H	-2.394	-2.28612	-1.58653
H	-1.64761	-3.89853	-1.40164
H	-1.24187	-0.36898	2.62661
H	-2.87218	1.45917	3.03987
H	-5.97599	-0.88525	1.16884
H	-4.33285	-2.72657	0.77017
H	-5.78655	1.57923	3.46966
H	-6.46522	1.39515	1.8372
H	-5.1073	2.51623	2.12956
C	2.21999	-2.68247	0.61215
N	1.99779	-1.53266	0.00478

C	3.2319	-1.06424	-0.4208
C	4.21821	-2.01001	-0.05125
N	3.53451	-3.02224	0.60875
C	3.58978	0.10884	-1.09957
C	4.93918	0.29263	-1.39772
C	5.91491	-0.66117	-1.03142
C	5.5732	-1.8298	-0.35031
C	4.12543	-4.2065	1.2005
H	2.83256	0.85076	-1.35633
H	5.2527	1.19894	-1.92178
H	6.96224	-0.4769	-1.28354
H	6.32686	-2.56533	-0.06216
H	3.33511	-4.80899	1.66673
H	4.85948	-3.92376	1.97097
H	4.62925	-4.81138	0.4304
C	-2.44507	0.74608	-1.08589
N	-1.24309	0.27653	-1.34646
C	-0.95096	0.65023	-2.64777
C	-2.05246	1.36986	-3.16876
N	-2.98622	1.41	-2.14333
C	0.18841	0.42077	-3.43055
C	0.18851	0.92664	-4.72856
C	-0.91651	1.64342	-5.24082
C	-2.05698	1.87857	-4.47258
C	-4.28714	2.04813	-2.19539
H	1.03768	-0.13201	-3.02355
H	1.06144	0.76843	-5.3664
H	-0.87554	2.0235	-6.26454
H	-2.90923	2.43326	-4.86988
H	-4.89845	1.60791	-2.9984
H	-4.17786	3.12822	-2.37988
H	-4.80164	1.90045	-1.2368
H	-2.96841	0.62718	-0.13931
H	1.43974	-3.27043	1.09393



TS 2

Thermal correction to Gibbs Free Energy = 0.418737

Single-point electronic energies = -3093.908240

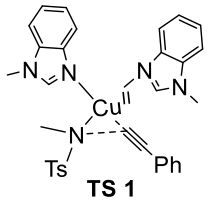
Free Energies (298K) = -3093.489502

Charge = 0 Multiplicity = 2

C	-2.84147	-0.55884	-0.32368
N	-1.8862	0.25619	0.26509
C	-2.54647	1.07568	1.05876

N	-3.88933	0.85662	1.04574
C	-4.11787	-0.19249	0.16715
Cu	0.16106	0.36838	0.02585
C	1.54683	1.53635	-0.77166
C	0.73138	2.07514	0.79864
C	0.72224	3.25543	1.21058
C	0.75555	4.58825	1.67795
C	1.86785	5.08083	2.41341
C	1.89359	6.39454	2.87524
C	0.82053	7.2616	2.62644
C	-0.28415	6.79407	1.90118
C	-0.32146	5.48313	1.43209
C	0.42319	-2.76792	0.23163
N	0.82373	-1.55122	-0.30074
C	1.85003	-1.8173	-1.08431
N	2.16123	-3.14094	-1.1163
C	3.23116	-3.7658	-1.86914
C	-4.89988	1.57772	1.7946
C	1.26058	-3.78752	-0.28201
C	2.64718	1.84621	-1.26493
C	3.89227	2.19972	-1.84289
C	5.06867	1.45856	-1.55501
C	6.2893	1.79963	-2.13441
C	6.38075	2.88581	-3.01463
C	5.23071	3.63142	-3.30615
C	4.00469	3.29906	-2.73329
C	-0.61063	-3.07828	1.12522
C	-0.77805	-4.41612	1.476
C	0.06122	-5.42694	0.95524
C	1.09691	-5.13298	0.06813
C	-2.70802	-1.59948	-1.25271
C	-3.86986	-2.2512	-1.66056
C	-5.13896	-1.88065	-1.16112
C	-5.28807	-0.84428	-0.23938
H	2.40289	-1.05963	-1.63966
H	2.82346	-4.49644	-2.5852
H	3.92742	-4.28173	-1.18979
H	3.78237	-2.99446	-2.42309
H	-5.44698	0.89236	2.46069
H	-5.6161	2.05739	1.10942
H	-4.41653	2.35348	2.40273
H	2.70781	4.4103	2.60877
H	2.7626	6.75009	3.43648
H	0.84615	8.29154	2.99152
H	-1.12476	7.46363	1.69662
H	-1.18228	5.12674	0.86079
H	5.00453	0.61588	-0.86201
H	7.18232	1.21506	-1.89475
H	7.34003	3.15106	-3.46653
H	5.29213	4.48417	-3.98833

H	3.11149	3.88462	-2.96254
H	-1.25041	-2.28741	1.519
H	-1.57585	-4.69372	2.1692
H	-0.10459	-6.46427	1.25661
H	1.74661	-5.91422	-0.33143
H	-2.07494	1.85616	1.65608
H	-1.72228	-1.87376	-1.63066
H	-3.80188	-3.06841	-2.38284
H	-6.02524	-2.41833	-1.50723
H	-6.26898	-0.55621	0.14384



TS 1

Thermal correction to Gibbs Free Energy = 0.488512

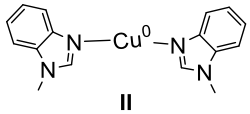
Single-point electronic energies = -3700.363195

Free Energies (298K) = -3699.874683

Charge = 0 Multiplicity = 2

C	2.10675	-1.38229	1.77833
C	2.05115	0.05787	3.38755
N	3.2673	-0.55203	3.49024
C	4.29811	-0.28822	4.47403
C	3.33684	-1.48526	2.46749
Cu	-0.50251	0.10371	1.70581
C	-2.34826	-0.40093	1.87354
C	-3.60392	-0.46482	2.00456
C	-5.01119	-0.55446	1.96848
C	-5.70034	-0.28838	0.75329
C	-7.08796	-0.37352	0.69362
C	-7.83086	-0.72117	1.83112
C	-7.1656	-0.99557	3.03366
C	-5.7766	-0.91811	3.10711
N	-0.29195	1.43754	0.06957
N	1.33095	-0.40032	2.38352
C	-1.42862	1.75454	-0.51843
C	0.65021	1.38458	-0.94842
N	-1.31175	1.92622	-1.8614
C	-2.4061	2.06225	-2.80063
C	0.01413	1.68065	-2.18142
C	2.01247	1.05772	-0.91921
C	2.70065	1.02766	-2.13181
C	2.05419	1.31682	-3.35402
C	0.69823	1.64692	-3.40135
C	1.83802	-2.18637	0.66312
C	2.8262	-3.08373	0.26722

C	4.05335	-3.18319	0.96249
C	4.33327	-2.38794	2.07416
S	-2.51717	-1.96773	-0.63354
O	-3.67392	-2.86994	-0.47315
O	-2.74781	-0.6243	-1.20254
H	1.73872	0.83892	4.07931
H	5.22704	0.03765	3.98022
H	4.50776	-1.19367	5.06485
H	3.96013	0.50686	5.15171
H	-5.11094	-0.05894	-0.13659
H	-7.60007	-0.17666	-0.25261
H	-8.92091	-0.78546	1.77851
H	-7.73871	-1.27455	3.92247
H	-5.25931	-1.13407	4.04493
H	-2.38897	1.80546	-0.0104
H	-2.60792	1.09468	-3.28493
H	-2.16473	2.8208	-3.56001
H	2.50046	0.81784	0.02561
H	3.76211	0.76745	-2.13991
H	2.6269	1.27645	-4.28408
H	0.19427	1.85716	-4.34677
H	-3.30905	2.37459	-2.26023
H	0.88512	-2.09139	0.14237
H	2.64797	-3.72349	-0.60019
H	4.80255	-3.9016	0.62018
H	5.28186	-2.46635	2.60899
N	-1.62933	-1.79825	0.76317
C	-1.33566	-2.795	-1.71067
C	-1.44283	-4.16731	-1.93712
C	-0.28686	-2.05487	-2.27036
C	-0.48187	-4.8052	-2.72902
H	-2.27653	-4.72126	-1.50183
C	0.66179	-2.70444	-3.05577
H	-0.21438	-0.98333	-2.08543
C	0.58319	-4.08998	-3.29686
H	-0.56512	-5.8807	-2.9088
H	1.48215	-2.12524	-3.48861
C	1.62482	-4.76992	-4.14842
H	1.45402	-5.8545	-4.21808
H	1.62675	-4.36099	-5.17316
H	2.63723	-4.61029	-3.7403
C	-1.52981	-3.00706	1.57034
H	-0.94678	-2.74774	2.46625
H	-2.51091	-3.40282	1.88445
H	-0.98456	-3.80284	1.02909



II

Thermal correction to Gibbs Free Energy = 0.238678

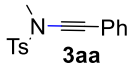
Single-point electronic energies = -2478.559333

Free Energies (298K) = -2478.320655

Charge = 0 Multiplicity = 2

C	2.10675	-1.38229	1.77833
C	2.05115	0.05787	3.38755
N	3.2673	-0.55203	3.49024
C	4.29811	-0.28822	4.47403
C	3.33684	-1.48526	2.46749
Cu	-0.50251	0.10371	1.70581
C	-2.34826	-0.40093	1.87354
C	-3.60392	-0.46482	2.00456
C	-5.01119	-0.55446	1.96848
C	-5.70034	-0.28838	0.75329
C	-7.08796	-0.37352	0.69362
C	-7.83086	-0.72117	1.83112
C	-7.1656	-0.99557	3.03366
C	-5.7766	-0.91811	3.10711
N	-0.29195	1.43754	0.06957
N	1.33095	-0.40032	2.38352
C	-1.42862	1.75454	-0.51843
C	0.65021	1.38458	-0.94842
N	-1.31175	1.92622	-1.8614
C	-2.4061	2.06225	-2.80063
C	0.01413	1.68065	-2.18142
C	2.01247	1.05772	-0.91921
C	2.70065	1.02766	-2.13181
C	2.05419	1.31682	-3.35402
C	0.69823	1.64692	-3.40135
C	1.83802	-2.18637	0.66312
C	2.8262	-3.08373	0.26722
C	4.05335	-3.18319	0.96249
C	4.33327	-2.38794	2.07416
S	-2.51717	-1.96773	-0.63354
O	-3.67392	-2.86994	-0.47315
O	-2.74781	-0.6243	-1.20254
H	1.73872	0.83892	4.07931
H	5.22704	0.03765	3.98022
H	4.50776	-1.19367	5.06485
H	3.96013	0.50686	5.15171
H	-5.11094	-0.05894	-0.13659
H	-7.60007	-0.17666	-0.25261
H	-8.92091	-0.78546	1.77851
H	-7.73871	-1.27455	3.92247
H	-5.25931	-1.13407	4.04493
H	-2.38897	1.80546	-0.0104
H	-2.60792	1.09468	-3.28493
H	-2.16473	2.8208	-3.56001

H	2.50046	0.81784	0.02561
H	3.76211	0.76745	-2.13991
H	2.6269	1.27645	-4.28408
H	0.19427	1.85716	-4.34677
H	-3.30905	2.37459	-2.26023
H	0.88512	-2.09139	0.14237
H	2.64797	-3.72349	-0.60019
H	4.80255	-3.9016	0.62018
H	5.28186	-2.46635	2.60899
N	-1.62933	-1.79825	0.76317
C	-1.33566	-2.795	-1.71067
C	-1.44283	-4.16731	-1.93712
C	-0.28686	-2.05487	-2.27036
C	-0.48187	-4.8052	-2.72902
H	-2.27653	-4.72126	-1.50183
C	0.66179	-2.70444	-3.05577
H	-0.21438	-0.98333	-2.08543
C	0.58319	-4.08998	-3.29686
H	-0.56512	-5.8807	-2.9088
H	1.48215	-2.12524	-3.48861
C	1.62482	-4.76992	-4.14842
H	1.45402	-5.8545	-4.21808
H	1.62675	-4.36099	-5.17316
H	2.63723	-4.61029	-3.7403
C	-1.52981	-3.00706	1.57034
H	-0.94678	-2.74774	2.46625
H	-2.51091	-3.40282	1.88445
H	-0.98456	-3.80284	1.02909



3aa

Thermal correction to Gibbs Free Energy = 0.220953

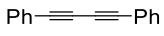
Single-point electronic energies = -1221.780281

Free Energies (298K) = -1221.559328

Charge = 0 Multiplicity = 1

C	-0.78702	1.35994	-0.53054
C	-1.85241	0.78061	-0.40704
N	0.39593	1.98425	-0.64338
C	0.92426	2.32275	-1.96989
C	-3.09527	0.10458	-0.2172
C	-3.53757	-0.21262	1.08688
C	-4.74369	-0.8865	1.27779
C	-5.53551	-1.24881	0.18199
C	-5.10853	-0.93338	-1.11281
C	-3.89978	-0.26732	-1.31661
C	2.11508	0.0621	0.37658
C	1.38593	-1.01073	0.90399

C	1.81339	-2.3088	0.63407
C	2.95697	-2.55413	-0.14837
C	3.67221	-1.45499	-0.65206
C	3.26016	-0.14572	-0.39739
C	3.3855	-3.9679	-0.44197
S	1.53223	1.72591	0.64973
O	0.74975	1.75911	1.88116
O	2.62385	2.66486	0.39041
H	1.26309	1.42556	-2.51686
H	1.75831	3.02493	-1.85141
H	0.12638	2.81488	-2.54347
H	-2.92413	0.07751	1.94293
H	-5.07106	-1.1268	2.29287
H	-6.4817	-1.77354	0.33665
H	-5.72171	-1.21178	-1.97412
H	-3.56673	-0.02799	-2.32902
H	0.50615	-0.82437	1.52148
H	1.25091	-3.1523	1.04365
H	4.5719	-1.62499	-1.24933
H	3.82583	0.70605	-0.77891
H	2.69189	-4.44327	-1.1572
H	3.37769	-4.58533	0.47067
H	4.39492	-4.00908	-0.87714



4a

Thermal correction to Gibbs Free Energy = 0.159035

Single-point electronic energies = -615.366169

Free Energies (298K) = -615.207134

Charge = 0 Multiplicity = 1

C	-5.44543	0.85736	0.85566
C	-4.05113	0.86186	0.85983
C	-3.33385	0.0001	-0.00016
C	-4.05122	-0.86178	-0.85997
C	-5.44551	-0.85753	-0.85541
C	-6.14674	-0.00015	0.00023
H	-5.98964	1.52829	1.52525
H	-3.50213	1.53017	1.52659
H	-3.50227	-1.52999	-1.52687
H	-5.98979	-1.52857	-1.52485
H	-7.23975	-0.00027	0.00039
C	-1.90797	0.00016	-0.00025
C	-0.68262	0.00012	-0.00024
C	0.6826	0.00015	-0.00013
C	1.90796	0.00015	-0.00004
C	3.33385	0.00007	0.
C	4.05108	-0.86096	0.86078
C	4.05128	0.86098	-0.86071

C	5.44537	-0.85671	0.85646
H	3.50203	-1.52858	1.52819
C	5.44558	0.8565	-0.8563
H	3.5024	1.52869	-1.52817
C	6.14675	-0.00017	0.00011
H	5.98954	-1.52711	1.52663
H	5.9899	1.5268	-1.52643
H	7.23975	-0.00026	0.00015

III

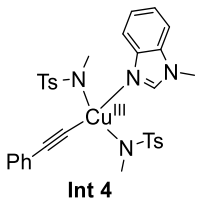
Thermal correction to Gibbs Free Energy = 0.126510

Single-point electronic energies = -914.040424

Free Energies (298K) = -913.913914

Charge = 0 Multiplicity = 2

N	-2.10319	-0.03157	1.20898
C	-3.5383	-0.01506	1.30769
C	0.20223	0.00537	-0.19562
C	0.87769	1.22356	-0.10639
C	2.26229	1.21337	0.07246
C	2.97491	0.00642	0.16031
C	2.26265	-1.2033	0.05939
C	0.88122	-1.2149	-0.11905
C	4.46916	-0.01053	0.34993
S	-1.56642	0.00433	-0.40633
O	-1.97466	-1.26306	-1.03239
O	-1.98137	1.28969	-0.98926
H	-3.8318	-0.0375	2.36683
H	-3.98207	-0.88454	0.7826
H	-3.96066	0.88846	0.82452
H	0.32627	2.16218	-0.18455
H	2.79962	2.1628	0.14169
H	2.8038	-2.15179	0.1182
H	0.33087	-2.15327	-0.20747
H	4.88325	1.00428	0.44088
H	4.96781	-0.50671	-0.49981
H	4.74516	-0.57478	1.25645



Int 4

Thermal correction to Gibbs Free Energy = 0.515585

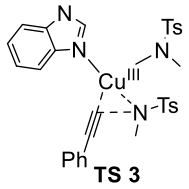
Single-point electronic energies = -4195.439750

Free Energies (298K) = -4194.924164

Charge = 0 Multiplicity = 1

Cu	-1.18715	0.07634	-0.68917
N	-1.22765	1.97717	-1.06426
C	-3.94177	1.0334	-0.91987
N	-3.21781	-0.0144	-0.56332
C	-4.12312	-0.97777	-0.1066
C	-5.42792	-0.43496	-0.22408
N	-5.26536	0.84152	-0.74303
C	-3.96164	-2.27119	0.41697
C	-5.10972	-2.96908	0.78817
C	-6.40065	-2.41675	0.65456
C	-6.582	-1.13233	0.14663
C	-6.32463	1.79678	-1.00458
C	0.62163	0.10504	-1.02626
C	1.80851	0.13302	-1.30882
C	3.21047	0.18143	-1.58586
C	3.86213	-0.89964	-2.21545
C	5.23798	-0.86019	-2.44227
C	5.98911	0.2507	-2.04027
C	5.3522	1.32865	-1.41471
C	3.9747	1.30046	-1.19158
C	-0.5338	2.54694	-2.2149
N	-0.95492	-1.80449	-0.41539
C	-0.80299	-2.65232	-1.58316
C	1.46429	-2.61421	0.84576
C	1.90082	-3.82187	0.29126
C	3.27031	-4.04131	0.13459
C	4.21286	-3.07938	0.53705
C	3.74398	-1.88598	1.10979
C	2.37961	-1.64671	1.26389
C	5.68909	-3.32949	0.36903
S	-0.29294	-2.30166	1.02097
O	-0.90358	-3.61448	1.31289
O	-0.46882	-1.17637	1.95281
S	-1.23383	2.91069	0.31626
C	0.44097	2.99324	0.95283
O	-1.62121	4.27465	-0.08856
O	-2.04147	2.17511	1.30056
C	1.27072	4.05449	0.58711
C	2.58371	4.08803	1.06663
C	3.07158	3.07963	1.91206
C	2.20448	2.03195	2.27363
C	0.89651	1.97393	1.79757
H	-2.9796	-2.71313	0.54989
H	-5.00072	-3.97408	1.20325
H	-7.27118	-3.00203	0.96104
H	-7.5738	-0.68737	0.04615
H	-5.88705	2.72502	-1.39425
H	-6.86943	2.02322	-0.07521
H	-7.03136	1.39273	-1.7458

H	-3.51081	1.96182	-1.28543
H	3.27956	-1.77519	-2.50824
H	5.73029	-1.70655	-2.92821
H	7.06787	0.27601	-2.21513
H	5.93204	2.20034	-1.09957
H	3.47638	2.13543	-0.69689
H	0.55193	2.67859	-2.06207
H	-0.98104	3.52324	-2.46306
H	-0.6743	1.87017	-3.06927
H	0.22786	-2.6731	-1.98173
H	-1.47308	-2.27587	-2.37127
H	-1.11877	-3.68165	-1.34085
H	1.17676	-4.58452	0.00038
H	3.61482	-4.98105	-0.30634
H	4.45808	-1.11869	1.41965
H	2.01872	-0.71121	1.68648
H	6.08091	-3.9385	1.203
H	6.25843	-2.38848	0.34888
H	5.90148	-3.87979	-0.561
H	0.8847	4.84979	-0.0527
H	3.23759	4.91664	0.78103
H	2.56641	1.24508	2.9415
H	0.23704	1.14635	2.06831
C	4.49629	3.08471	2.40185
H	5.01006	4.02785	2.16338
H	4.54632	2.93246	3.49237
H	5.06796	2.26298	1.9363



TS 3

Thermal correction to Gibbs Free Energy = 0.512605

Single-point electronic energies = -4195.418286

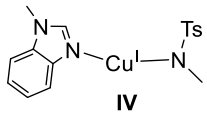
Free Energies (298K) = -4194.905682

Charge = 0 Multiplicity = 1

Cu	-0.30946	-1.13249	-1.07418
N	-1.56495	-2.58983	-0.88603
C	0.18831	1.7403	-1.43026
N	0.56371	0.5099	-1.71965
C	1.7512	0.60356	-2.42788
C	2.07642	1.97363	-2.5532
N	1.06209	2.66387	-1.90063
C	2.58368	-0.38218	-2.97289
C	3.72739	0.04424	-3.64138
C	4.04441	1.41557	-3.76465

C	3.22695	2.40624	-3.22244
C	0.97226	4.10459	-1.75359
C	-2.0571	-0.73253	-1.59286
C	-3.15	-0.30825	-1.95357
C	-4.46381	0.15343	-2.2692
C	-5.53878	-0.23978	-1.439
C	-6.83411	0.19365	-1.71967
C	-7.08193	1.01531	-2.8261
C	-6.02395	1.40361	-3.65626
C	-4.7228	0.98048	-3.38264
C	-2.02472	-3.44839	-1.96879
N	1.3202	-2.004	-0.35494
C	1.6342	-3.38422	-0.67396
C	3.75495	-0.86572	0.2742
C	4.05841	0.47039	-0.00204
C	5.30982	0.79816	-0.52047
C	6.27416	-0.19152	-0.77795
C	5.95287	-1.52439	-0.47631
C	4.70642	-1.86602	0.05557
C	7.60574	0.18399	-1.37674
S	2.10969	-1.30333	0.87146
O	2.34354	-2.26444	1.97631
O	1.42102	-0.0312	1.17119
S	-2.4855	-2.61866	0.54927
C	-1.77648	-4.04462	1.35562
O	-2.11687	-1.41493	1.29833
O	-3.89348	-2.91348	0.2385
C	-0.51946	-3.91105	1.95693
C	0.05271	-5.02626	2.56131
C	-0.60947	-6.26872	2.58091
C	-1.87131	-6.36568	1.97208
C	-2.46368	-5.25979	1.35627
H	2.34177	-1.43696	-2.84658
H	4.4065	-0.69806	-4.0667
H	4.95638	1.70563	-4.29208
H	3.47361	3.46572	-3.31272
H	0.91444	4.58708	-2.74141
H	1.85387	4.48736	-1.21702
H	0.07108	4.35562	-1.17945
H	-0.71273	1.99522	-0.87496
H	-5.33335	-0.89721	-0.59098
H	-7.65864	-0.11619	-1.07213
H	-8.09945	1.35121	-3.0425
H	-6.21477	2.04279	-4.52245
H	-3.89471	1.2849	-4.02703
H	-3.06011	-3.23494	-2.27966
H	-1.94809	-4.50174	-1.64555
H	-1.35182	-3.31137	-2.82628
H	0.74698	-3.84216	-1.13983
H	1.87196	-3.98294	0.22105

H	2.47875	-3.48047	-1.38693
H	3.30772	1.23665	0.19292
H	5.54271	1.84421	-0.73872
H	6.69382	-2.30956	-0.652
H	4.47974	-2.90239	0.31226
H	8.28947	-0.67641	-1.43139
H	8.10108	0.97534	-0.78986
H	7.47782	0.57744	-2.40037
H	0.01762	-2.96382	1.94284
H	1.03812	-4.92294	3.02337
H	-2.40332	-7.32083	1.98177
H	-3.44771	-5.32994	0.88968
C	0.02852	-7.45456	3.25655
H	-0.54041	-8.38077	3.08698
H	1.05808	-7.61132	2.8947
H	0.09514	-7.2936	4.34632



IV

Thermal correction to Gibbs Free Energy = 0.262532

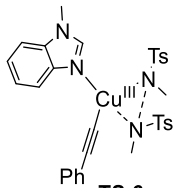
Single-point electronic energies = -2973.702333

Free Energies (298K) = -2973.439802

Charge = 0 Multiplicity = 1

Cu	-0.48341	-1.09438	-0.40419
C	-2.24275	0.21062	1.36789
N	-2.09505	-0.23329	0.12967
C	-3.2764	0.06271	-0.534
C	-4.14786	0.71158	0.37143
N	-3.45342	0.78811	1.57081
C	-3.66937	-0.18114	-1.85606
C	-4.94227	0.23867	-2.23457
C	-5.80715	0.88628	-1.32311
C	-5.42793	1.1353	-0.00456
C	-3.94515	1.36987	2.80571
N	1.23269	-1.8659	-0.54749
C	1.95335	-2.41529	-1.68402
C	3.01407	0.03492	0.30852
C	2.29221	1.21042	0.06299
C	2.96948	2.363	-0.32555
C	4.37022	2.36843	-0.47913
C	5.06906	1.17923	-0.22965
C	4.39983	0.01384	0.16279
C	5.08245	3.63039	-0.89616
S	2.11088	-1.46815	0.75445
O	3.13571	-2.48045	1.0792
O	1.14546	-1.06246	1.80814

H	-1.48017	0.12577	2.14186
H	-2.99035	-0.6837	-2.54811
H	-5.28361	0.06456	-3.25783
H	-6.79817	1.19899	-1.66104
H	-6.09704	1.63407	0.69902
H	-3.17014	1.28754	3.57892
H	-4.84731	0.8383	3.14559
H	-4.18937	2.43287	2.65638
H	1.21729	-2.80627	-2.40258
H	2.61807	-3.24735	-1.39115
H	2.57058	-1.66223	-2.21783
H	1.20498	1.20879	0.17529
H	2.40642	3.28196	-0.51542
H	6.15692	1.16027	-0.34214
H	4.94227	-0.91214	0.362
H	4.95297	4.42639	-0.14276
H	4.67951	4.02124	-1.84581
H	6.16225	3.46616	-1.0289



TS 6

Thermal correction to Gibbs Free Energy = 0.509529

Single-point electronic energies = -4195.353388

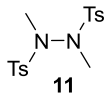
Free Energies (298K) = -4194.843860

Charge = 0 Multiplicity = 1

Cu	-0.42297	0.64117	-0.08725
N	-1.48869	-0.95303	0.61269
C	0.62665	2.7419	-1.88322
N	0.43849	1.43851	-1.81637
C	0.89806	0.9208	-3.01869
C	1.39689	1.98625	-3.80844
N	1.20211	3.13248	-3.0512
C	0.94063	-0.39475	-3.50069
C	1.49433	-0.60477	-4.76151
C	1.99934	0.46419	-5.53507
C	1.95801	1.78027	-5.07417
C	1.53801	4.48657	-3.44753
C	-1.39521	2.16165	0.68246
C	-2.18979	2.86296	1.31288
C	-3.14441	3.54288	2.13349
C	-3.37581	4.93244	2.0303
C	-4.31759	5.56208	2.84639
C	-5.05018	4.82317	3.78211
C	-4.8314	3.44418	3.89496

C	-3.89212	2.80702	3.08429
C	-2.5949	-1.05916	-0.32194
N	0.17933	-1.45404	-0.26805
C	-0.15322	-2.78164	-0.75308
C	2.86415	-1.45382	-0.57713
C	3.3162	-0.26193	-1.15408
C	4.27727	-0.32232	-2.15883
C	4.78885	-1.55348	-2.60666
C	4.33209	-2.73195	-1.9921
C	3.37747	-2.69252	-0.97476
C	5.78377	-1.5918	-3.73585
S	1.60193	-1.37053	0.68506
O	1.7572	-2.55547	1.53692
O	1.59236	-0.00452	1.22687
S	-1.77133	-1.29844	2.23044
C	-2.00386	-3.07226	2.33697
O	-0.57156	-0.94271	2.97798
O	-3.07968	-0.69285	2.52523
C	-0.90716	-3.88619	2.64071
C	-1.08759	-5.26809	2.68732
C	-2.34362	-5.85204	2.44225
C	-3.42767	-5.00632	2.15389
C	-3.27036	-3.61975	2.10702
C	-2.52518	-7.34536	2.52995
H	0.56321	-1.21614	-2.89471
H	1.54669	-1.62044	-5.1611
H	2.42756	0.25571	-6.51867
H	2.3425	2.60828	-5.67289
H	0.98958	4.76634	-4.36041
H	2.61897	4.5743	-3.63847
H	1.26213	5.17799	-2.64084
H	0.33835	3.43529	-1.09305
H	-2.80473	5.51235	1.30095
H	-4.48121	6.63954	2.75186
H	-5.78664	5.31878	4.42055
H	-5.39876	2.85906	4.62452
H	-3.71641	1.73124	3.16591
H	-3.32811	-0.26605	-0.09802
H	-3.0838	-2.04924	-0.31079
H	-2.2226	-0.86751	-1.33949
H	-0.99346	-2.71382	-1.45487
H	-0.39661	-3.50019	0.04405
H	0.70403	-3.17001	-1.32938
H	2.91157	0.69033	-0.81297
H	4.62841	0.6048	-2.61943
H	4.7354	-3.69701	-2.30995
H	3.04406	-3.60731	-0.48161
H	6.60796	-0.87978	-3.56744
H	5.29736	-1.30182	-4.68352
H	6.21627	-2.59405	-3.871

H	0.07087	-3.43629	2.81205
H	-0.23314	-5.90887	2.92307
H	-4.41571	-5.43867	1.97327
H	-4.12171	-2.96543	1.91296
H	-2.65985	-7.65859	3.58038
H	-3.4107	-7.68317	1.97047
H	-1.64502	-7.8832	2.14382



11

Thermal correction to Gibbs Free Energy = 0.287955

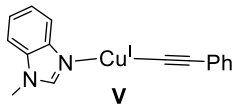
Single-point electronic energies = -1828.179014

Free Energies (298K) = -1827.891059

Charge = 0 Multiplicity = 1

N	-0.75969	-0.49836	0.49669
C	-1.67448	0.0251	-0.51333
N	0.40296	-1.07524	0.07135
C	0.76065	-2.38056	0.61871
C	-2.01179	-0.56674	2.9329
C	-3.29343	-0.02796	3.05089
C	-4.27001	-0.74815	3.74462
C	-3.97984	-1.99164	4.32617
C	-2.67326	-2.50186	4.19898
C	-1.68777	-1.79985	3.51018
C	-5.02308	-2.76429	5.09043
S	-0.7551	0.3342	2.02824
O	0.55174	0.0368	2.62002
O	-1.24515	1.70249	1.84154
C	2.00206	-0.47787	-2.07248
C	3.06927	-1.31095	-2.4084
C	3.26187	-1.65816	-3.74879
C	2.40738	-1.17941	-4.75316
C	1.34517	-0.33205	-4.38146
C	1.13727	0.02415	-3.05188
C	2.61587	-1.53946	-6.20113
S	1.73257	-0.03404	-0.35743
O	2.92553	-0.43404	0.39368
O	1.18637	1.3245	-0.30718
H	-2.67164	0.1552	-0.06785
H	-1.7489	-0.72017	-1.31742
H	-1.33755	0.99147	-0.92074
H	-0.14278	-3.00612	0.61079
H	1.16347	-2.30816	1.64137
H	1.5151	-2.85206	-0.02793
H	-3.51595	0.94718	2.61438
H	-5.27555	-0.32975	3.83978
H	-2.42638	-3.4646	4.65538

H	-0.67388	-2.19548	3.4264
H	-5.07609	-3.81015	4.74617
H	-6.02267	-2.31737	4.98588
H	-4.77778	-2.79316	6.1661
H	3.74385	-1.6708	-1.62968
H	4.09771	-2.3098	-4.01702
H	0.67525	0.05834	-5.15283
H	0.31945	0.69077	-2.77214
H	3.42854	-2.26933	-6.32981
H	2.86782	-0.64419	-6.79488
H	1.69889	-1.96644	-6.64013



V

Thermal correction to Gibbs Free Energy = 0.199831

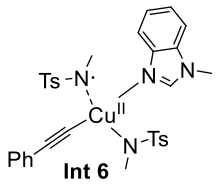
Single-point electronic energies = -2367.258328

Free Energies (298K) = -2367.058495

Charge = 0 Multiplicity = 1

Cu	-0.0646	-0.38844	-0.00009
C	-2.71831	-1.67197	-0.00011
N	-1.98958	-0.56974	-0.00015
C	-2.89193	0.48751	-0.00009
C	-4.20341	-0.03842	-0.00001
N	-4.05208	-1.41759	-0.00004
C	-2.6748	1.87179	-0.00005
C	-3.79731	2.6957	0.00008
C	-5.10596	2.16093	0.00017
C	-5.33528	0.78568	0.00013
C	-5.12802	-2.39063	0.00008
C	1.784	-0.20901	0.00005
C	3.01299	-0.10566	0.00004
C	4.43922	0.00827	0.00004
C	5.16627	0.06422	1.21206
C	6.55744	0.17156	1.20844
C	7.2617	0.22569	0.00004
C	6.55742	0.17183	-1.20837
C	5.16626	0.06449	-1.21199
H	-2.32082	-2.6855	-0.00013
H	-1.65729	2.26854	-0.0001
H	-3.66686	3.78047	0.00012
H	-5.95912	2.84378	0.00027
H	-6.34626	0.37409	0.00021
H	-5.75493	-2.26671	0.89648
H	-4.70425	-3.40329	-0.00031
H	-5.75549	-2.26628	-0.89587
H	4.62024	0.02159	2.1574
H	7.09804	0.21293	2.15833

H	8.35176	0.30921	0.00004
H	7.098	0.21341	-2.15827
H	4.62021	0.02207	-2.15733



Int 6

Thermal correction to Gibbs Free Energy = 0.512558

Single-point electronic energies = -4195.409298

Free Energies (298K) = -4194.896742

Charge = 0 Multiplicity = 3

Cu	-1.28952	0.20595	-0.7909
N	-1.75973	2.15144	-1.11286
C	-4.17807	0.51849	-0.89509
N	-3.23414	-0.34998	-0.57132
C	-3.89616	-1.48643	-0.10905
C	-5.29078	-1.24811	-0.18804
N	-5.42457	0.03826	-0.69143
C	-3.42864	-2.70926	0.39156
C	-4.37462	-3.6569	0.7804
C	-5.76017	-3.41011	0.68299
C	-6.24391	-2.19512	0.19931
C	-6.67193	0.74367	-0.91163
C	0.59542	0.35753	-1.27596
C	1.81587	0.42762	-1.48592
C	3.21694	0.55817	-1.66829
C	3.91304	-0.23516	-2.60975
C	5.29605	-0.12249	-2.74023
C	6.00934	0.78732	-1.94868
C	5.32952	1.58725	-1.0204
C	3.94905	1.47532	-0.87526
C	-1.07165	2.81852	-2.21527
N	-0.32403	-1.69561	-0.48533
C	-0.18689	-2.60257	-1.60378
C	2.06808	-2.42566	0.80028
C	2.57811	-3.66803	0.41359
C	3.95929	-3.8141	0.26603
C	4.83256	-2.74235	0.51041
C	4.28603	-1.50894	0.91036
C	2.91205	-1.33931	1.05386
C	6.32252	-2.88714	0.3453
S	0.30618	-2.22489	1.00269
O	-0.26863	-3.56589	1.22847
O	0.05794	-1.14262	1.95759
S	-1.91758	3.05265	0.25021
C	-0.29689	3.08313	1.04058

O	-2.24354	4.4485	-0.10793
O	-2.81523	2.31615	1.16065
C	0.60043	4.11706	0.76414
C	1.88702	4.06949	1.30944
C	2.28727	3.00671	2.13592
C	1.35938	1.98464	2.40428
C	0.0764	2.01426	1.86094
H	-2.3676	-2.91329	0.50385
H	-4.02907	-4.61331	1.18043
H	-6.46655	-4.18103	1.00072
H	-7.31395	-1.98976	0.13047
H	-6.45546	1.74561	-1.30413
H	-7.22479	0.84497	0.03501
H	-7.29765	0.20052	-1.63678
H	-3.95768	1.52148	-1.25325
H	3.35484	-0.94573	-3.22301
H	5.82429	-0.74677	-3.46545
H	7.09339	0.87489	-2.05792
H	5.88197	2.3013	-0.40405
H	3.4118	2.0885	-0.15028
H	-0.01141	3.05398	-2.00131
H	-1.58632	3.75393	-2.49107
H	-1.08552	2.14361	-3.08402
H	0.85414	-2.93173	-1.76986
H	-0.54213	-2.0864	-2.50697
H	-0.8112	-3.4994	-1.43886
H	1.90329	-4.50963	0.2496
H	4.36496	-4.78271	-0.03765
H	4.95144	-0.66226	1.09423
H	2.48825	-0.37816	1.34475
H	6.84711	-2.67365	1.29179
H	6.70209	-2.16909	-0.40052
H	6.60424	-3.89961	0.02084
H	0.28448	4.95134	0.13537
H	2.59262	4.87583	1.08924
H	1.64224	1.14461	3.04404
H	-0.62382	1.20337	2.06353
C	3.67107	2.96163	2.73431
H	4.37489	3.60748	2.18681
H	3.65833	3.30485	3.78378
H	4.07604	1.93685	2.73873

Int 7^{MECP}

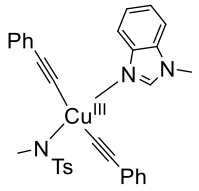
Single-point electronic energies = -4195.401722

Charge = 0 Multiplicity = 3

Cu	-1.1967	0.06615	-0.83696
N	-1.60538	2.03652	-1.02548
C	-4.08298	0.46537	-0.94317

N	-3.18776	-0.4623	-0.65881
C	-3.9125	-1.55856	-0.18951
C	-5.29098	-1.23297	-0.22883
N	-5.35615	0.06506	-0.7151
C	-3.51404	-2.81396	0.29291
C	-4.50871	-3.70259	0.69885
C	-5.87667	-3.36807	0.63856
C	-6.29244	-2.12056	0.17643
C	-6.55446	0.86257	-0.88211
C	0.66782	0.20338	-1.41585
C	1.87093	0.32351	-1.69818
C	3.24732	0.54321	-1.97875
C	3.89697	-0.10525	-3.05568
C	5.25048	0.11595	-3.30367
C	5.98281	0.99426	-2.49537
C	5.35066	1.65495	-1.43439
C	4.00053	1.4322	-1.17213
C	-0.97129	2.8208	-2.0831
N	-0.28431	-1.89492	-0.6421
C	-0.10558	-2.82316	-1.73653
C	2.02088	-2.63799	0.81116
C	2.52696	-3.91681	0.56412
C	3.91144	-4.09952	0.51213
C	4.79383	-3.02652	0.71155
C	4.25153	-1.7556	0.97843
C	2.87537	-1.5514	1.029
C	6.28883	-3.21439	0.64348
S	0.2528	-2.38556	0.89316
O	-0.36672	-3.70095	1.13793
O	-0.01955	-1.24821	1.77323
S	-1.85996	2.8376	0.38832
C	-0.26321	3.09468	1.19365
O	-2.39971	4.17973	0.0981
O	-2.61637	1.9205	1.25949
C	0.44273	4.28442	0.99834
C	1.69621	4.44585	1.59716
C	2.25348	3.43864	2.40142
C	1.514	2.25781	2.59225
C	0.26582	2.07816	1.99616
H	-2.46511	-3.0867	0.38799
H	-4.21474	-4.68136	1.08559
H	-6.62348	-4.09341	0.97014
H	-7.34995	-1.85001	0.13954
H	-6.2784	1.84866	-1.27808
H	-7.06266	1.00117	0.08524
H	-7.24993	0.37633	-1.58458
H	-3.81751	1.46129	-1.29346
H	3.32283	-0.7848	-3.68877
H	5.73896	-0.39464	-4.1376
H	7.04259	1.16978	-2.69627

H	5.91536	2.35262	-0.81053
H	3.50046	1.94842	-0.34995
H	0.08447	3.08194	-1.87673
H	-1.53055	3.75546	-2.25513
H	-0.98564	2.23328	-3.01321
H	0.92912	-3.19949	-1.82546
H	-0.37417	-2.31199	-2.67177
H	-0.77584	-3.69256	-1.60405
H	1.84304	-4.75723	0.43462
H	4.31185	-5.09814	0.3185
H	4.92243	-0.90795	1.14132
H	2.45732	-0.5643	1.23091
H	6.76536	-2.95856	1.60452
H	6.73229	-2.55404	-0.12003
H	6.55954	-4.2509	0.39653
H	0.00078	5.08009	0.39569
H	2.24658	5.37881	1.44369
H	1.91613	1.46314	3.22806
H	-0.29298	1.15471	2.15464
C	3.59196	3.62382	3.07513
H	4.21567	4.36083	2.54643
H	3.46886	3.9823	4.11239
H	4.14951	2.67513	3.12883



Int 5

Thermal correction to Gibbs Free Energy = 0.444945

Single-point electronic energies = -3588.968456

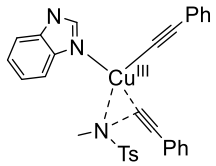
Free Energies (298K) = -3588.968456

Charge = 0 Multiplicity = 1

Cu	0.56951	0.49476	-0.35805
C	2.31587	-0.22002	-0.41306
C	3.39436	-0.79762	-0.40363
C	4.59098	-1.58295	-0.36538
C	4.49127	-2.96524	-0.08838
C	5.64041	-3.75488	-0.04192
C	6.90022	-3.18811	-0.27051
C	7.00703	-1.82024	-0.54651
C	5.86398	-1.02034	-0.59352
N	-0.06265	-1.24396	-0.8656
C	0.26889	-1.72749	-2.19258
C	-1.53972	-3.07552	0.38902
C	-2.66162	-2.26969	0.62353
C	-3.9247	-2.85202	0.60364

C	-4.09001	-4.22943	0.35492
C	-2.9468	-5.0087	0.12493
C	-1.66832	-4.44033	0.13804
C	-5.4707	-4.83301	0.33831
S	0.08304	-2.30921	0.40839
O	0.18366	-1.47685	1.62046
O	1.06911	-3.37784	0.16057
C	2.07466	2.37463	1.24885
N	1.23841	2.23344	0.2338
C	0.92512	3.50701	-0.22078
C	1.62626	4.43232	0.5863
N	2.33852	3.67414	1.50794
C	0.10426	3.94847	-1.26631
C	0.01225	5.32292	-1.46891
C	0.71371	6.24162	-0.65627
C	1.53356	5.81431	0.38649
C	3.21117	4.19446	2.54519
C	-1.24898	1.08037	-0.34095
C	-2.45034	1.31811	-0.28963
C	-3.8585	1.55925	-0.21017
C	-4.57996	1.20741	0.95307
C	-5.95718	1.4204	1.02686
C	-6.6445	1.98961	-0.05134
C	-5.94059	2.34568	-1.20724
C	-4.5636	2.13478	-1.28969
H	3.50063	-3.39158	0.08741
H	5.55241	-4.8231	0.17428
H	7.79768	-3.81145	-0.23401
H	7.98867	-1.37359	-0.72683
H	5.94558	0.04755	-0.80998
H	-0.37526	-2.59213	-2.43695
H	1.32502	-2.02179	-2.31087
H	0.03164	-0.9298	-2.91243
H	-2.53662	-1.20039	0.80068
H	-4.80439	-2.22569	0.77765
H	-3.05377	-6.07937	-0.06973
H	-0.77698	-5.04346	-0.04232
H	-6.10953	-4.33752	-0.41212
H	-5.96884	-4.70614	1.31457
H	-5.44626	-5.90843	0.10787
H	-0.44354	3.23171	-1.87818
H	-0.62139	5.70248	-2.27395
H	0.61023	7.31194	-0.85013
H	2.07689	6.52128	1.01606
H	3.63393	3.35865	3.1173
H	2.64308	4.84497	3.22732
H	4.03236	4.77286	2.09526
H	2.51555	1.54687	1.80055
H	-4.04532	0.76505	1.79689
H	-6.49837	1.14103	1.93502

H	-7.72319	2.15574	0.00925
H	-6.46979	2.79131	-2.05399
H	-4.01757	2.40998	-2.19494



TS 4

Thermal correction to Gibbs Free Energy = 0.445780

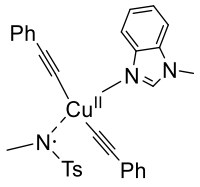
Single-point electronic energies = -3588.960726

Free Energies (298K) = -3588.514945

Charge = 0 Multiplicity = 1

Cu	-0.56403	-1.0685	0.29249
C	1.02933	-0.04101	0.12744
C	2.07327	0.60078	0.04906
C	3.27709	1.36974	-0.05154
C	3.25983	2.67544	-0.59168
C	4.43534	3.42062	-0.69127
C	5.65201	2.88416	-0.25439
C	5.68343	1.59287	0.28463
C	4.51209	0.84137	0.38628
N	-1.78733	-2.50949	0.78878
C	-2.19538	-3.48962	-0.21473
C	-3.91516	-2.4785	2.45318
C	-4.28557	-1.18982	2.85049
C	-5.63765	-0.84464	2.85551
C	-6.62767	-1.76932	2.47626
C	-6.2242	-3.06277	2.10077
C	-4.87728	-3.42796	2.09495
C	-8.08744	-1.39903	2.51328
S	-2.17225	-2.90318	2.40539
O	-1.45381	-1.95891	3.26214
O	-2.0728	-4.35495	2.61313
C	-3.2429	0.08427	-0.31767
N	-1.96181	0.13917	-0.62817
C	-1.83462	1.15819	-1.56589
C	-3.11552	1.71483	-1.79757
N	-3.98619	1.00354	-0.98186
C	-0.71454	1.64482	-2.25518
C	-0.91912	2.68867	-3.1548
C	-2.20104	3.24179	-3.37274
C	-3.3248	2.76428	-2.69993
C	-5.41607	1.21572	-0.86321
C	0.17222	-2.68093	0.88667
C	0.86433	-3.64479	1.19551
C	1.65294	-4.75969	1.61127

C	1.18848	-5.57851	2.66607
C	1.9447	-6.67028	3.09206
C	3.16392	-6.97262	2.47355
C	3.6276	-6.17127	1.42372
C	2.88479	-5.07021	0.99603
H	0.27032	1.21504	-2.07279
H	-0.06634	3.09166	-3.70665
H	2.30983	3.09736	-0.92823
H	4.40211	4.42982	-1.11116
H	6.57145	3.4705	-0.33199
H	6.62966	1.16731	0.63002
H	4.53623	-0.16591	0.80819
H	-3.29606	-3.56759	-0.23805
H	-1.76189	-4.48516	-0.0294
H	-1.86242	-3.1287	-1.19755
H	-3.5194	-0.47398	3.15372
H	-5.93121	0.16102	3.1691
H	-6.97946	-3.80078	1.81703
H	-4.57119	-4.44083	1.82797
H	-8.53519	-1.68955	3.47996
H	-8.65706	-1.91489	1.7248
H	-8.23661	-0.31462	2.39799
H	-2.31415	4.06129	-4.08686
H	-4.31722	3.18639	-2.86932
H	-5.82789	0.506	-0.13357
H	-5.90991	1.05818	-1.83461
H	-5.623	2.24111	-0.51975
H	-3.67045	-0.61847	0.3943
H	0.22649	-5.34292	3.1263
H	1.5768	-7.29472	3.91084
H	3.75174	-7.8312	2.80907
H	4.57969	-6.40262	0.93836
H	3.24971	-4.43657	0.1845



Int 9

Thermal correction to Gibbs Free Energy = 0.441377

Single-point electronic energies = -3588.951181

Free Energies (298K) = -3588.509803

Charge = 0 Multiplicity = 3

Cu	0.55827	0.71329	-0.77643
C	2.51384	0.36636	-0.8541
C	3.62257	-0.18679	-0.79273
C	4.87906	-0.85164	-0.67826

C	5.04954	-1.8658	0.29401
C	6.27219	-2.52519	0.41309
C	7.34486	-2.18698	-0.42097
C	7.18571	-1.18703	-1.388
C	5.96493	-0.52649	-1.52274
N	0.82551	-1.34531	-0.66943
C	0.87015	-2.21518	-1.8164
C	-0.68362	-2.69308	1.08946
C	-1.68163	-1.80294	1.50589
C	-2.9892	-2.26601	1.6119
C	-3.31817	-3.60026	1.30671
C	-2.2928	-4.46919	0.89742
C	-0.97381	-4.02522	0.78289
C	-4.74789	-4.05949	1.40618
S	0.97538	-2.07749	0.87335
O	1.21171	-0.9899	1.82582
O	1.90441	-3.21585	0.78902
C	1.64712	3.03322	0.7079
N	0.6554	2.6659	-0.08166
C	-0.24736	3.7218	-0.0902
C	0.26149	4.74884	0.74162
N	1.46854	4.27141	1.23253
C	-1.4698	3.89284	-0.75614
C	-2.14816	5.0936	-0.55714
C	-1.63293	6.10887	0.27942
C	-0.41668	5.95636	0.94371
C	2.3595	4.97549	2.13427
C	-1.36677	0.54057	-1.01826
C	-2.5678	0.27598	-1.06036
C	-3.95861	-0.05724	-1.06343
C	-4.92437	0.8397	-0.55336
C	-6.27581	0.49217	-0.52628
C	-6.69741	-0.75208	-1.00945
C	-5.7521	-1.6499	-1.52004
C	-4.39864	-1.31085	-1.5455
H	4.20286	-2.1416	0.92516
H	6.38855	-3.31243	1.16271
H	8.30235	-2.70491	-0.32078
H	8.01944	-0.92255	-2.04395
H	5.83725	0.25166	-2.27873
H	-0.07741	-2.78336	-1.89178
H	1.70527	-2.93261	-1.75921
H	0.96875	-1.59134	-2.71551
H	-1.43452	-0.76401	1.72461
H	-3.77782	-1.5762	1.92199
H	-2.52933	-5.51056	0.6636
H	-0.17536	-4.70043	0.47005
H	-5.38841	-3.46574	0.73266
H	-5.13837	-3.91597	2.42757
H	-4.86012	-5.12159	1.14301

H	-1.86392	3.1005	-1.39218
H	-3.10425	5.2559	-1.06118
H	-2.19947	7.03465	0.40733
H	-0.01391	6.73941	1.58911
H	3.23073	4.34385	2.35121
H	1.84288	5.20696	3.07865
H	2.70471	5.91517	1.67571
H	2.51857	2.41533	0.92017
H	-4.59645	1.81024	-0.17349
H	-7.0076	1.19902	-0.12547
H	-7.75695	-1.02024	-0.9892
H	-6.07235	-2.62356	-1.90102
H	-3.66047	-2.016	-1.93354

Int 10^{MECP}

Single-point electronic energies = -3588.947741

Charge = 0 Multiplicity = 3

Cu	0.45377	0.60499	-0.63157
C	2.36882	0.24863	-0.73269
C	3.51882	-0.20336	-0.73217
C	4.84094	-0.73915	-0.67499
C	5.13085	-1.78129	0.2373
C	6.41596	-2.31761	0.30444
C	7.43243	-1.82959	-0.52506
C	7.1558	-0.80014	-1.43181
C	5.87269	-0.25975	-1.51245
N	0.54257	-1.40189	-0.61223
C	0.70601	-2.28481	-1.74129
C	-0.80737	-2.82697	1.23875
C	-1.93022	-2.04235	1.53296
C	-3.16248	-2.66639	1.69985
C	-3.29748	-4.06214	1.5801
C	-2.15053	-4.82297	1.30491
C	-0.90342	-4.21599	1.12998
C	-4.6519	-4.705	1.74282
S	0.75937	-2.00949	0.95148
O	0.82916	-0.82653	1.81705
O	1.81872	-3.03003	0.96887
C	1.65274	2.85953	0.83039
N	0.65579	2.54338	0.02858
C	-0.13449	3.68266	-0.08078
C	0.45029	4.70614	0.70342
N	1.58618	4.14293	1.27224
C	-1.31084	3.93246	-0.80286
C	-1.86373	5.20773	-0.71066
C	-1.27277	6.21963	0.07619
C	-0.10371	5.98792	0.79848

C	2.52008	4.80431	2.16195
C	-1.47092	0.59239	-0.92989
C	-2.68165	0.40393	-1.04426
C	-4.08659	0.1643	-1.18159
C	-5.04023	0.99401	-0.54863
C	-6.40611	0.73922	-0.67684
C	-6.85655	-0.34505	-1.43797
C	-5.92535	-1.17578	-2.07079
C	-4.55853	-0.92721	-1.94599
H	4.32568	-2.16864	0.86584
H	6.62622	-3.12617	1.00946
H	8.4381	-2.25418	-0.46819
H	7.94675	-0.4173	-2.08229
H	5.65234	0.54147	-2.2212
H	-0.12958	-3.01092	-1.78443
H	1.65586	-2.84329	-1.69818
H	0.67727	-1.68368	-2.66055
H	-1.83561	-0.95932	1.61266
H	-4.043	-2.05523	1.91514
H	-2.23241	-5.9103	1.22325
H	-0.00938	-4.80692	0.92258
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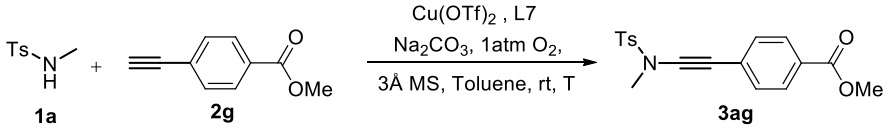
H	-2.78127	5.4325	-1.25989
H	-1.74183	7.20545	0.11999
H	0.3532	6.77129	1.4064
H	3.31354	4.09985	2.44269
H	2.01008	5.14526	3.07666
H	2.97811	5.67485	1.66622
H	2.45242	2.17438	1.1111
H	-4.69122	1.84071	0.04688
H	-7.12783	1.39285	-0.17903
H	-7.9273	-0.54097	-1.53832
H	-6.26768	-2.02539	-2.66815
H	-3.83236	-1.57673	-2.43882

4. Kinetic Studies of The Copper-catalyzed CDC Reaction



1a **2g** **3ag**

Following the general procedure, nine parallel CDC reactions of amide **1a** and terminal alkyne **2g** were performed. These reactions were quenched and worked up every 2 hours from 2h to 18h. The variations in substrate and product concentrations were monitored via integrating ^{1}H-NMR resonances of amide N-C<u>H</u>$_3$ (δ 2.63 ppm, 3H), alkyne C$_{sp}$-<u>H</u> (δ 3.26 ppm, 1H) and ynamide N-C<u>H</u>$_3$ (δ 3.17 ppm, 3H) with respect to the 1,3,5-Trimethoxybenzene Ph-<u>H</u> (0.5 eq of **2g**, δ 6.08 ppm, 3H) internal standard (Table *S5*). The data were plotted in Origin 2015pro. Plots of [amide], [alkyne] and

[ynamide] versus time gave three straight lines which indicates that the reaction rate is independent of [amide] and [alkyne] under the general procedure as shown in Figure *S8*.

Table *S5*. Concentrations of substrates and products in the CDC reaction with time

Entry	time	terminal alkyne (mol/L)	Amide (mol/L)	Ynamide (mol/L)
1	2	0.153	0.708	0.018
2	4	0.125	0.680	0.053
3	6	0.105	0.645	0.083
4	8	0.063	0.625	0.105
5	10	0.040	0.615	0.110
6	12	0.030	0.603	0.133
7	14	0.020	0.565	0.145
8	16	0.019	0.545	0.155
9	18	0.017	0.513	0.175

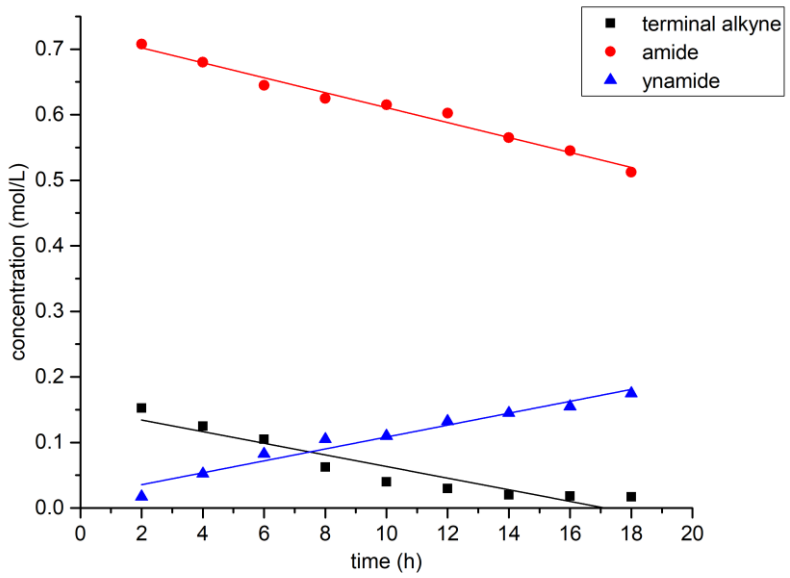
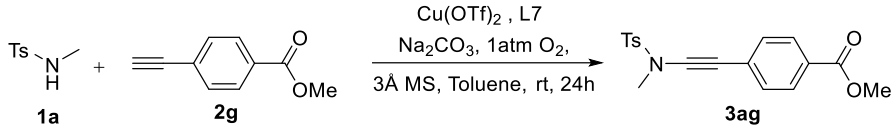


Figure *S8*. Concentrations of substrates and product as a function of time (h) for the CDC reaction to determine the reaction order in [amide] and [alkyne] under the general procedure

Effect of different dosage of 3Å molecular sieves on the CDC reaction



Following the general procedure, different 3Å molecular sieves loadings were employed from 60mg to 180mg. The yields of ynamide were listed in Table *S6* and k_{obs} were obtained. Plot of *kobs* vs dosage of 3Å molecular sieves gave a straight line, which suggested an apparent first-order reaction rate in 3Å MS (Figure *S9*).

Table *S6.* Effect of different dosage of 3Å molecular sieves on the CDC reaction

Entry	3Å MS (mg)	Yield (%)	M (mol/L)	K_{obs} (M h^{-1})*10^{-3}
1	60	0.31	0.078	3.229
2	90	0.43	0.108	4.479
3	120	0.56	0.140	5.833
4	150	0.70	0.175	7.292
5	180	0.87	0.218	9.063

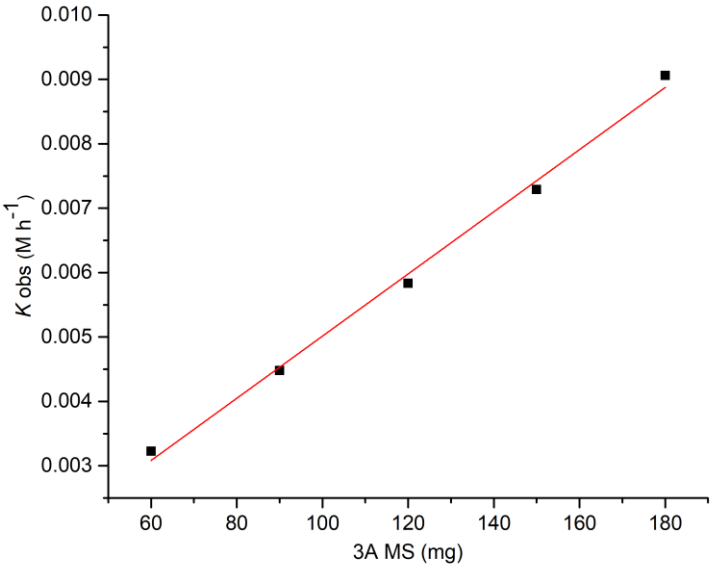
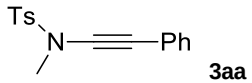
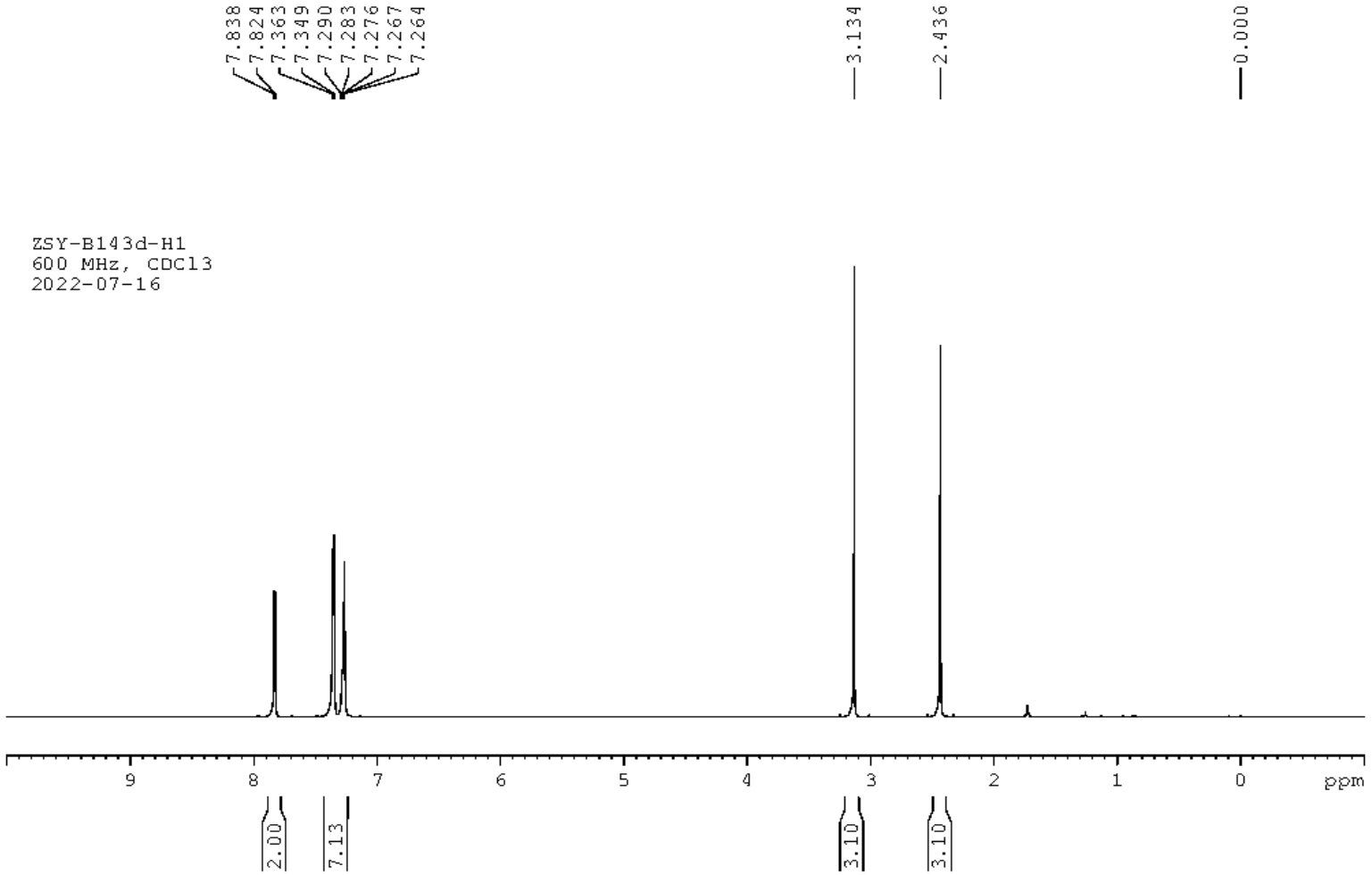


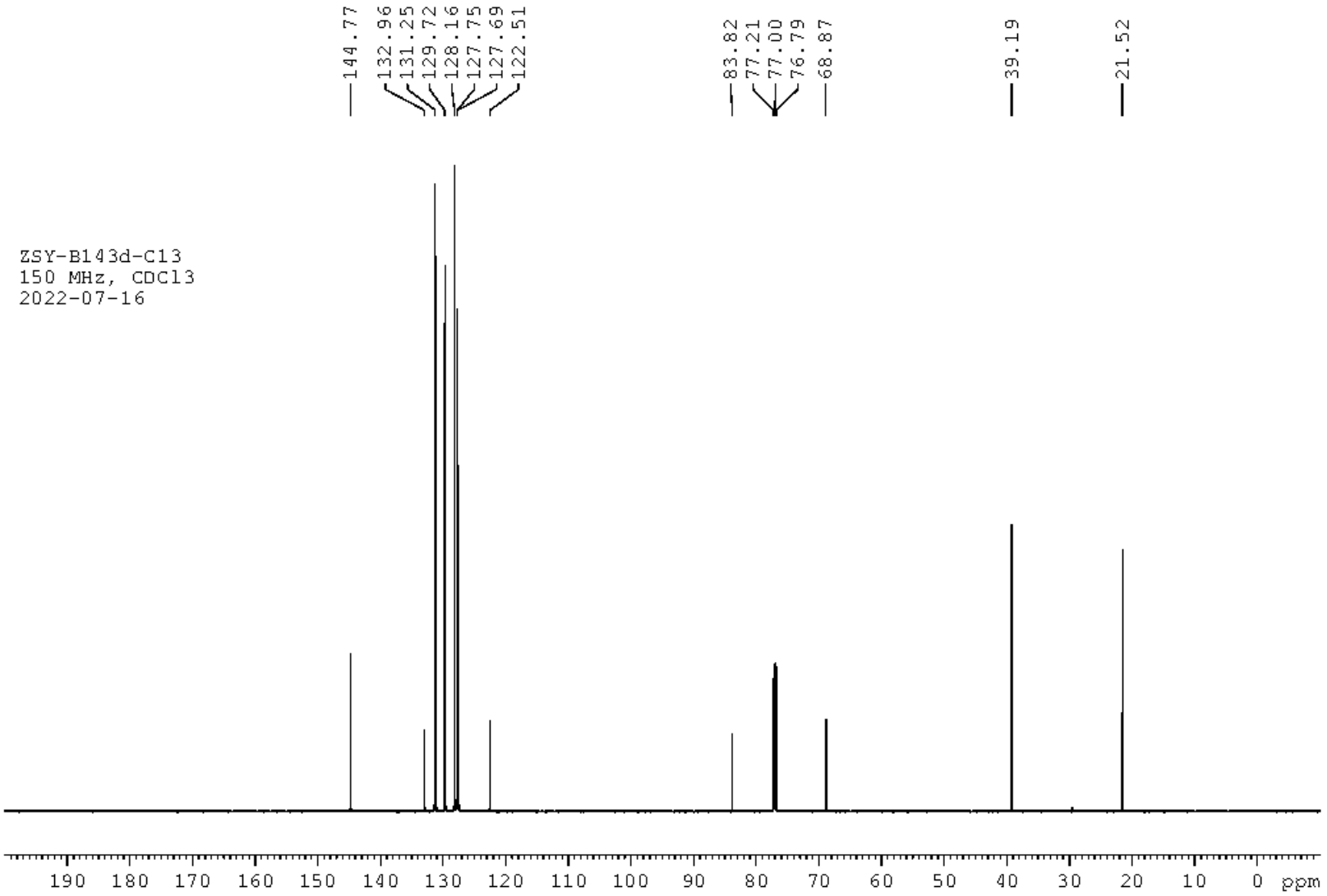
Figure *S9.* The apparent first-order reaction rate in 3Å MS

5. ^{1}H and ^{13}C NMR spectra



3aa

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131.25
129.72
128.16
127.75
127.69
122.51
83.82
77.21
77.00
76.79
68.87
39.19
21.52
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2022-07-16
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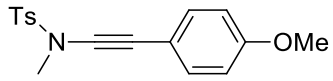
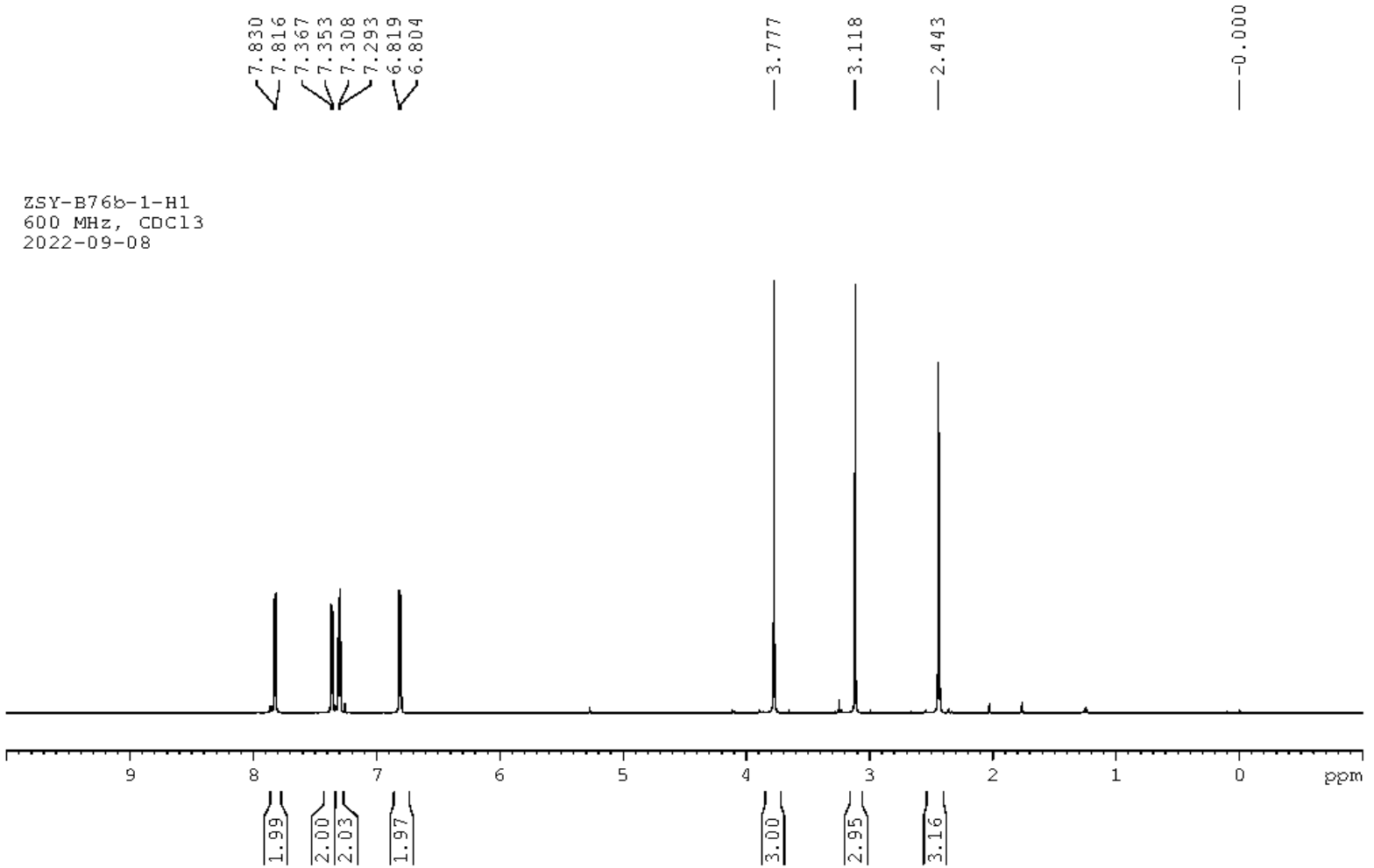

Ts
N
OMe

3ab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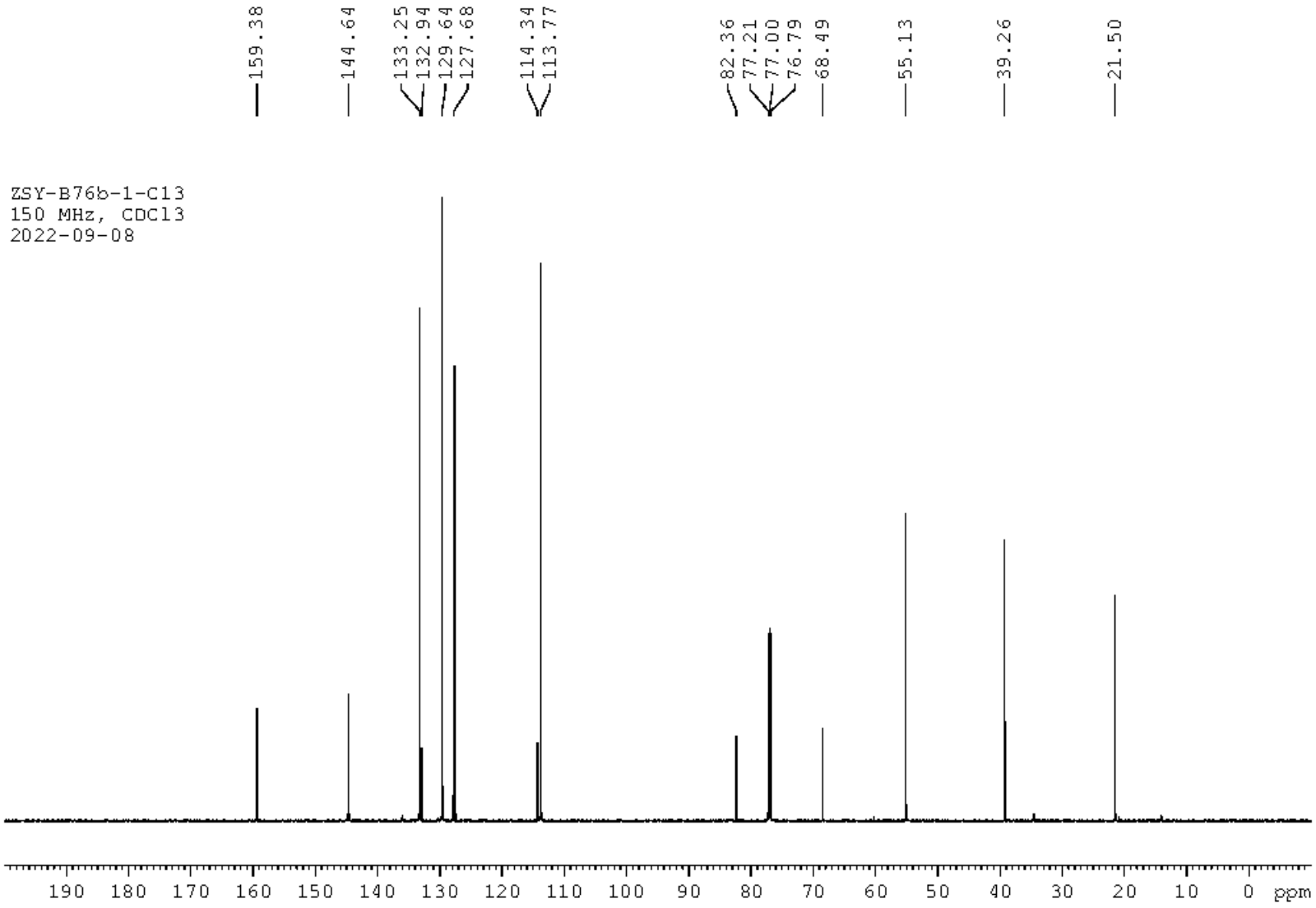
7.816
7.367
7.353
7.308
7.293
6.819
6.804
3.777
3.118
2.443
0.000
ZSY-B76b-1-H1
600 MHz, CDCl3
2022-09-08
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.00
2.03
1.97
3.00
2.95
3.16


159.38
144.64
133.25
132.94
129.64
127.68
114.34
113.77
82.36
77.21
77.00
76.79
68.49
55.13
39.26
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2022-09-08
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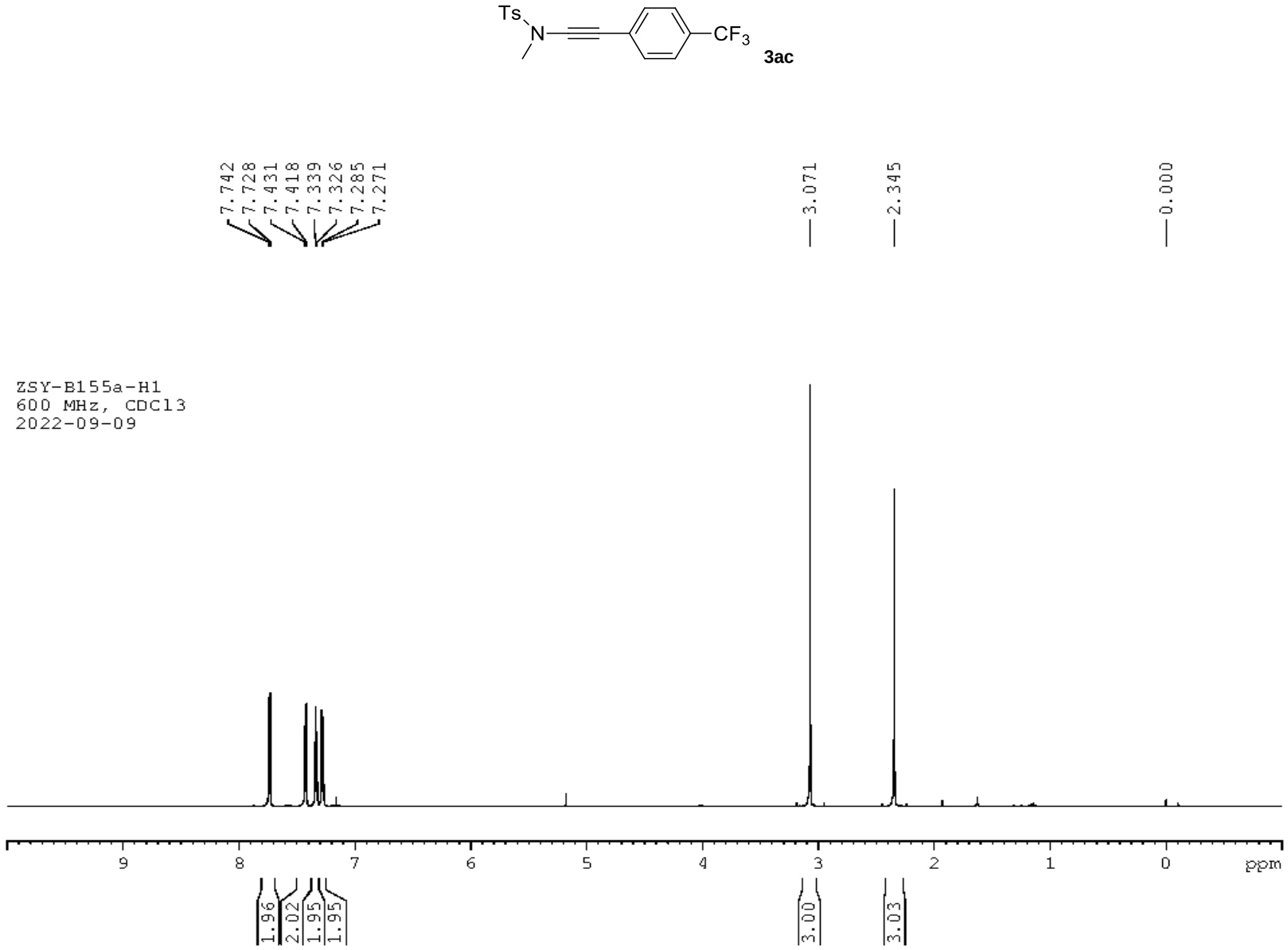
Ts
N
CF3
3ac
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7.728
7.431
7.418
7.339
7.326
7.285
7.271
3.071
2.345
0.000
ZSY-B155a-H1
600 MHz, CDCl3
2022-09-09
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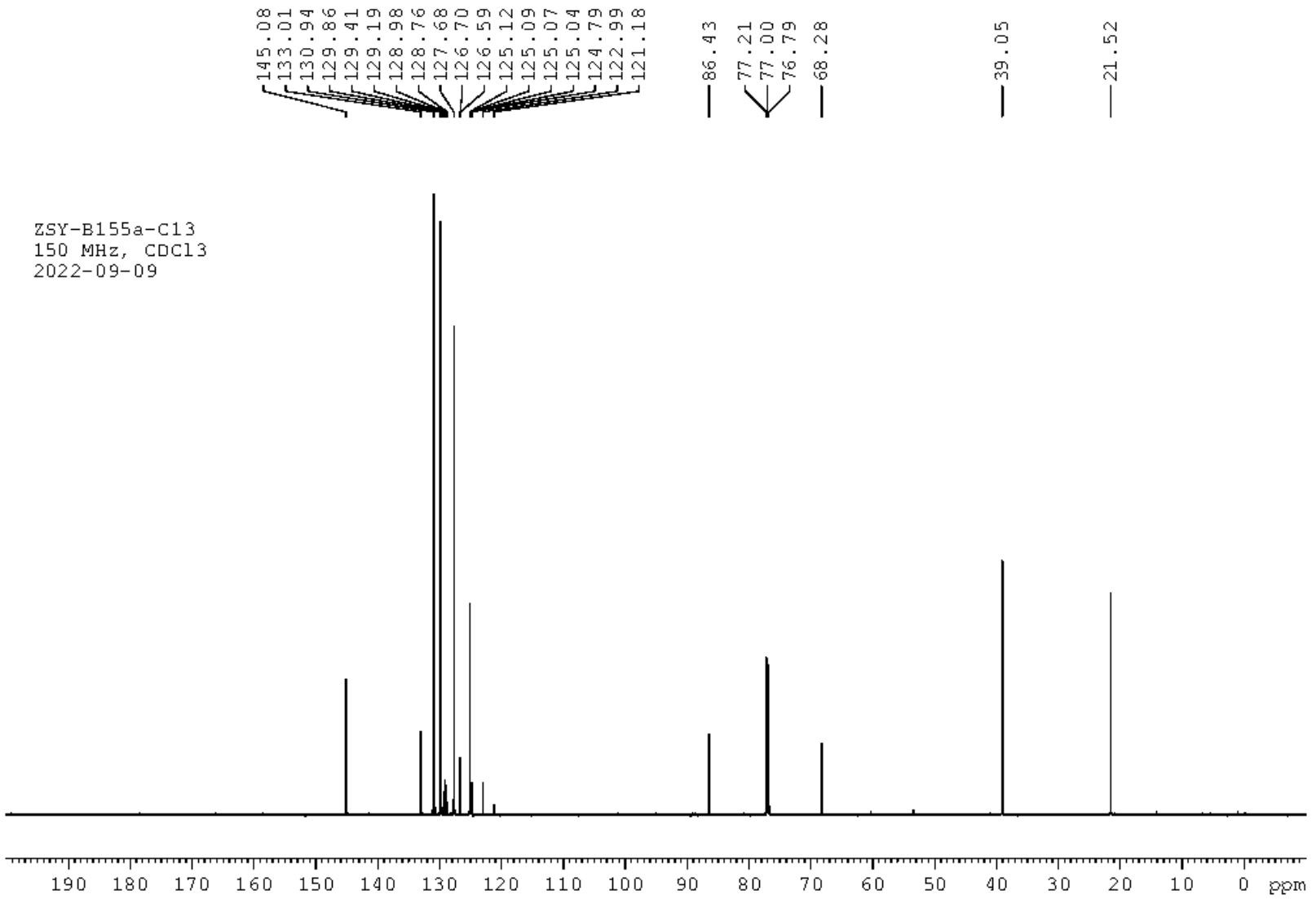
8
7
6
5
4
3
2
1
0
ppm
1.96
2.02
1.95
1.95
3.00
3.03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129.41
129.19
128.98
128.76
127.68
126.70
126.59
125.12
125.09
125.07
125.04
124.79
122.99
121.18
86.43
77.21
77.00
76.79
68.28
39.05
21.52
ZSY-B155a-C13
150 MHz, CDCl3
2022-09-09
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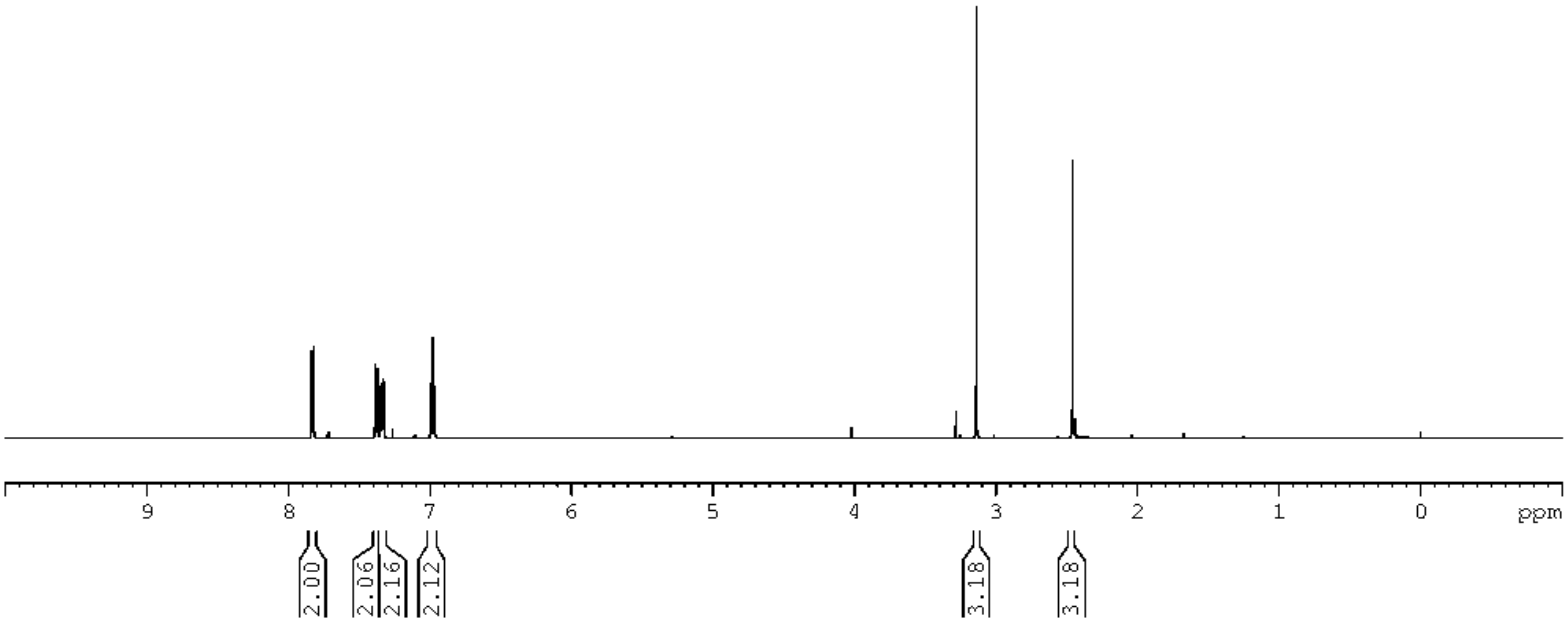
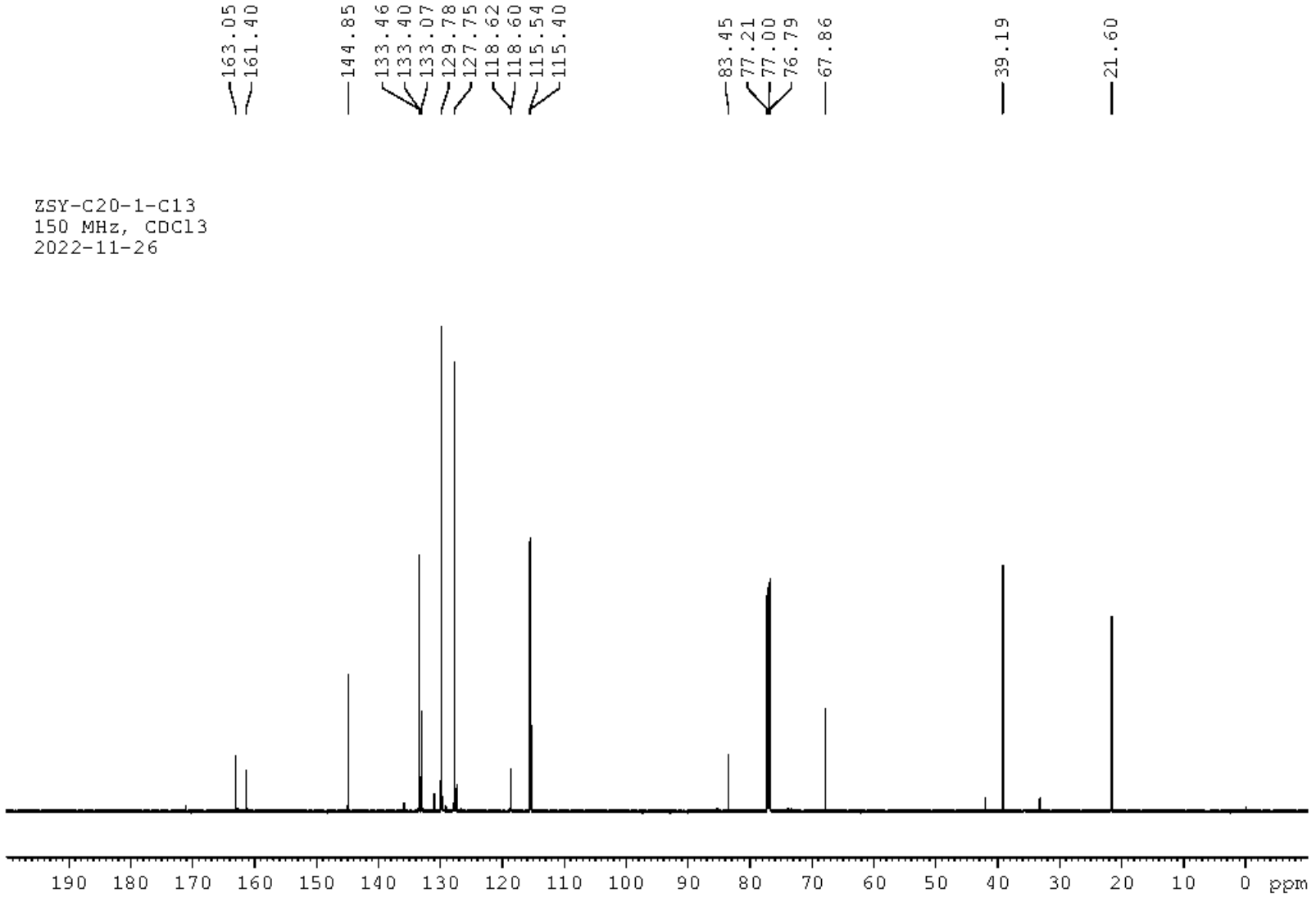
3ad

ZSY-C20-1-H1
600 MHz, CDCl3
2022-11-26

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133.40
133.07
129.78
127.75
118.62
118.60
115.54
115.40
83.45
77.21
77.00
76.79
67.86
39.19
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150 MHz, CDCl3
2022-11-26
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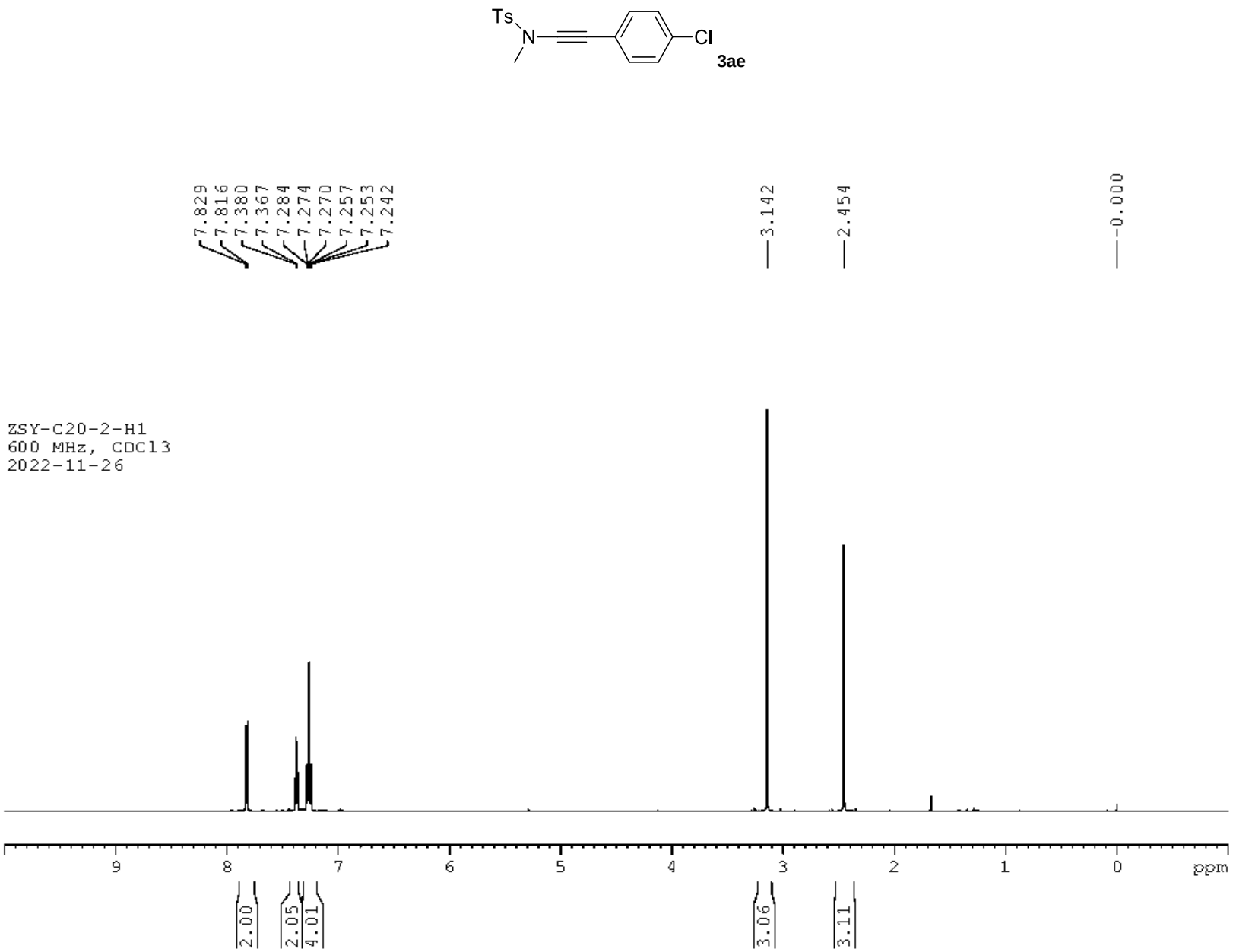
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7.257
7.253
7.242
3.142
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0.000
ZSY-C20-2-H1
600 MHz, CDCl3
2022-11-26
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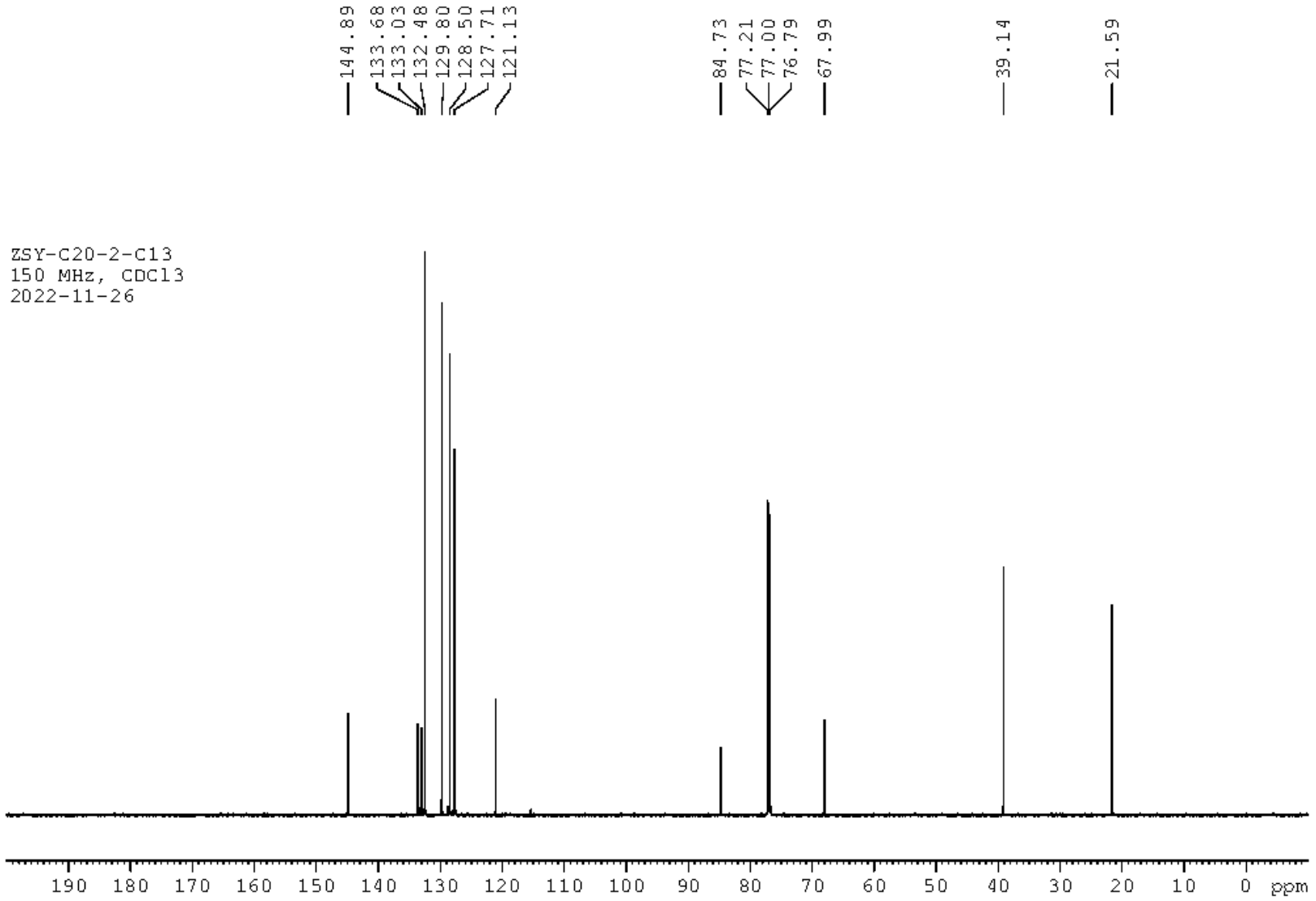
8
7
6
5
4
3
2
1
0
ppm
2.00
2.05
4.01
3.06
3.11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129.80
128.50
127.71
121.13
84.73
77.21
77.00
76.79
67.99
39.14
21.59
ZSY-C20-2-C13
150 MHz, CDCl3
2022-11-26
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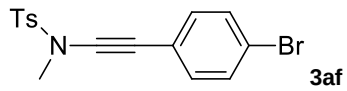
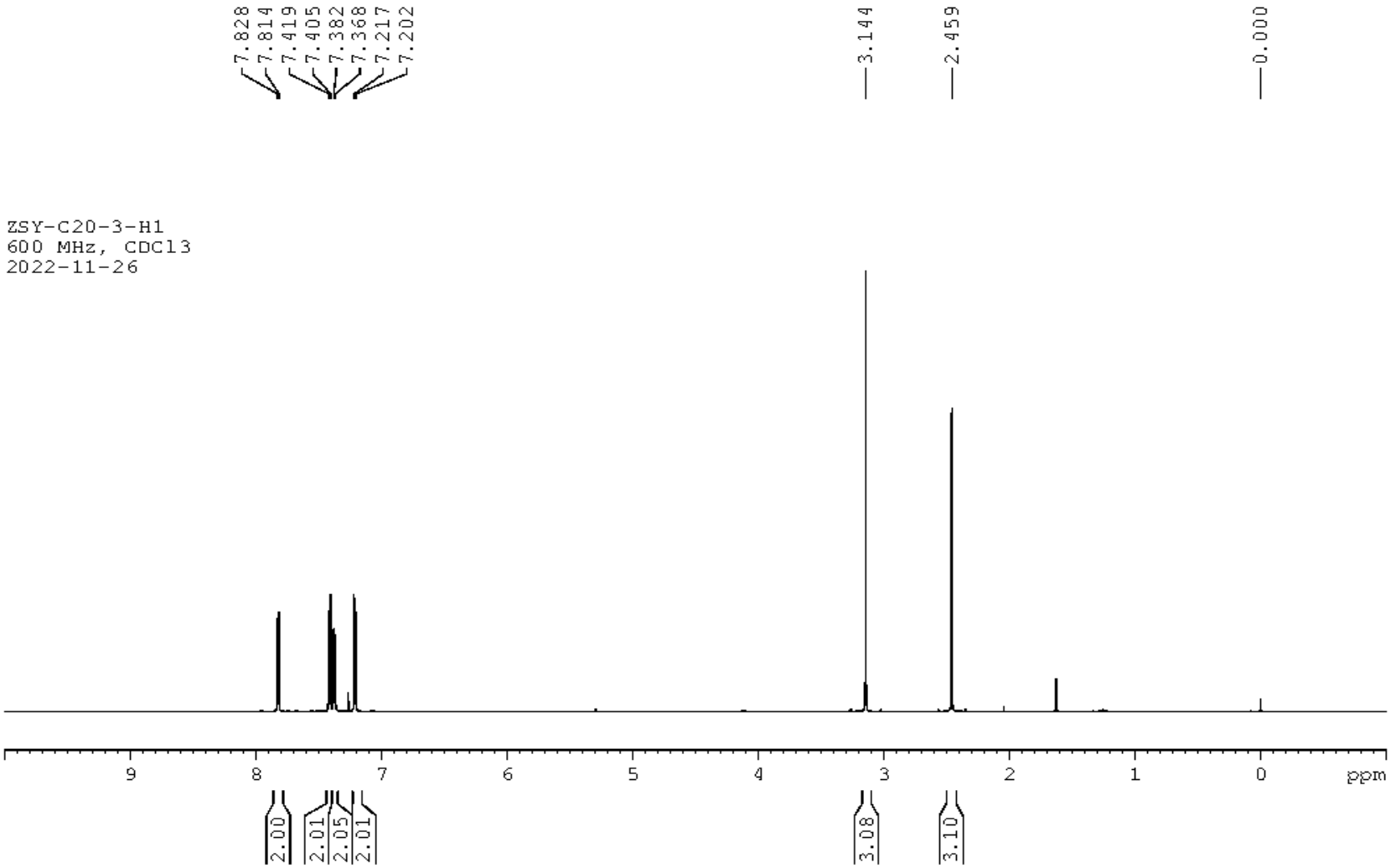

Ts
N
Br

3af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7.419
7.405
7.382
7.368
7.217
7.202
3.144
2.459
0.000
ZSY-C20-3-H1
600 MHz, CDCl3
2022-11-26
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8
7
6
5
4
3
2
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ppm
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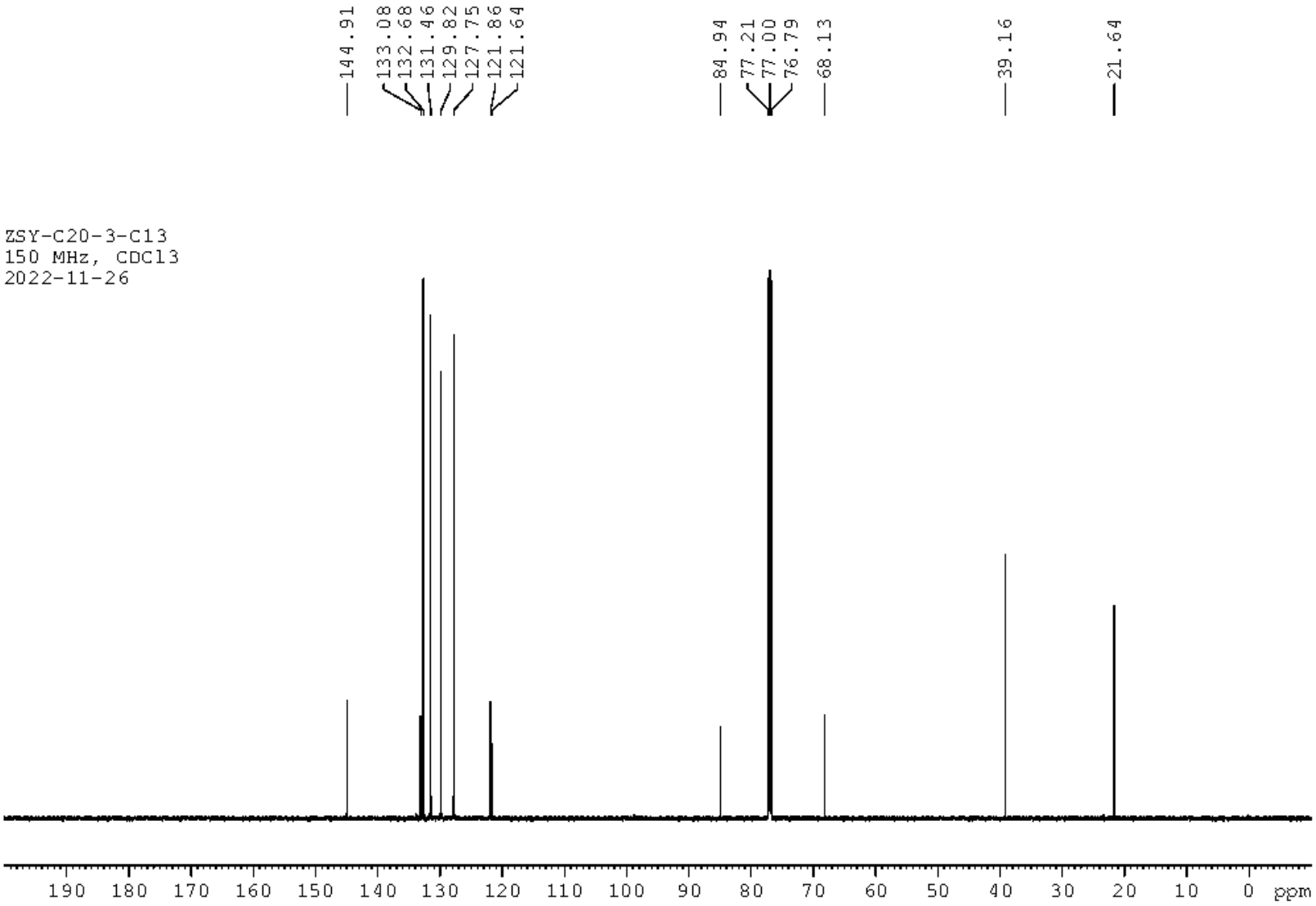
2.01
2.05
2.01
3.08
3.10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77.00
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68.13
39.16
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2022-11-26
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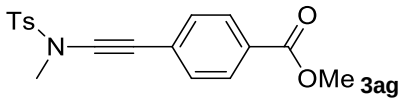
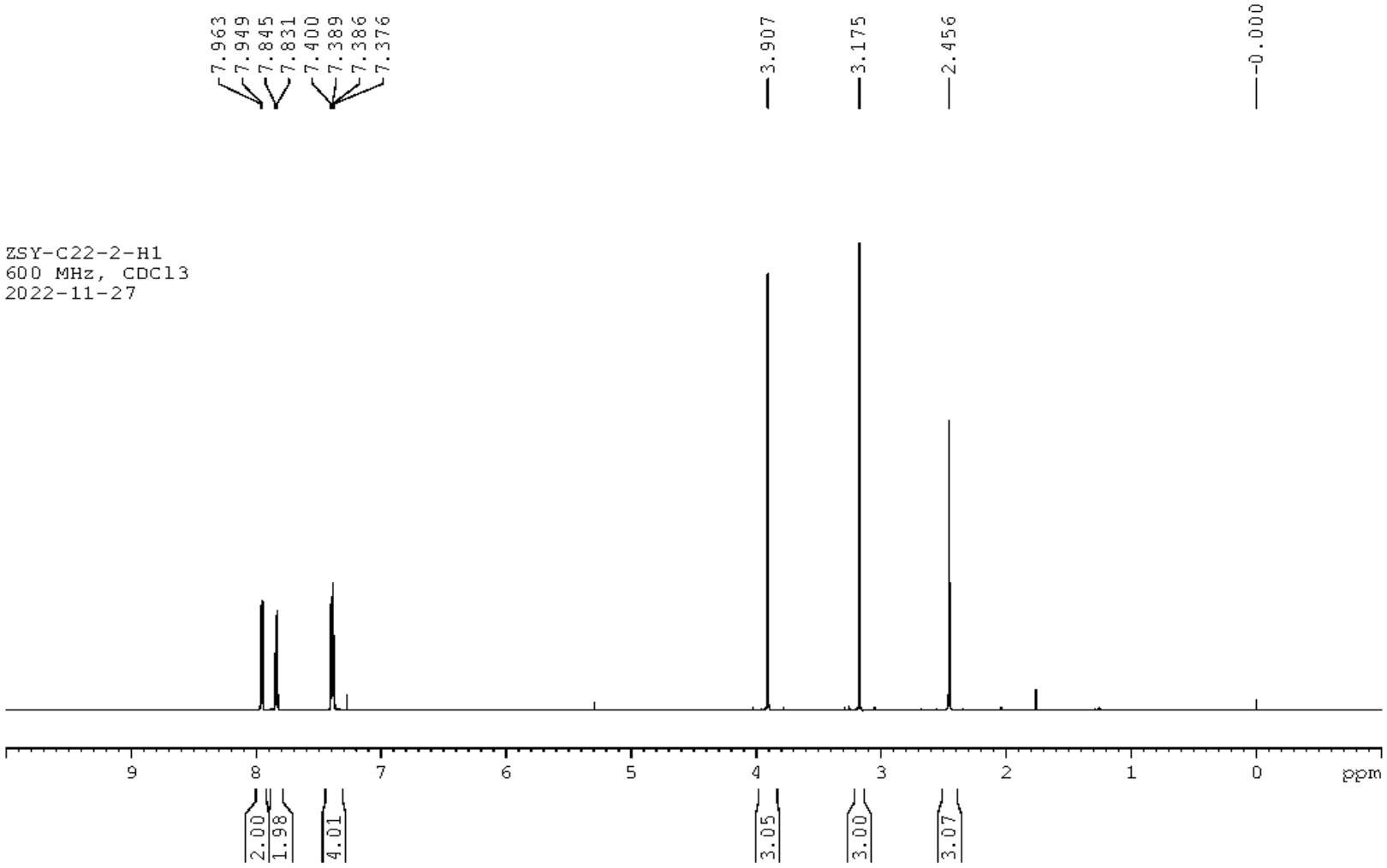

Ts
N
O
OMe

3ag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ZSY-C22-2-H1
600 MHz, CDCl3
2022-11-27
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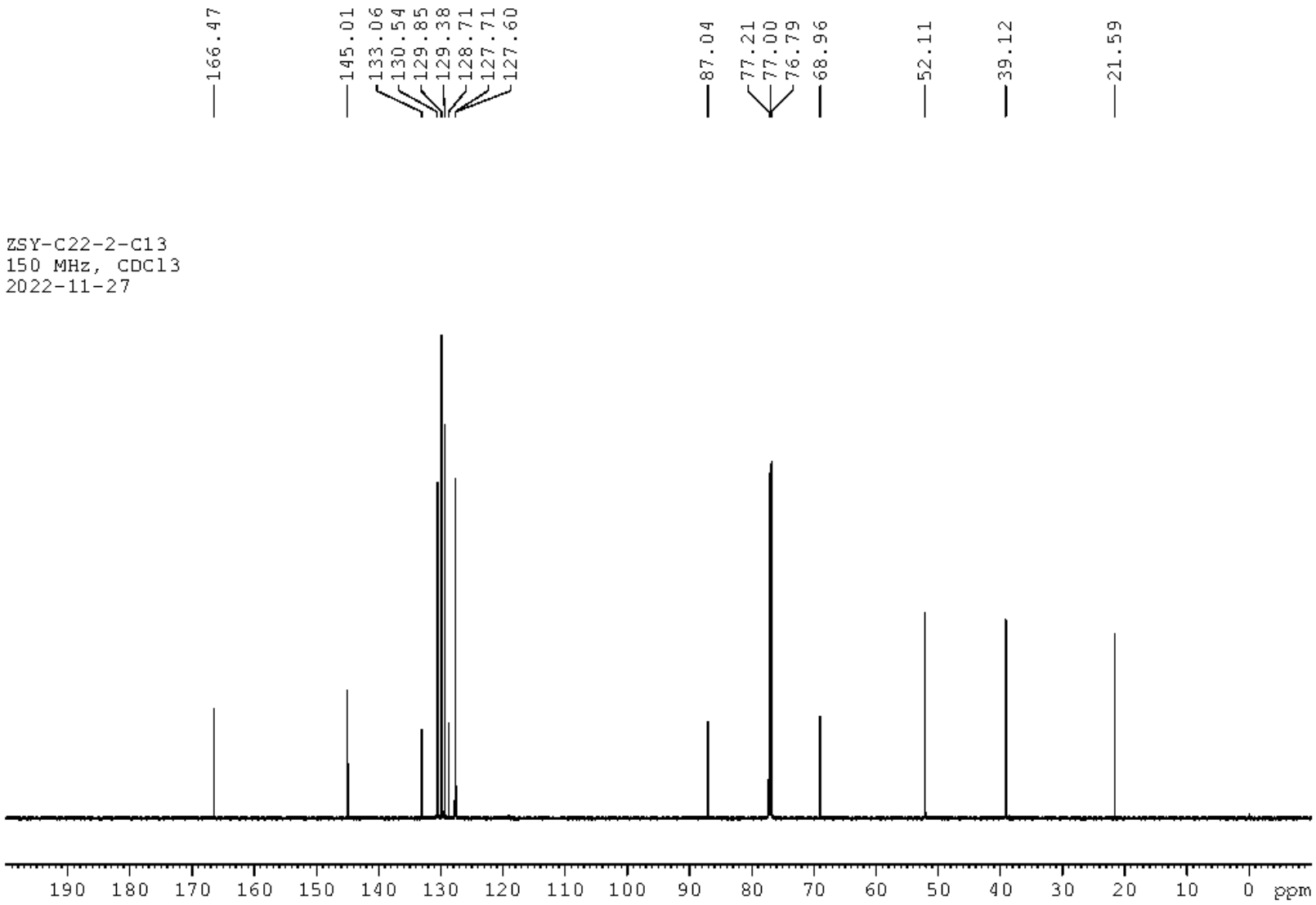
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127.71
127.60
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68.96
52.11
39.12
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150 MHz, CDCl3
2022-11-27
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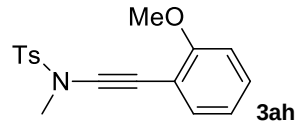
MeO
Ts
N

3ah


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7.246
7.235
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6.841
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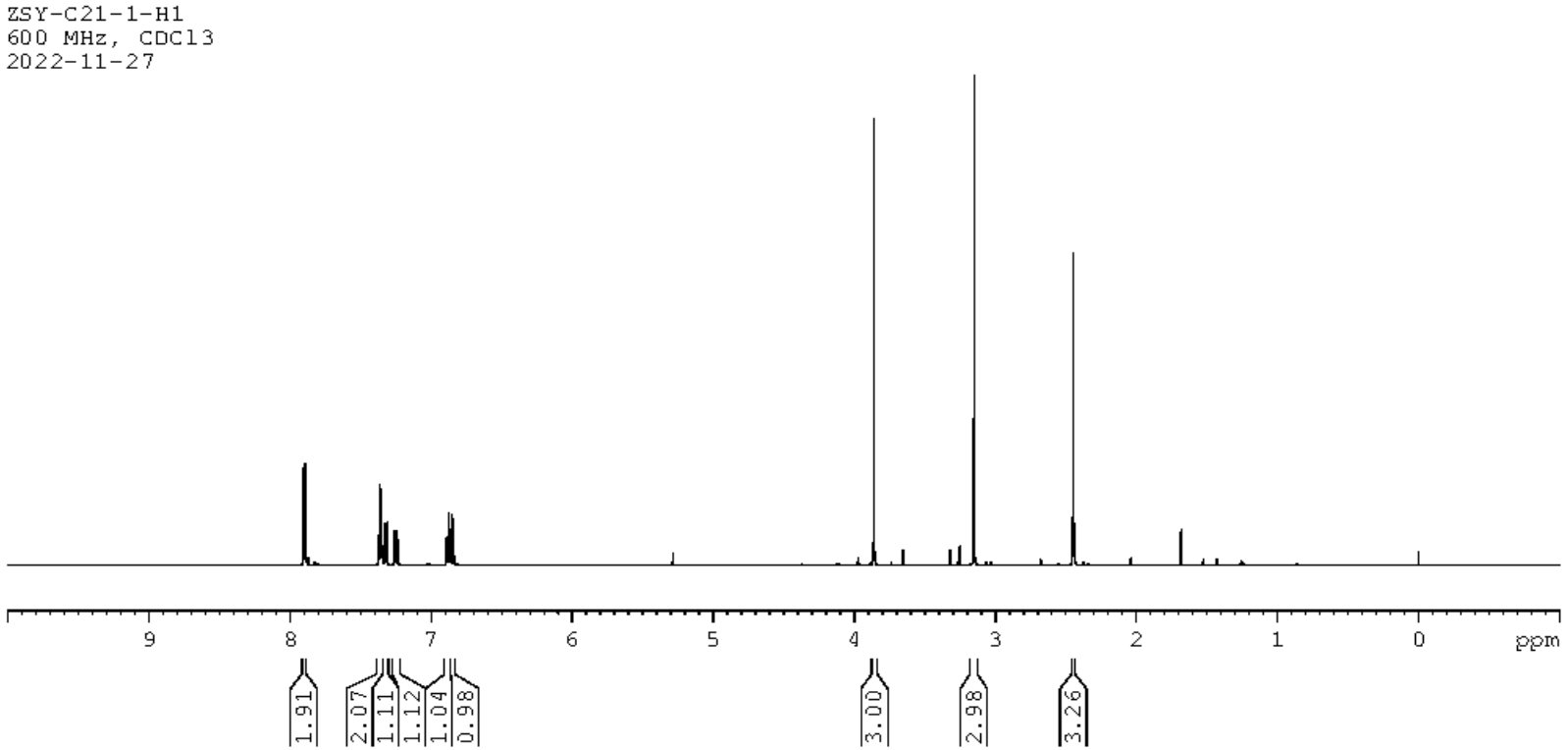
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600 MHz, CDCl3
2022-11-27
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ppm
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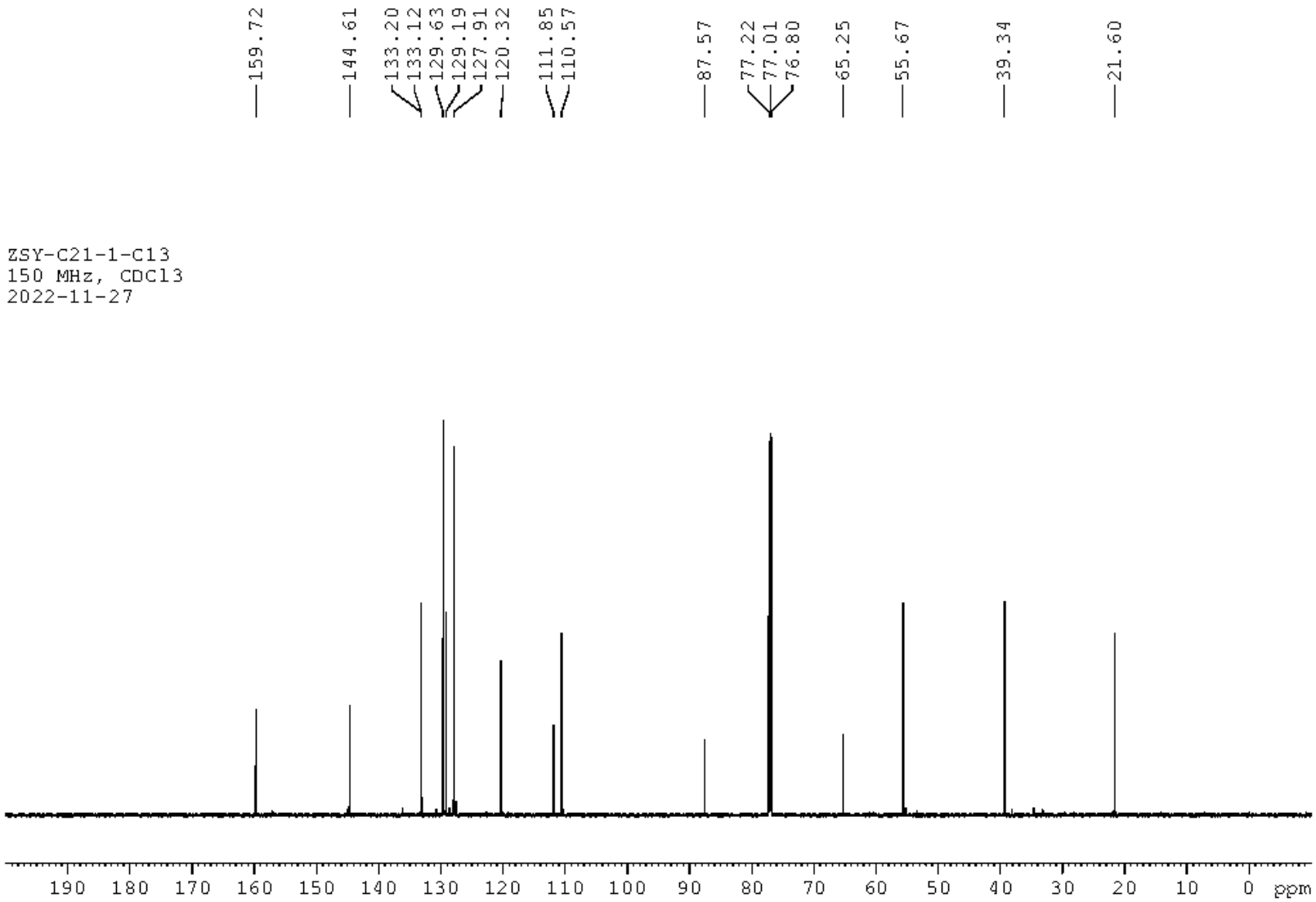
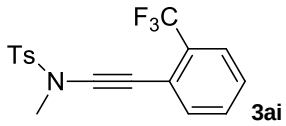
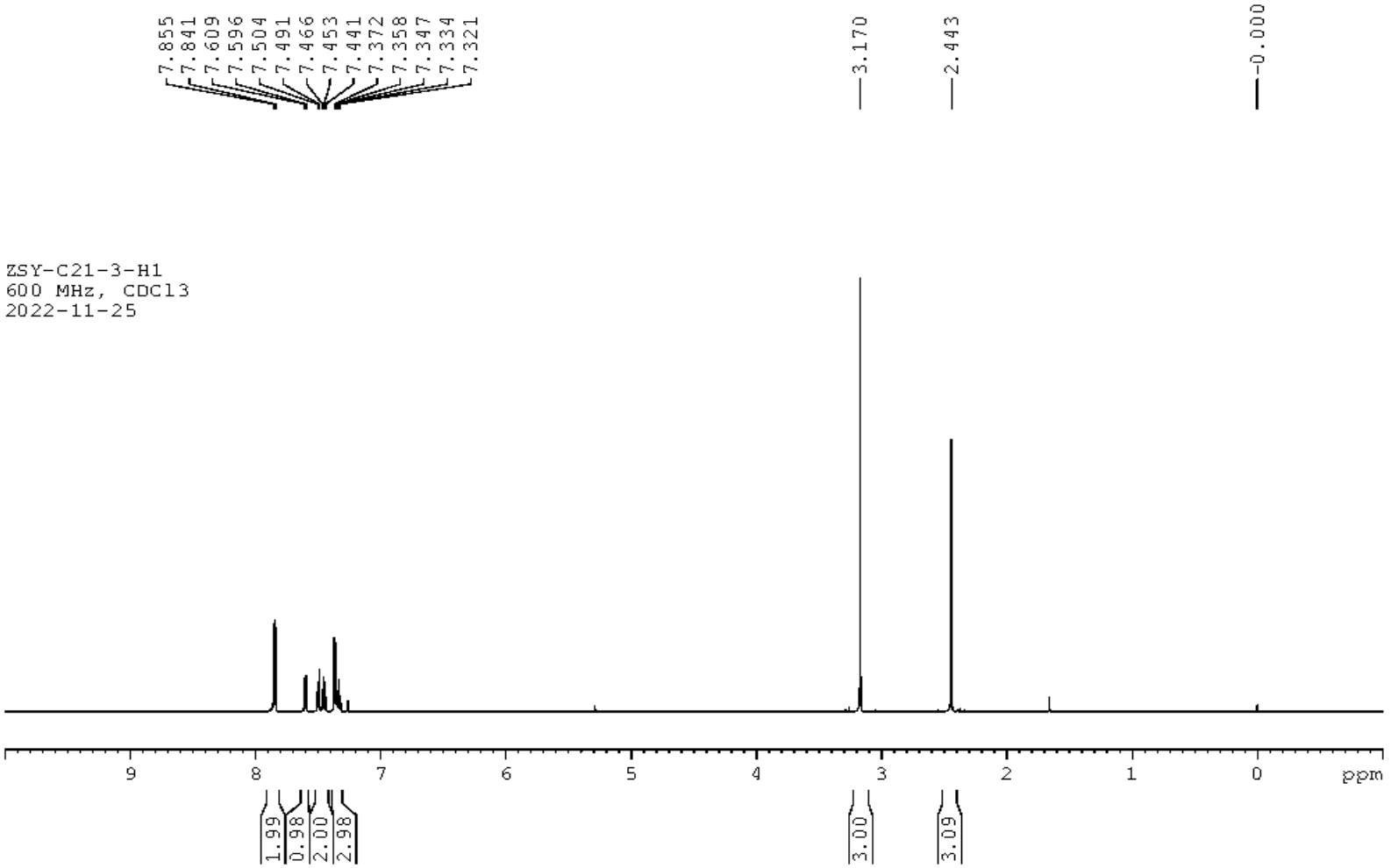
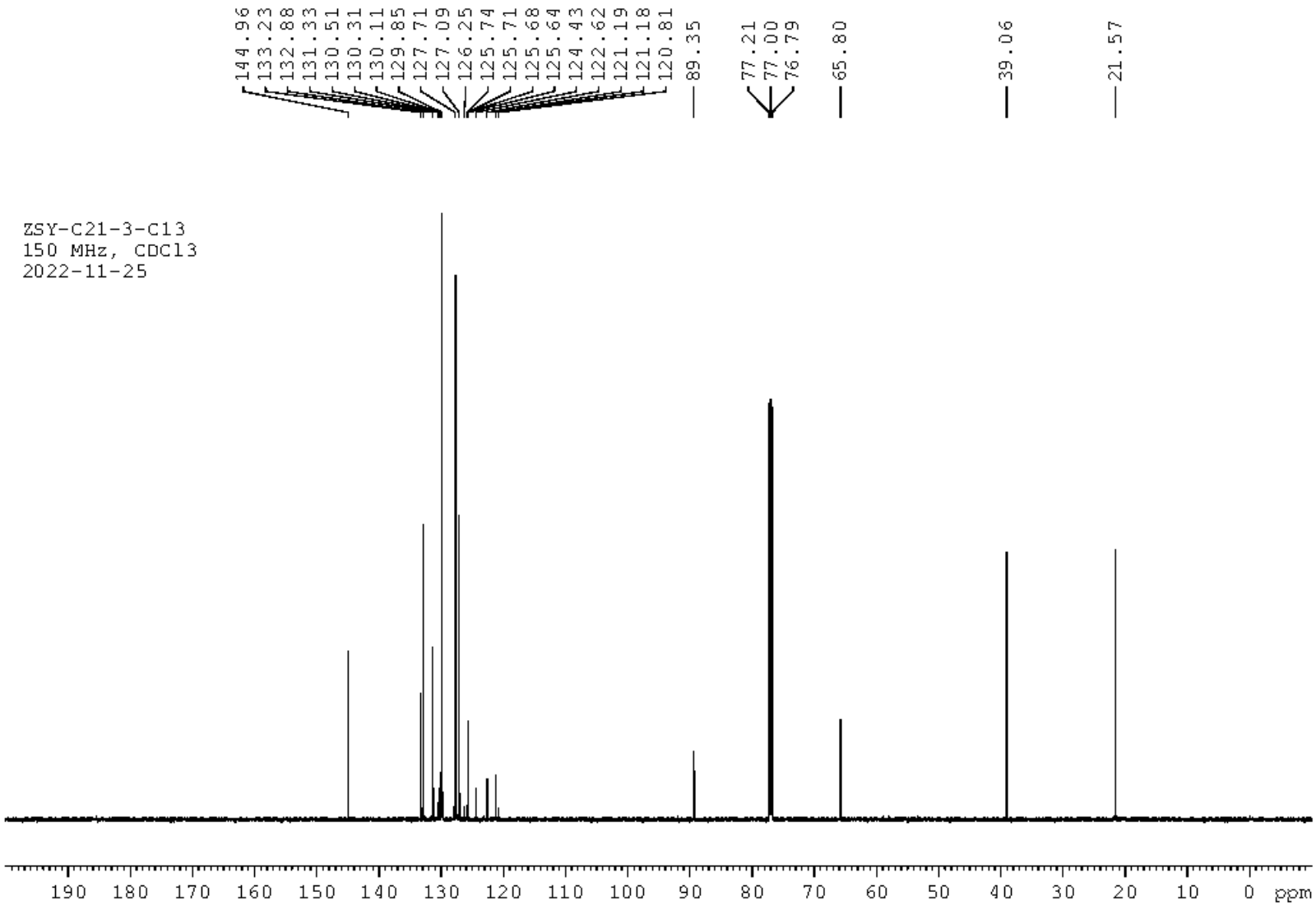
1.11
1.12
1.04
0.98
3.00
2.98
3.26

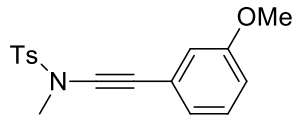

159.72
144.61
133.20
133.12
129.63
129.19
127.91
120.32
111.85
110.57
87.57
77.22
77.01
76.80
65.25
55.67
39.34
21.60
ZSY-C21-1-C13
150 MHz, CDCl3
2022-11-27
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


F3C
Ts
N

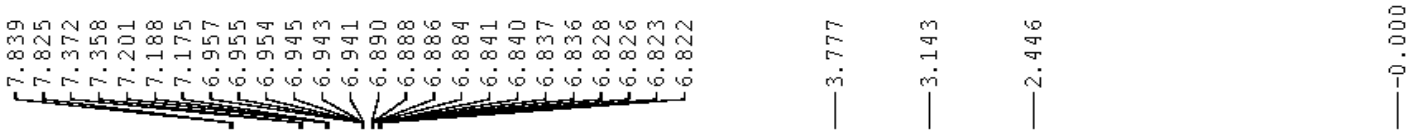
3ai

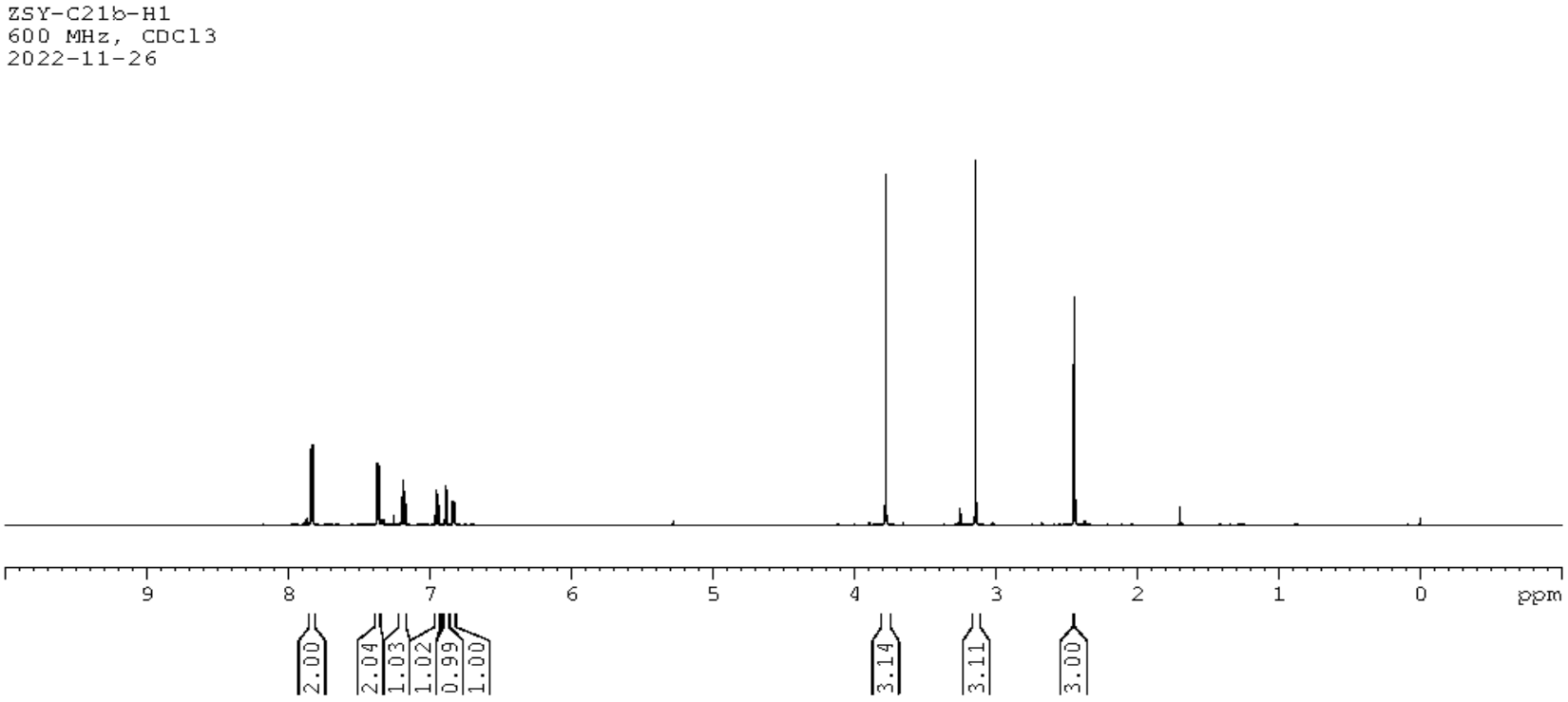

7.855
7.841
7.609
7.596
7.504
7.491
7.466
7.453
7.441
7.372
7.358
7.347
7.334
7.321
3.170
2.443
0.000
ZSY-C21-3-H1
600 MHz, CDCl3
2022-11-25
9
8
7
6
5
4
3
2
1
0
ppm
1.99
0.98
2.00
2.98
3.00
3.09

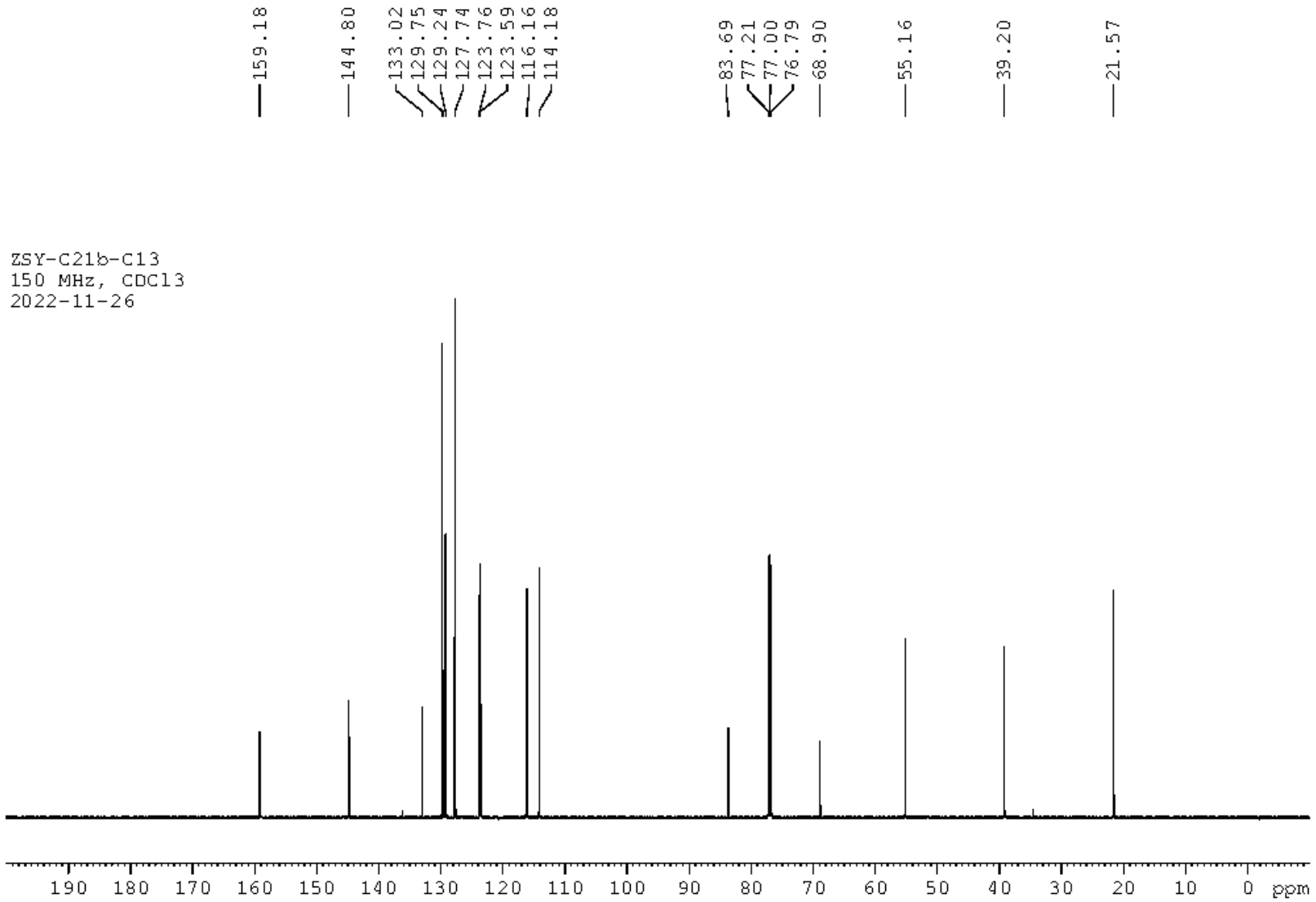

144.96
133.23
132.88
131.33
130.51
130.31
130.11
129.85
127.71
127.09
126.25
125.74
125.71
125.68
125.64
124.43
122.62
121.19
121.18
120.81
89.35
77.21
77.00
76.79
65.80
39.06
21.57
ZSY-C21-3-C13
150 MHz, CDCl3
2022-11-25
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

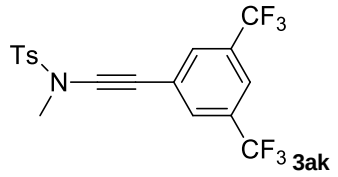

OMe
Ts
N

3aj

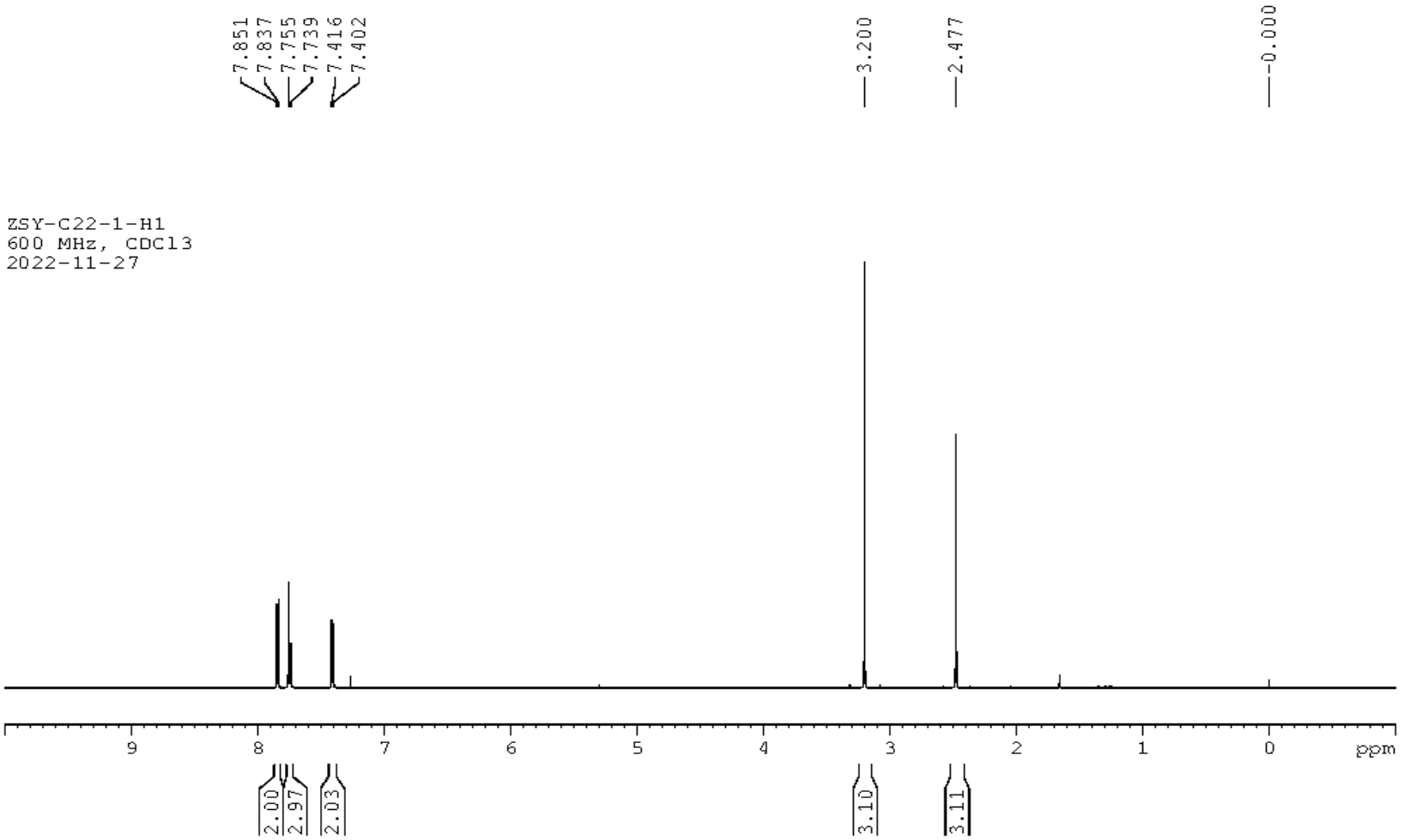

7.839
7.825
7.372
7.358
7.201
7.188
7.175
6.957
6.955
6.954
6.945
6.943
6.941
6.890
6.888
6.886
6.884
6.841
6.840
6.837
6.836
6.828
6.826
6.823
6.822
3.777
3.143
2.446
0.000

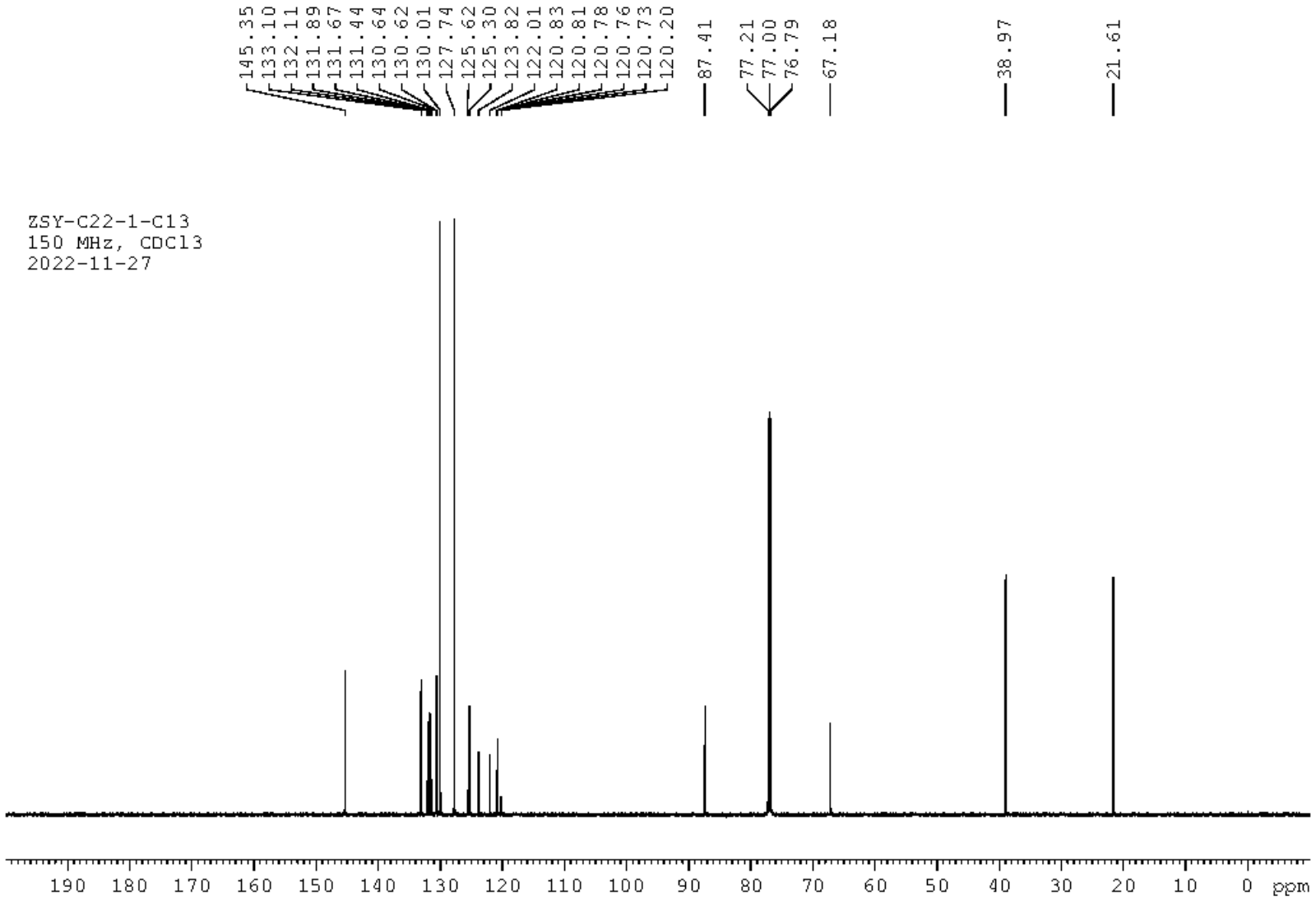

ZSY-C21b-H1
600 MHz, CDCl3
2022-11-26
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.04
1.03
1.02
0.99
1.00
3.14
3.11
3.00

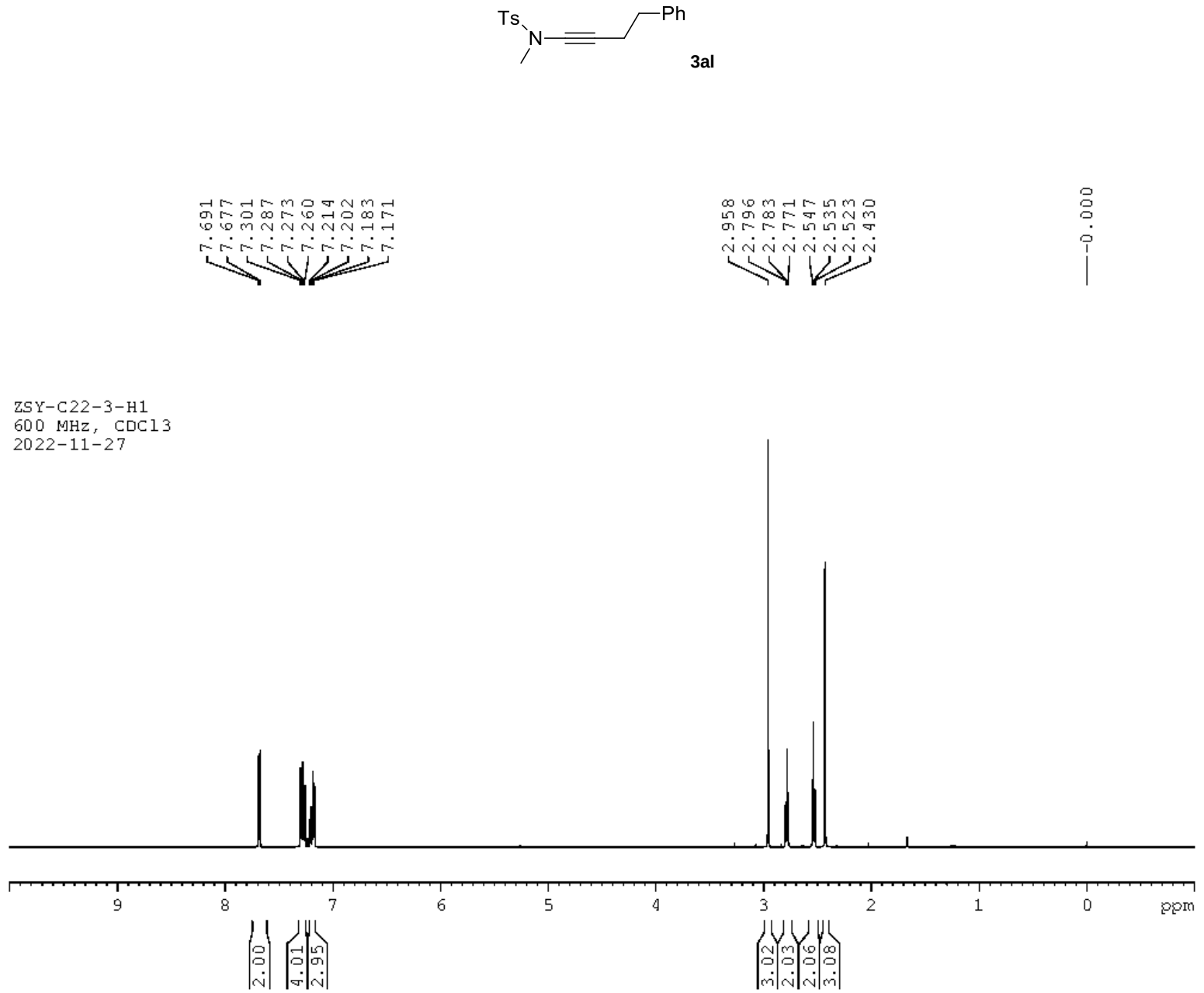

159.18
144.80
133.02
129.75
129.24
127.74
123.76
123.59
116.16
114.18
83.69
77.21
77.00
76.79
68.90
55.16
39.20
21.57
ZSY-C21b-C13
150 MHz, CDCl3
2022-11-26
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

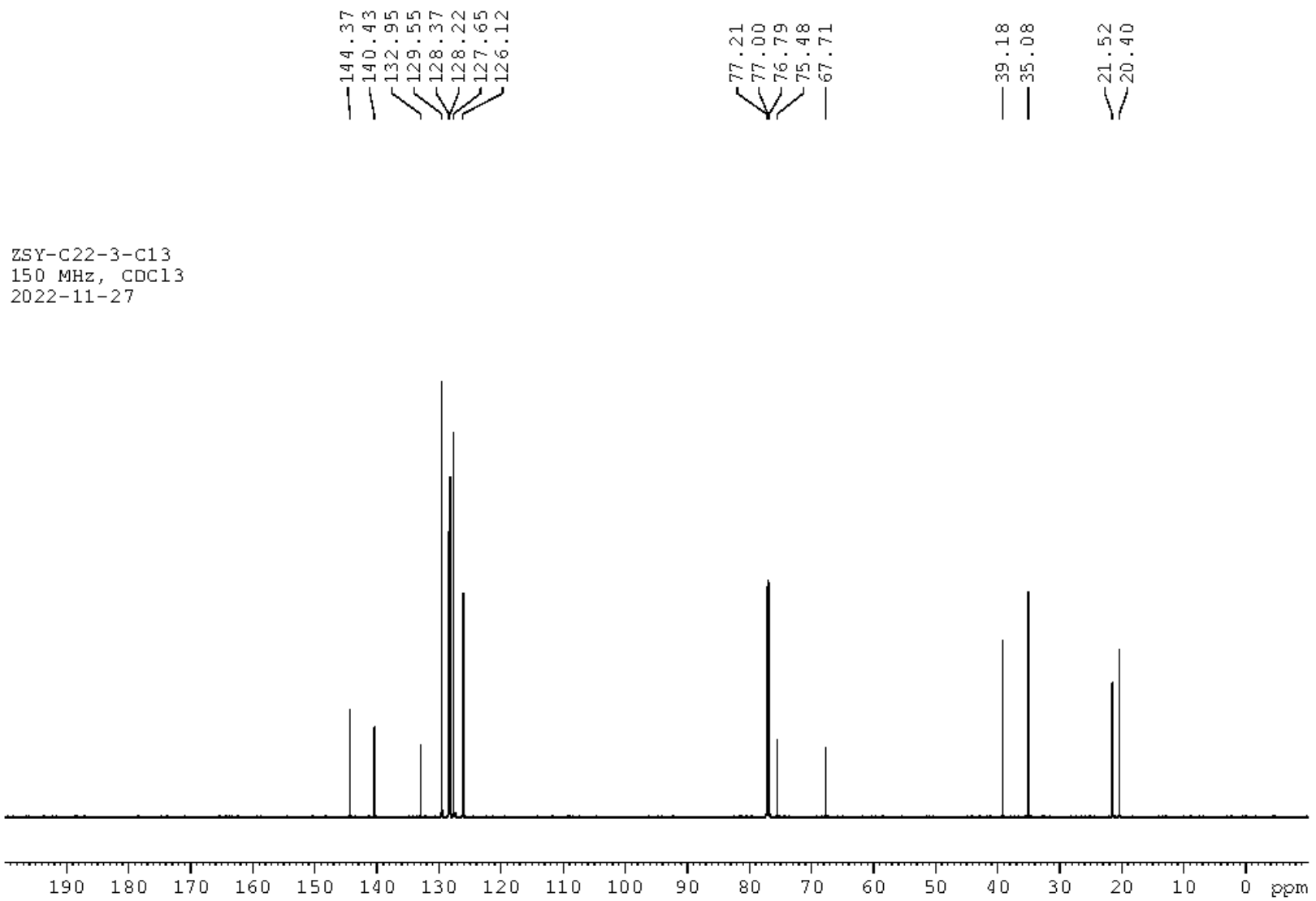

Ts
N
CF3
CF3

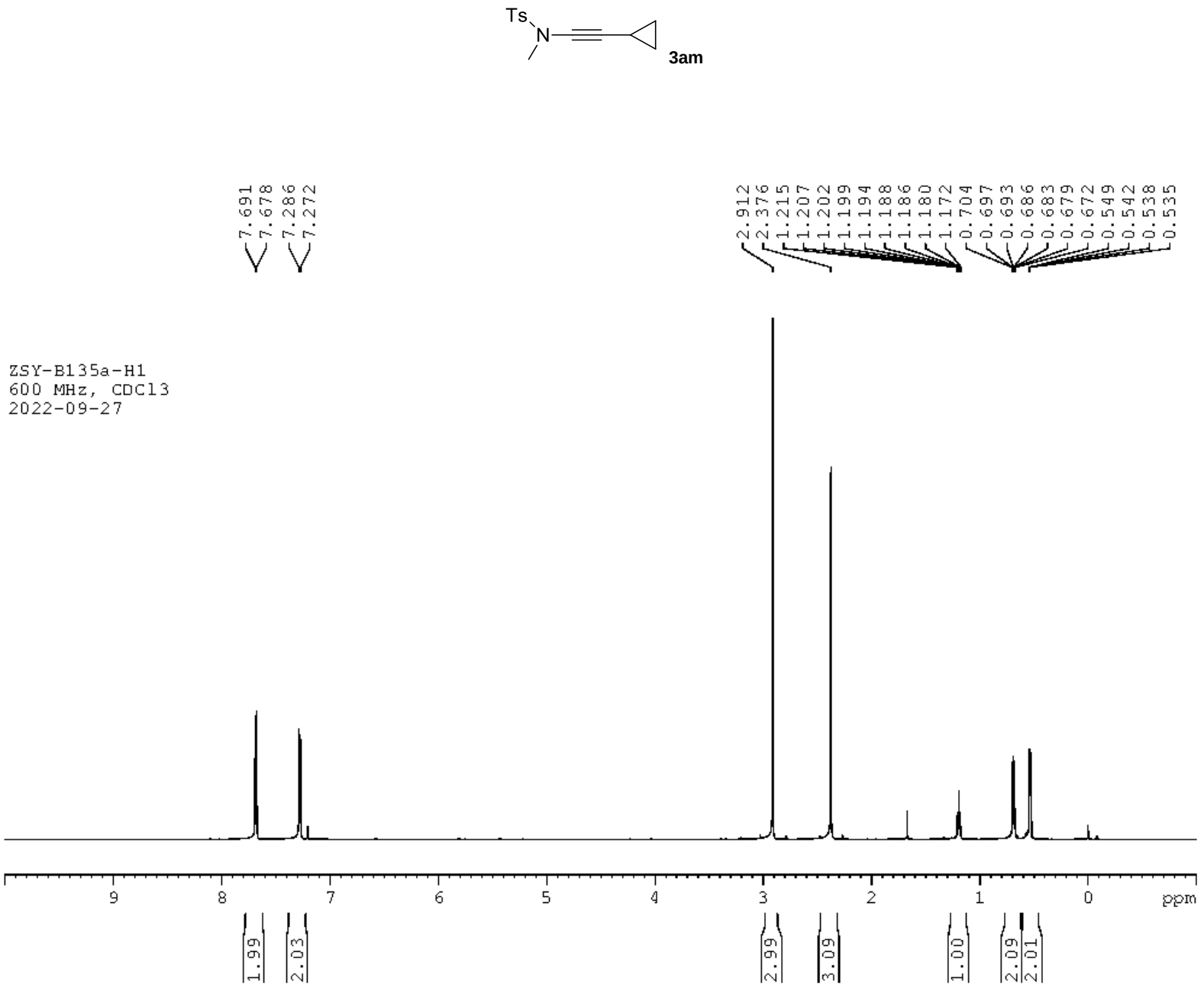
3ak

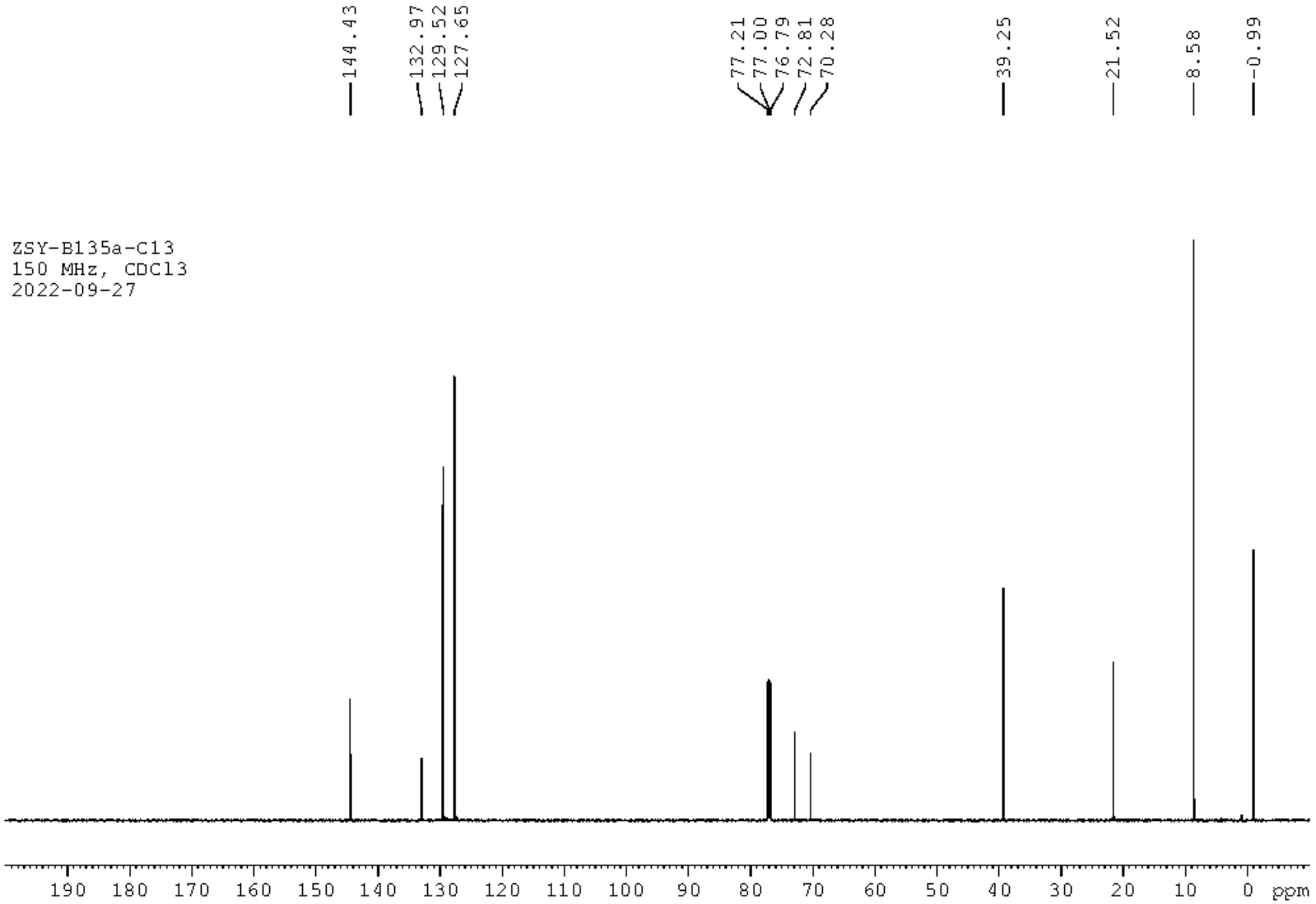

7.851
7.837
7.755
7.739
7.416
7.402
3.200
2.477
0.000
ZSY-C22-1-H1
600 MHz, CDCl3
2022-11-27
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.97
2.03
3.10
3.11

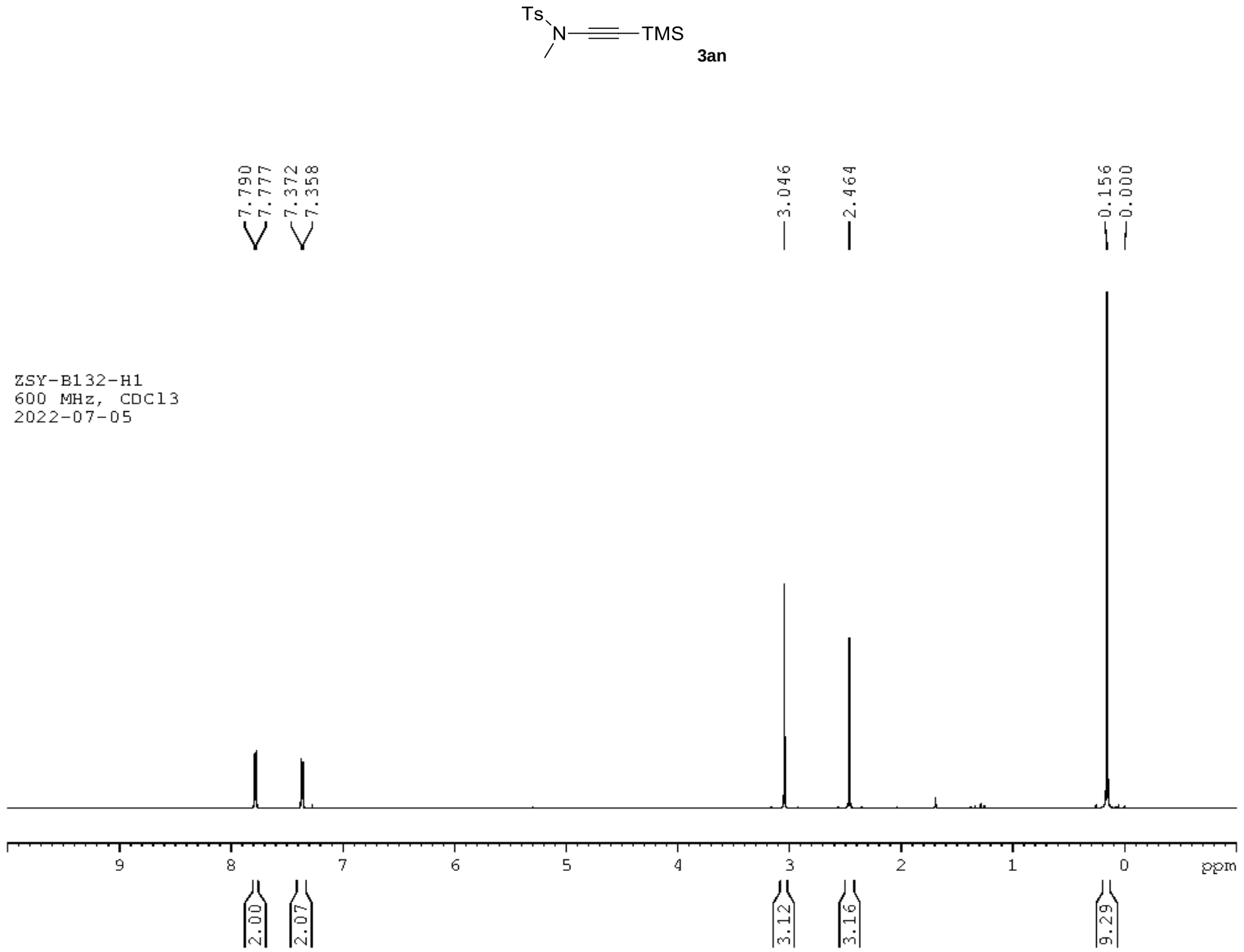

145.35
133.10
132.11
131.89
131.67
131.44
130.64
130.62
130.01
127.74
125.62
125.30
123.82
122.01
120.83
120.81
120.78
120.76
120.73
120.20
87.41
77.21
77.00
76.79
67.18
38.97
21.61
ZSY-C22-1-C13
150 MHz, CDCl3
2022-11-27
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

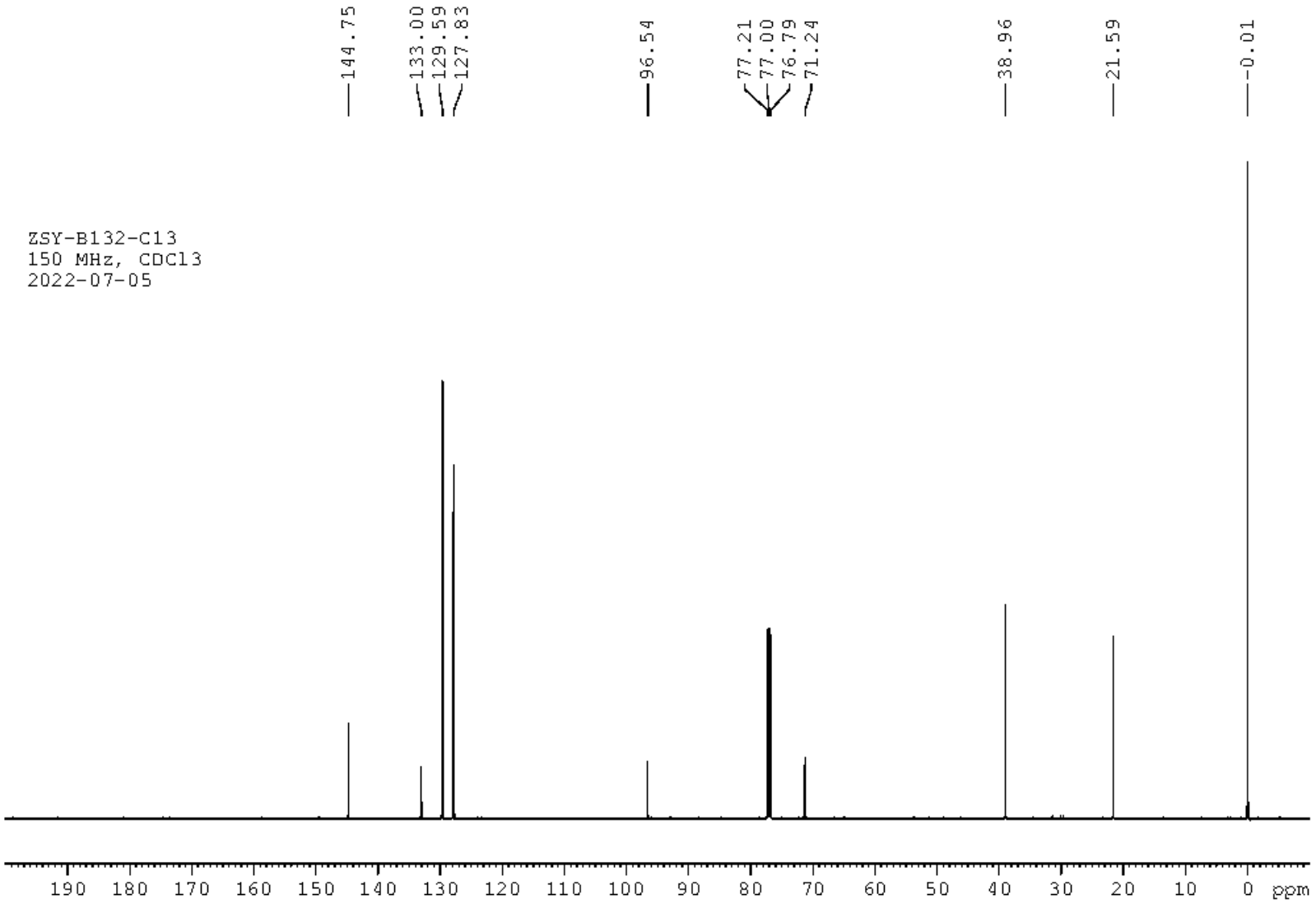

Ts
N
Ph
3al
7.691
7.677
7.301
7.287
7.273
7.260
7.214
7.202
7.183
7.171
2.958
2.796
2.783
2.771
2.547
2.535
2.523
2.430
0.000
ZSY-C22-3-H1
600 MHz, CDCl3
2022-11-27
9
8
7
6
5
4
3
2
1
0
ppm
2.00
4.01
2.95
3.02
2.03
2.06
3.08

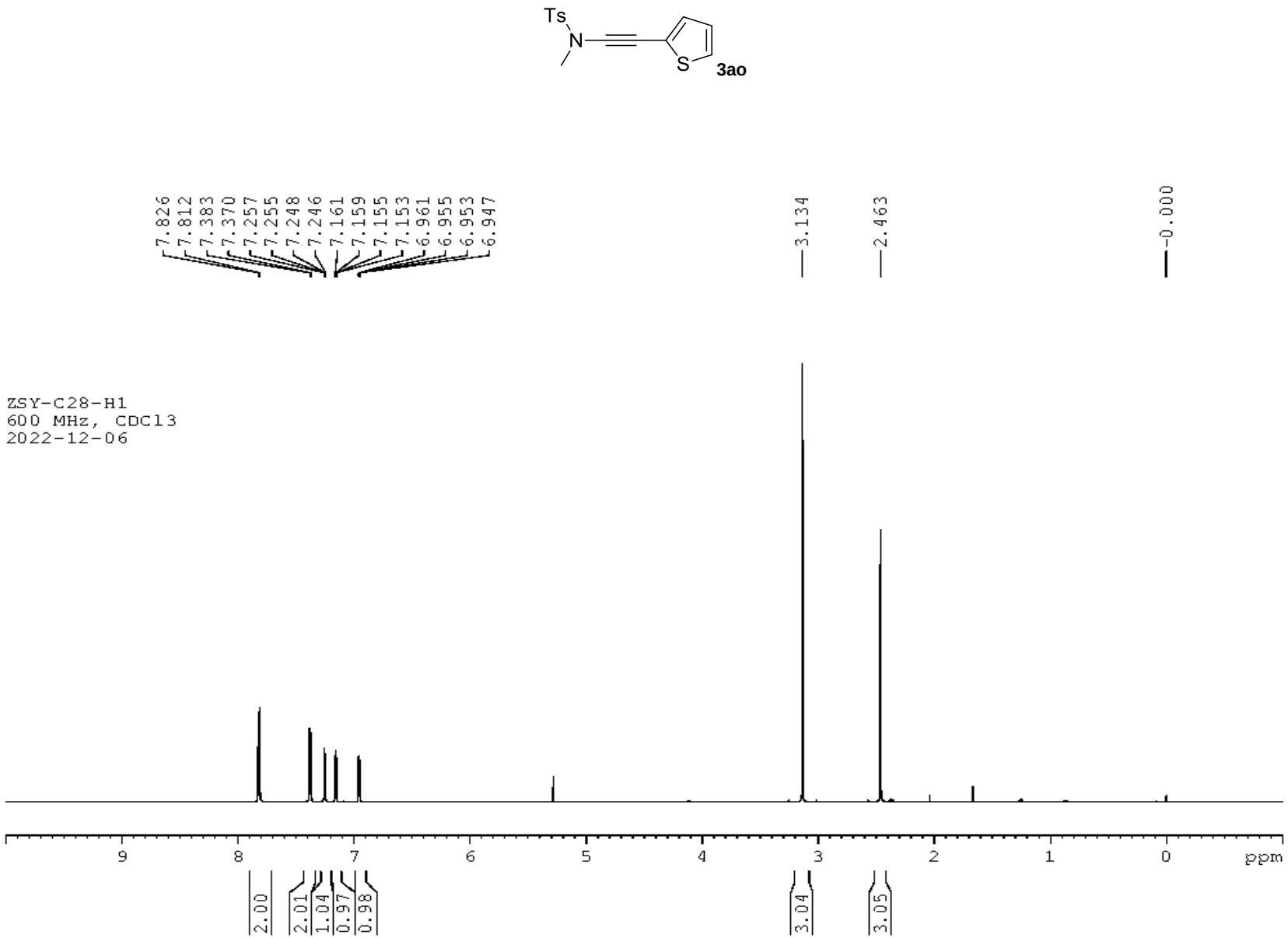

144.37
140.43
132.95
129.55
128.37
128.22
127.65
126.12
77.21
77.00
76.79
75.48
67.71
39.18
35.08
21.52
20.40
ZSY-C22-3-C13
150 MHz, CDCl3
2022-11-27
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

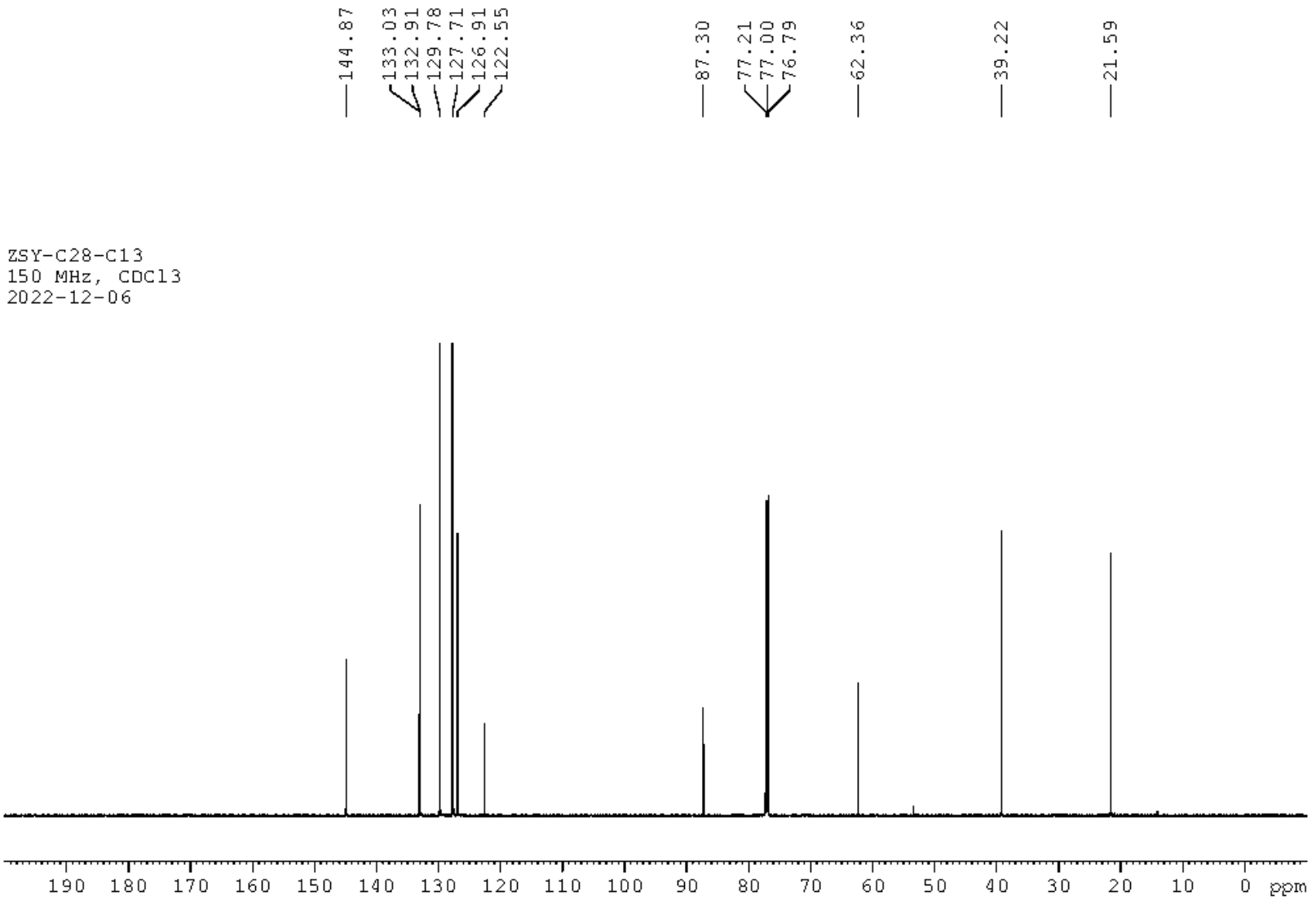

Ts
N
3am
7.691
7.678
7.286
7.272
2.912
2.376
1.215
1.207
1.202
1.199
1.194
1.188
1.186
1.180
1.172
0.704
0.697
0.693
0.686
0.683
0.679
0.672
0.549
0.542
0.538
0.535
ZSY-B135a-H1
600 MHz, CDCl3
2022-09-27
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.03
2.99
3.09
1.00
2.09
2.01

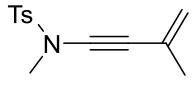

144.43
132.97
129.52
127.65
77.21
77.00
76.79
72.81
70.28
39.25
21.52
8.58
-0.99
ZSY-B135a-C13
150 MHz, CDCl3
2022-09-27
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ts
N
TMS
3an
7.790
7.777
7.372
7.358
3.046
2.464
0.156
0.000
ZSY-B132-H1
600 MHz, CDCl3
2022-07-05
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.07
3.12
3.16
9.29

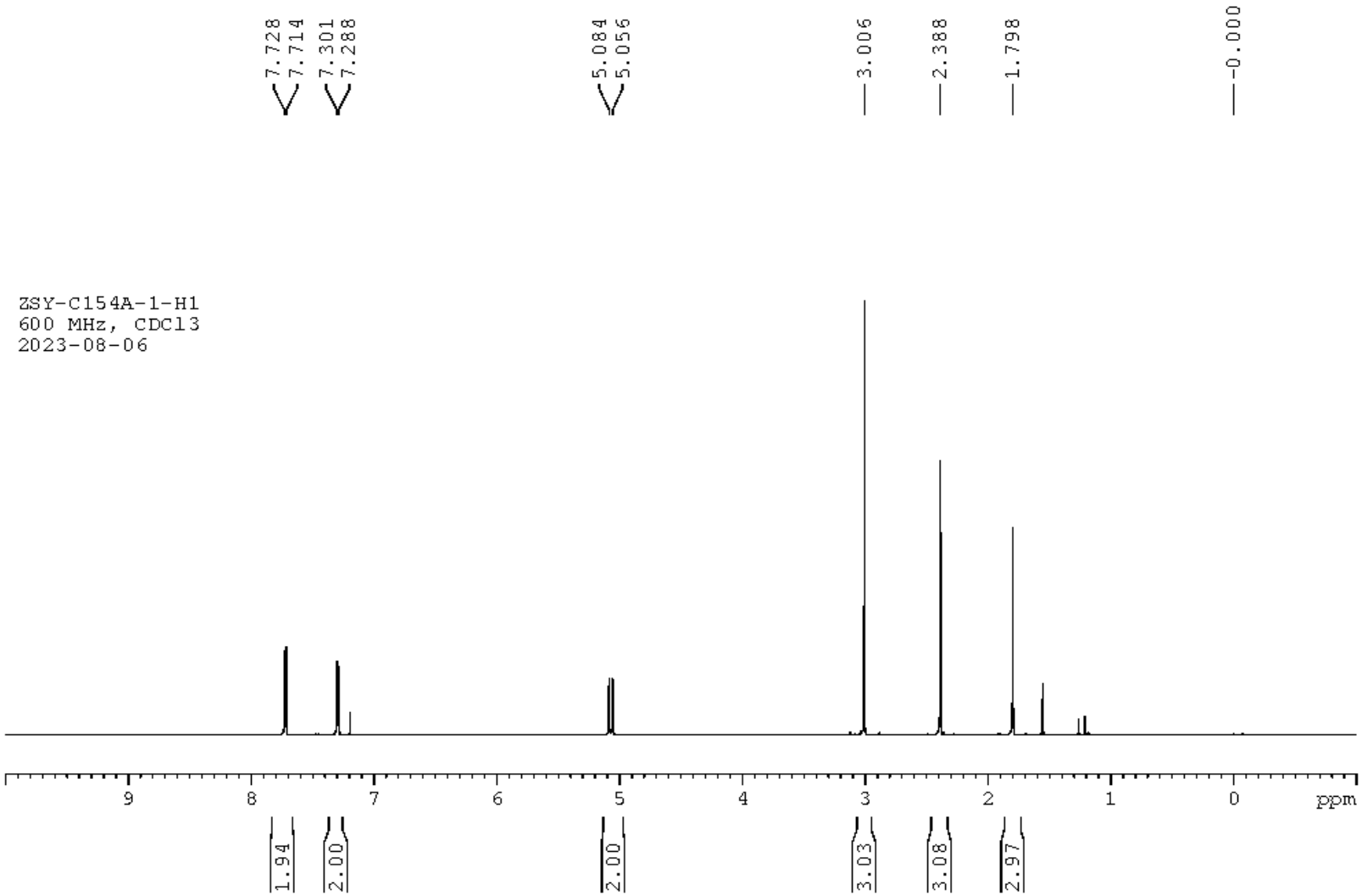

144.75
133.00
129.59
127.83
96.54
77.21
77.00
76.79
71.24
38.96
21.59
-0.01
ZSY-B132-C13
150 MHz, CDCl3
2022-07-05
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

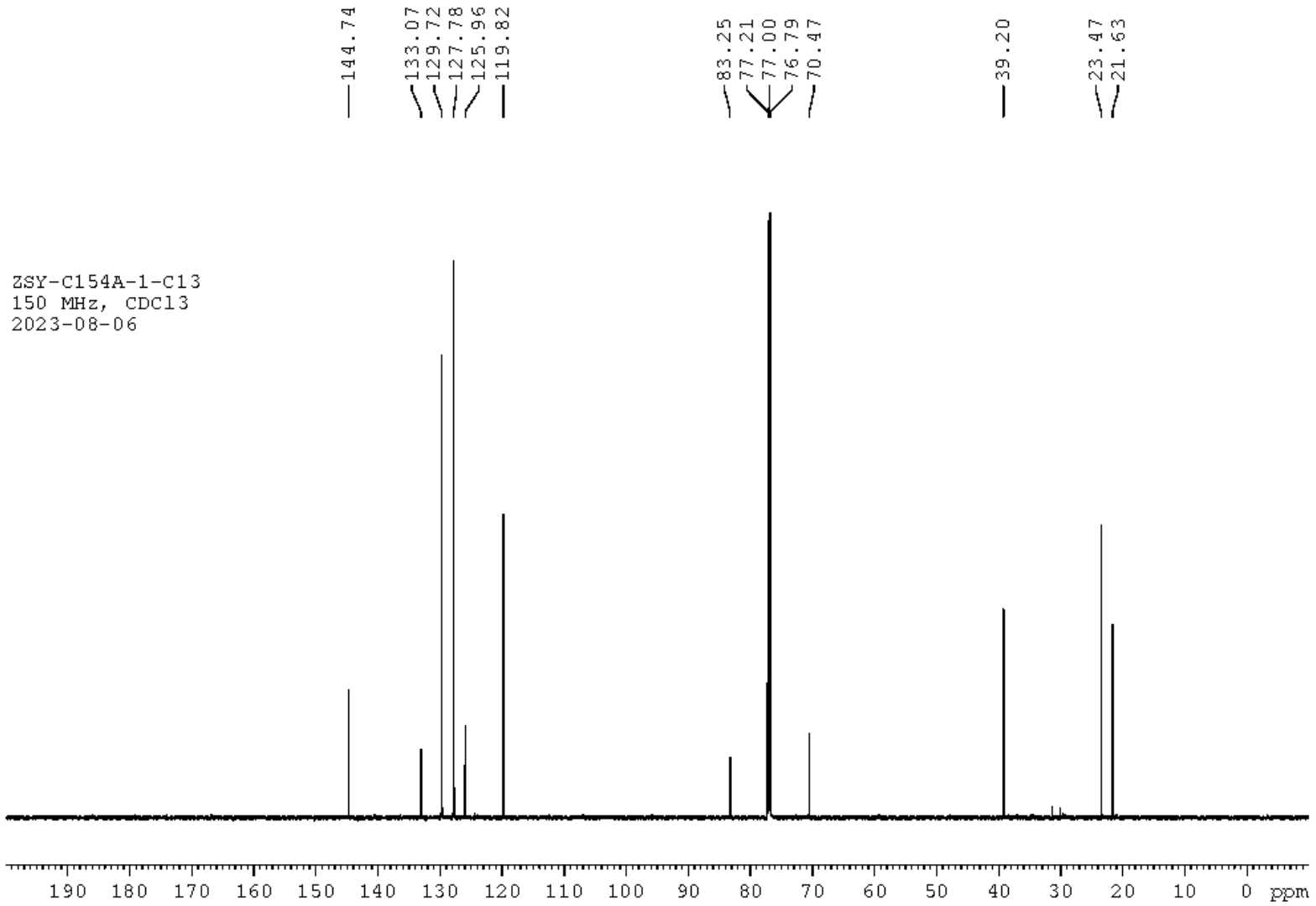

Ts
N
S
3ao
7.826
7.812
7.383
7.370
7.257
7.255
7.248
7.246
7.161
7.159
7.155
7.153
6.961
6.955
6.953
6.947
3.134
2.463
0.000
ZSY-C28-H1
600 MHz, CDCl3
2022-12-06
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
1.04
0.97
0.98
3.04
3.05

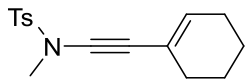

144.87
133.03
132.91
129.78
127.71
126.91
122.55
87.30
77.21
77.00
76.79
62.36
39.22
21.59
ZSY-C28-C13
150 MHz, CDCl3
2022-12-06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ts
N

3ap

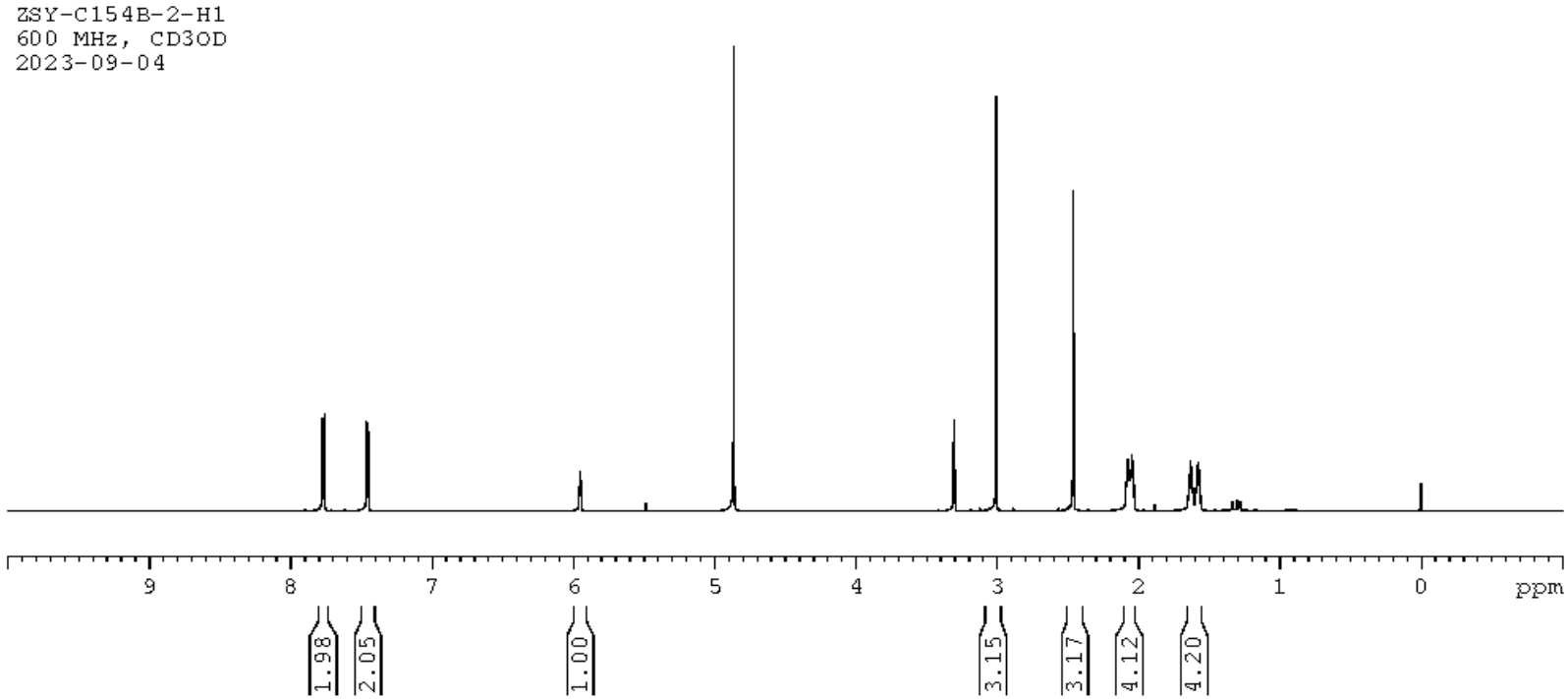

7.728
7.714
7.301
7.288
5.084
5.056
3.006
2.388
1.798
-0.000
ZSY-C154A-1-H1
600 MHz, CDCl3
2023-08-06
9
8
7
6
5
4
3
2
1
0
ppm
1.94
2.00
2.00
3.03
3.08
2.97

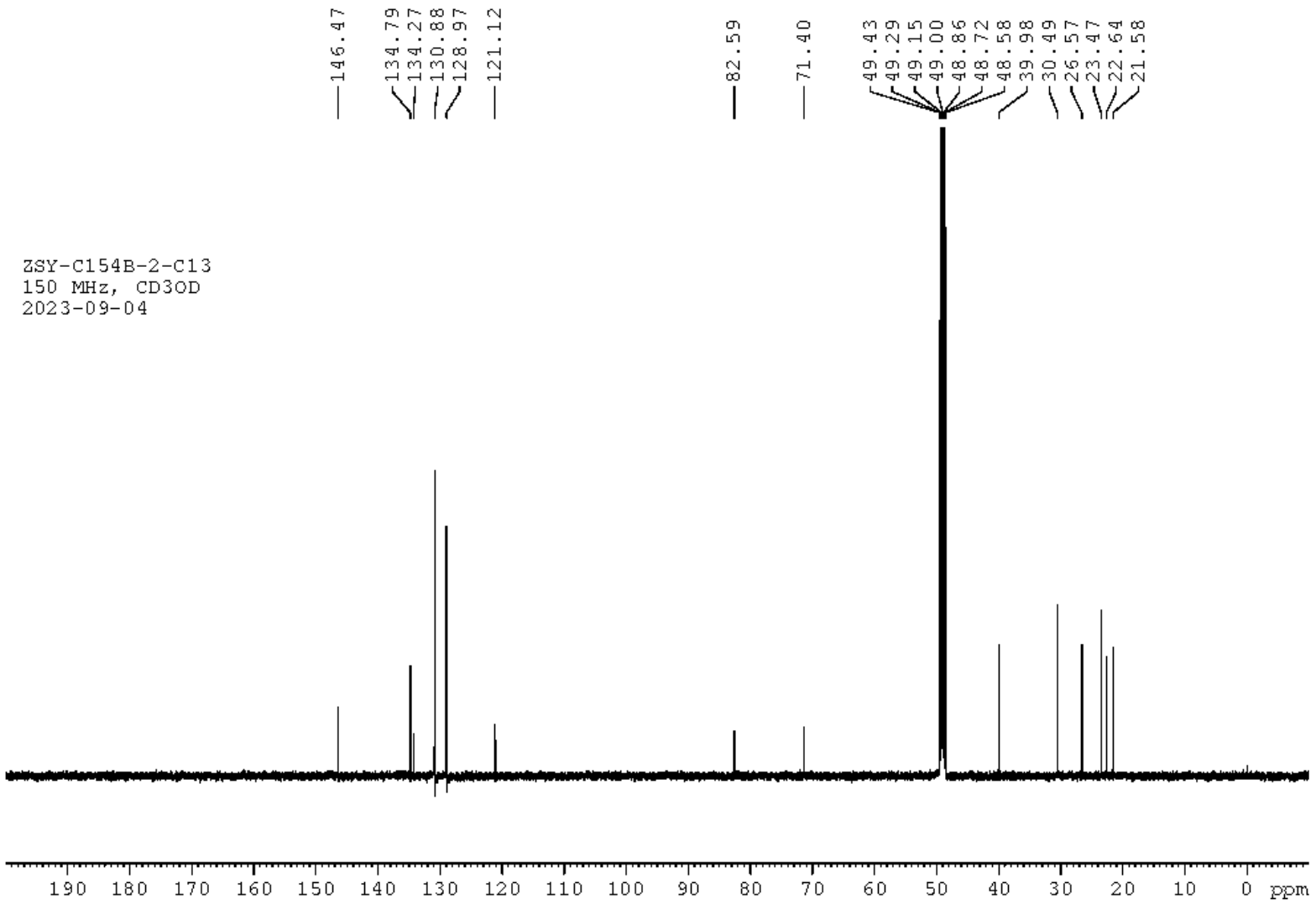

144.74
133.07
129.72
127.78
125.96
119.82
83.25
77.21
77.00
76.79
70.47
39.20
23.47
21.63
ZSY-C154A-1-C13
150 MHz, CDCl3
2023-08-06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

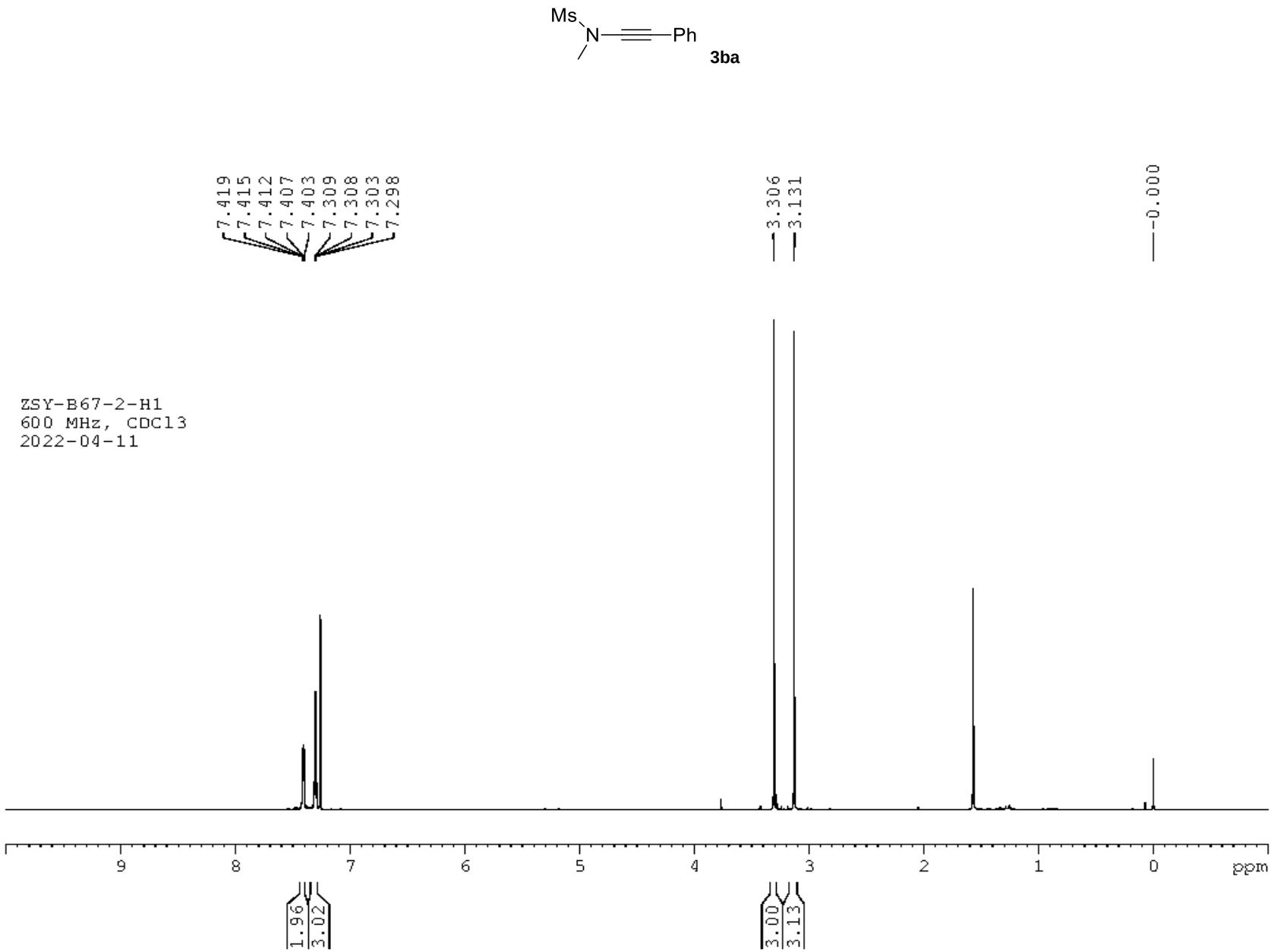

Ts
N

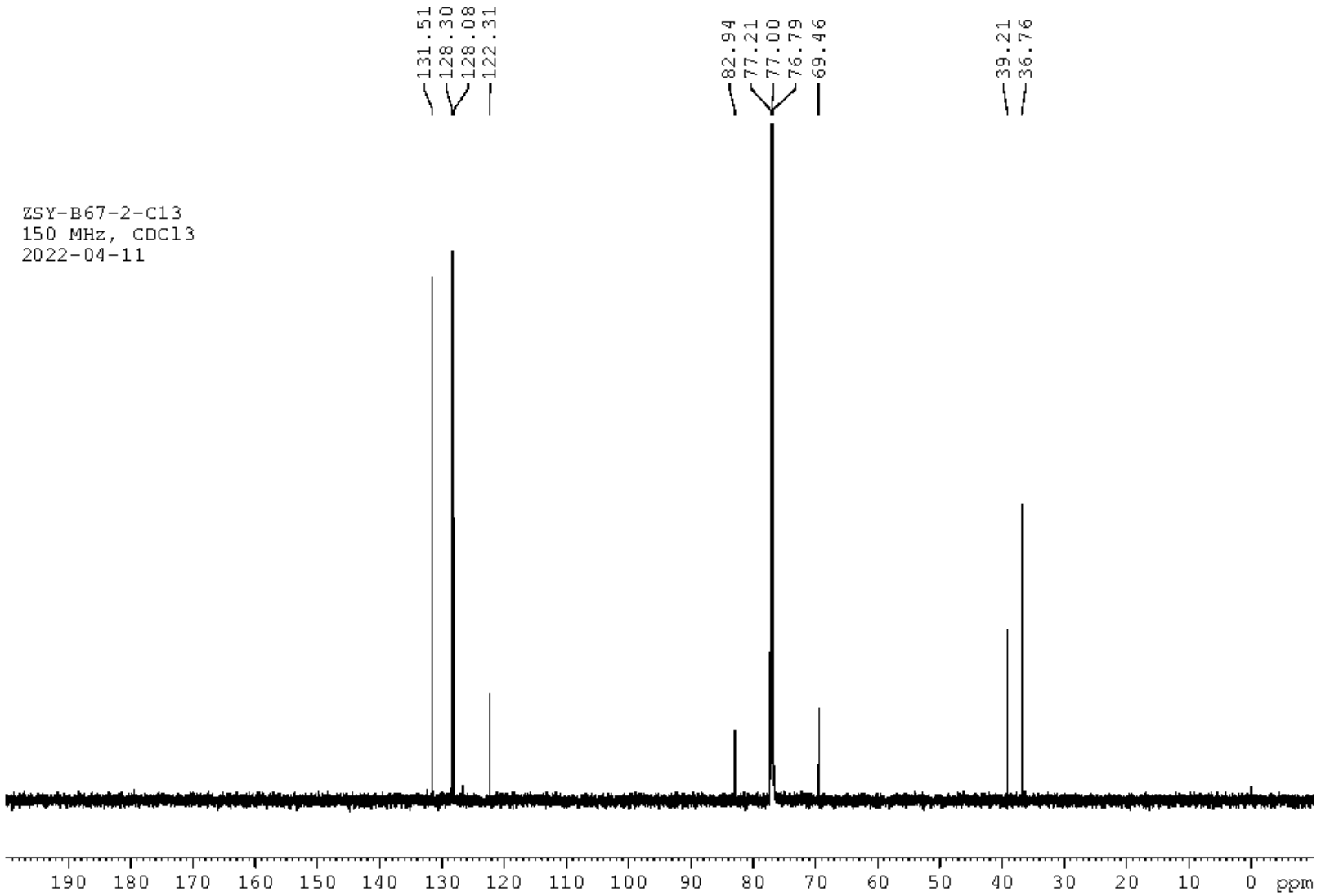
3aq

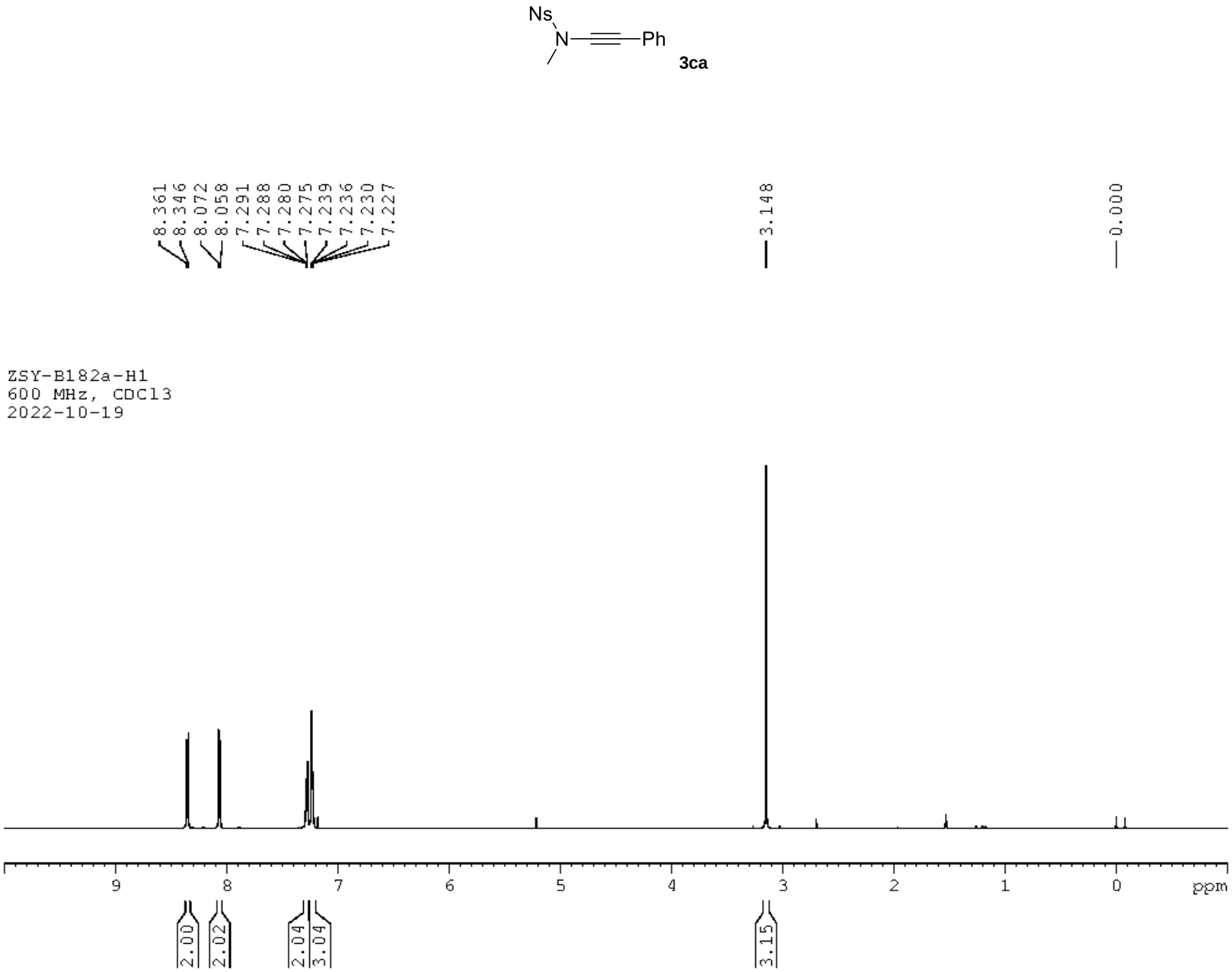

7.775
7.761
7.462
7.449
5.957
5.951
5.944
3.009
2.464
2.090
2.084
2.080
2.074
2.070
2.063
2.058
2.048
2.044
2.034
1.652
1.643
1.634
1.627
1.624
1.617
1.614
1.592
1.586
1.583
1.576
1.567
0.000

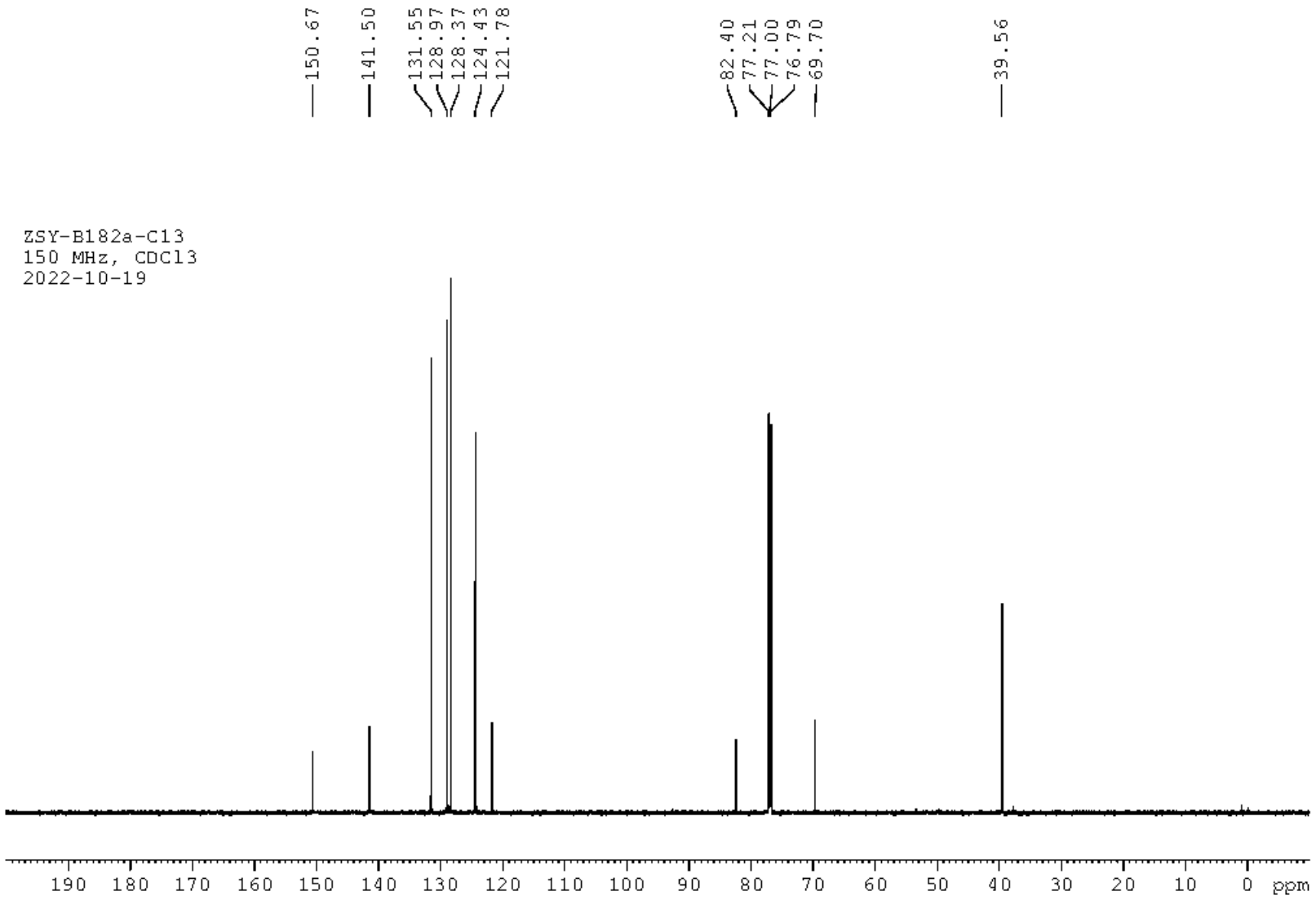

ZSY-C154B-2-H1
600 MHz, CD3OD
2023-09-04
9
8
7
6
5
4
3
2
1
0
ppm
1.98
2.05
1.00
3.15
3.17
4.12
4.20

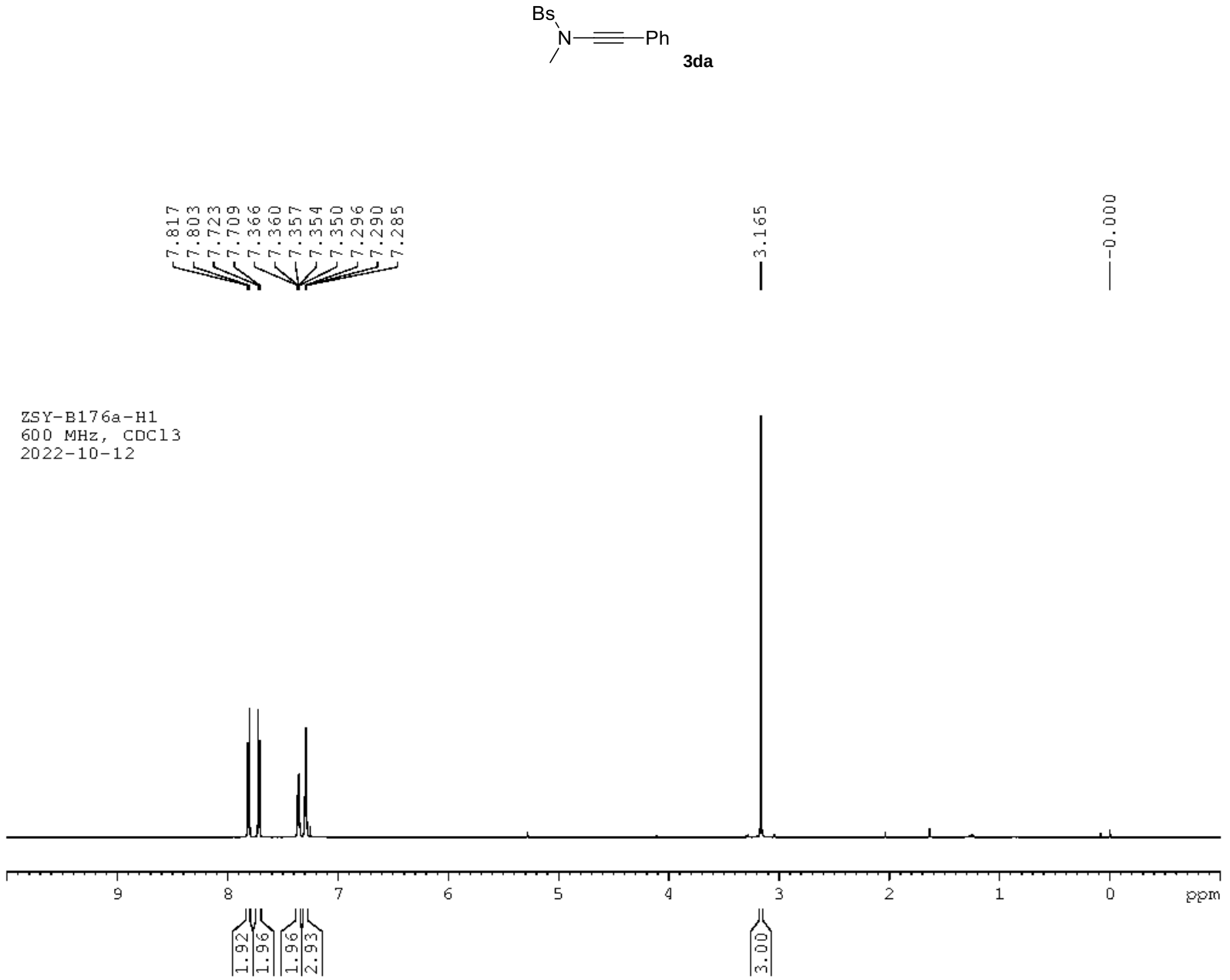

146.47
134.79
134.27
130.88
128.97
121.12
82.59
71.40
49.43
49.29
49.15
49.00
48.86
48.72
48.58
39.98
30.49
26.57
23.47
22.64
21.58
ZSY-C154B-2-C13
150 MHz, CD3OD
2023-09-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

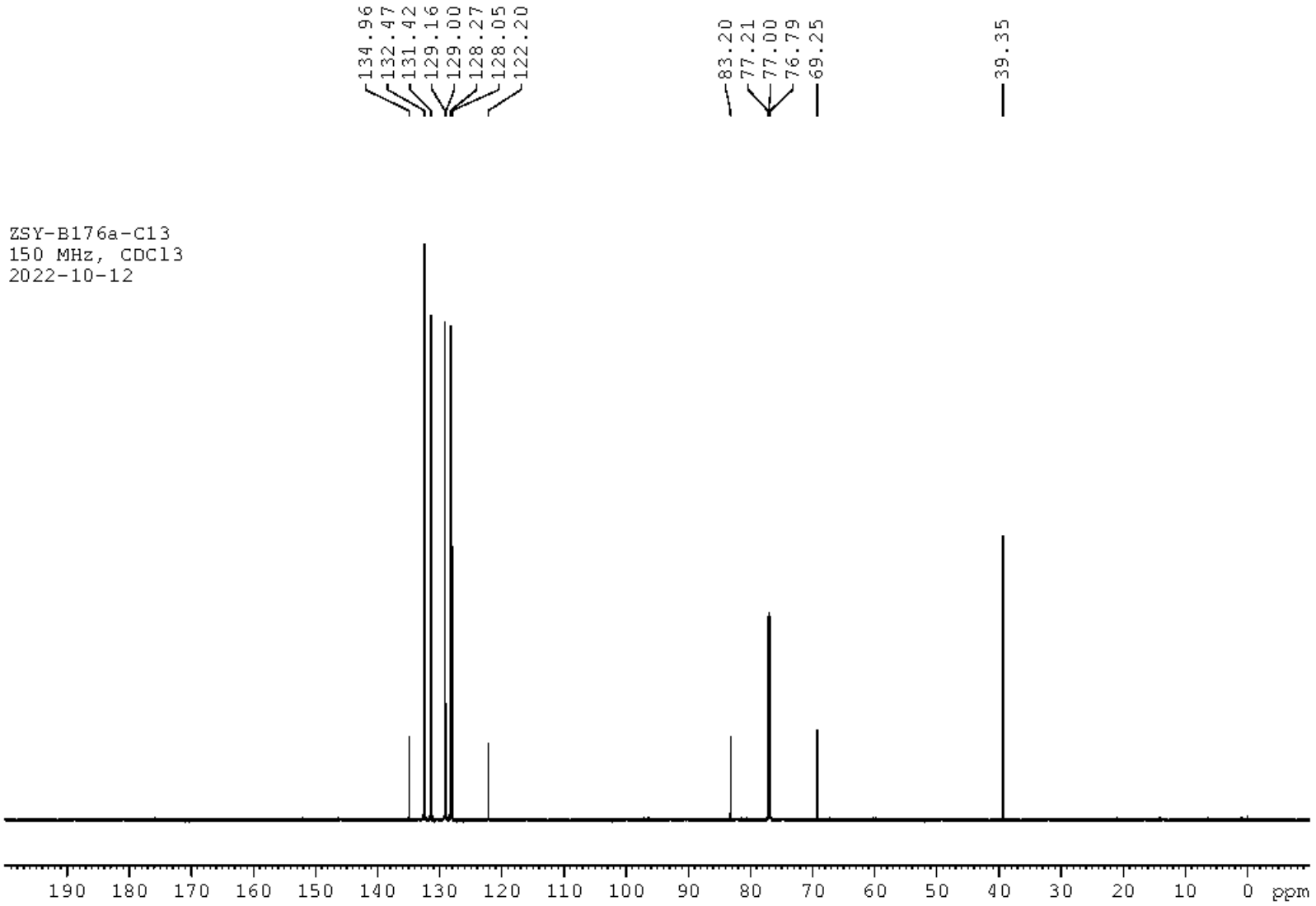

Ms
N
Ph
3ba
7.419
7.415
7.412
7.407
7.403
7.309
7.308
7.303
7.298
3.306
3.131
0.000
ZSY-B67-2-H1
600 MHz, CDCl3
2022-04-11
9
8
7
6
5
4
3
2
1
0
ppm
1.96
3.02
3.00
3.13

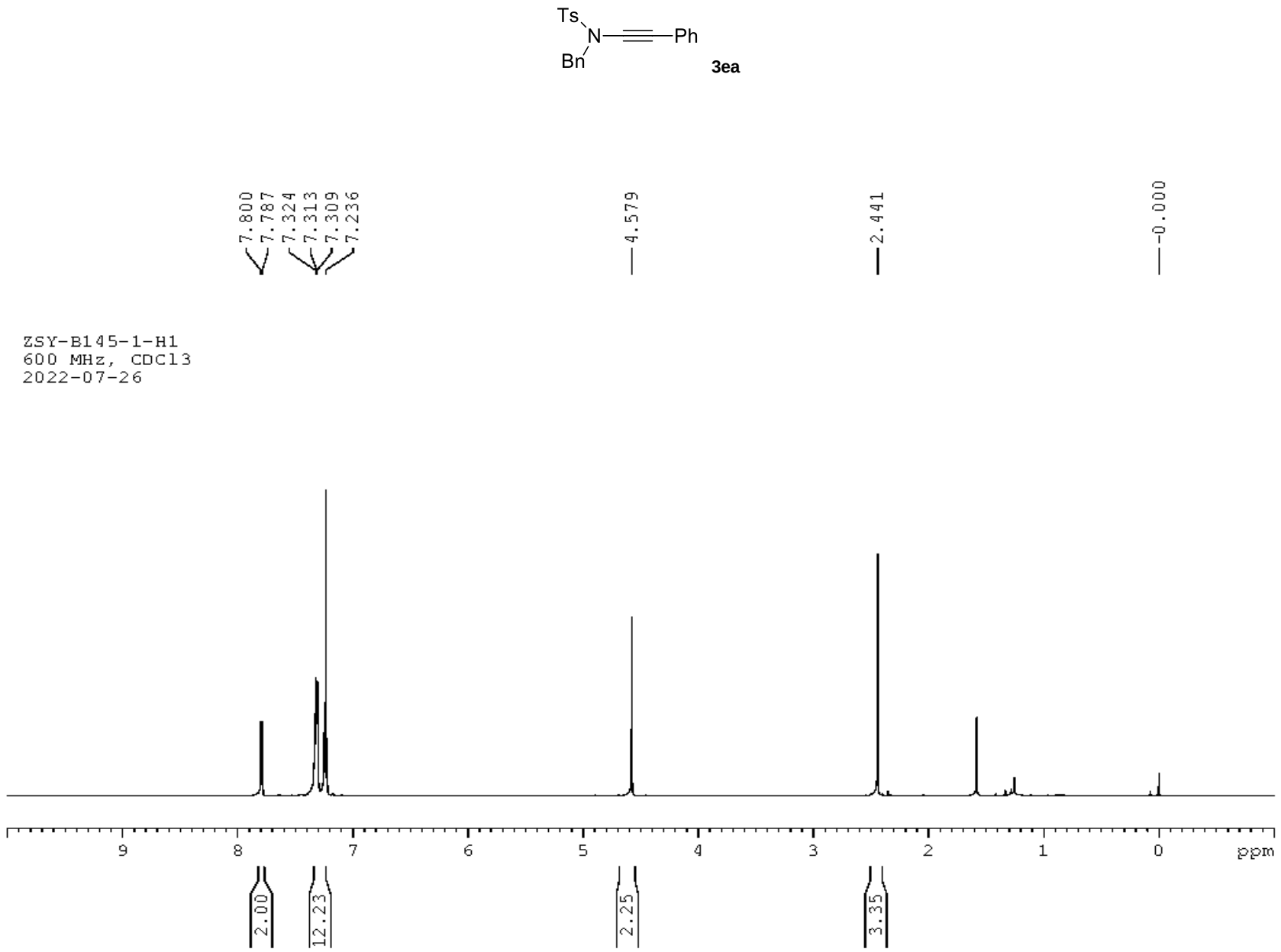

131.51
128.30
128.08
122.31
82.94
77.21
77.00
76.79
69.46
39.21
36.76
ZSY-B67-2-C13
150 MHz, CDCl3
2022-04-11
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

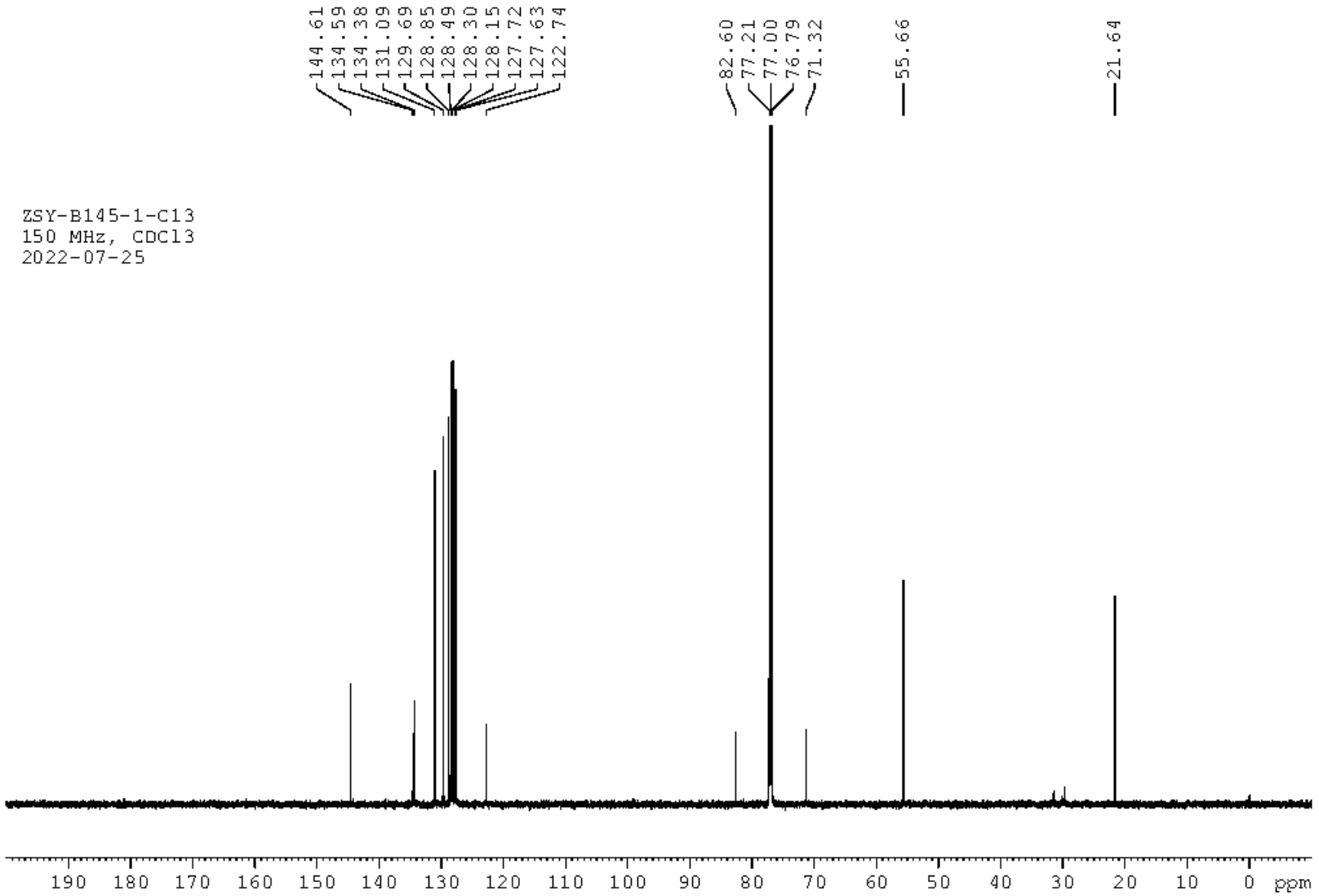

Ns
N
Ph
3ca
8.361
8.346
8.072
8.058
7.291
7.288
7.280
7.275
7.239
7.236
7.230
7.227
3.148
0.000
ZSY-B182a-H1
600 MHz, CDCl3
2022-10-19
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02
2.04
3.04
3.15

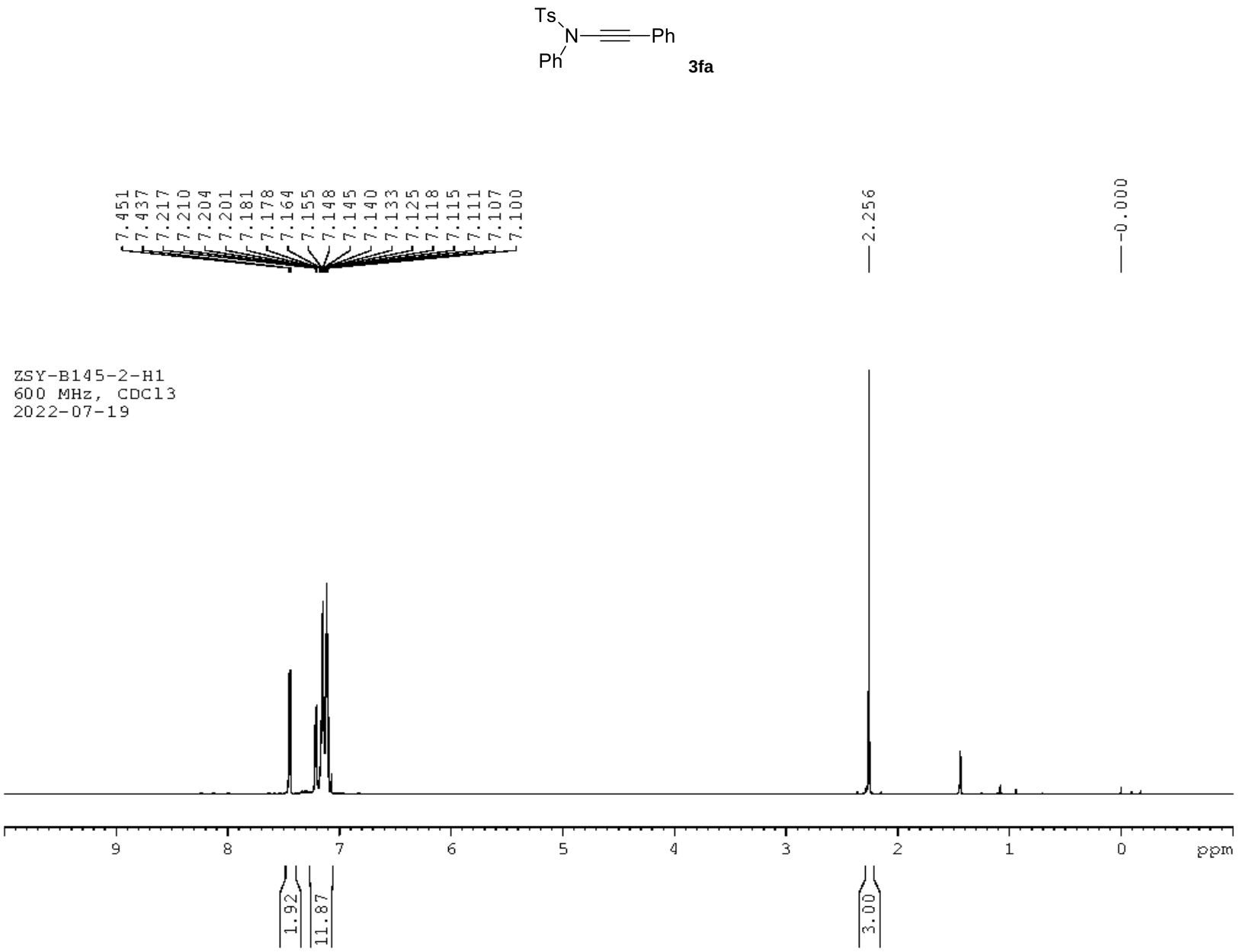

150.67
141.50
131.55
128.97
128.37
124.43
121.78
82.40
77.21
77.00
76.79
69.70
39.56
ZSY-B182a-C13
150 MHz, CDCl3
2022-10-19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

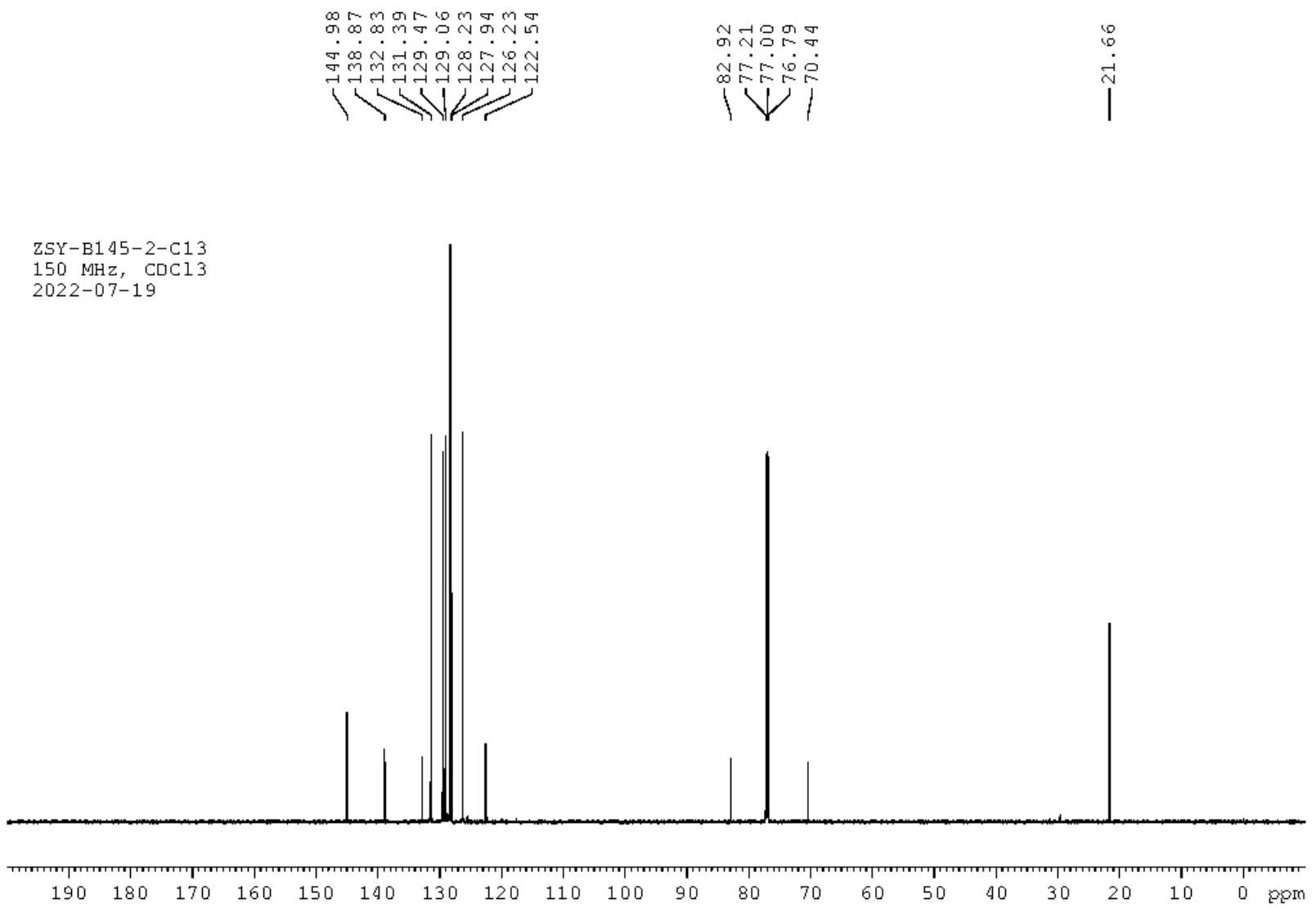

Bs
N
Ph
3da
7.817
7.803
7.723
7.709
7.366
7.360
7.357
7.354
7.350
7.296
7.290
7.285
3.165
0.000
ZSY-B176a-H1
600 MHz, CDCl3
2022-10-12
9
8
7
6
5
4
3
2
1
0
ppm
1.92
1.96
1.96
2.93
3.00

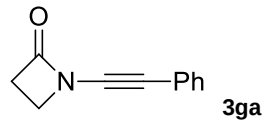

134.96
132.47
131.42
129.16
129.00
128.27
128.05
122.20
83.20
77.21
77.00
76.79
69.25
39.35
ZSY-B176a-C13
150 MHz, CDCl3
2022-10-12
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ts
N
Ph
Bn
3ea
7.800
7.787
7.324
7.313
7.309
7.236
4.579
2.441
-0.000
ZSY-B145-1-H1
600 MHz, CDCl3
2022-07-26
9
8
7
6
5
4
3
2
1
0
ppm
2.00
12.23
2.25
3.35

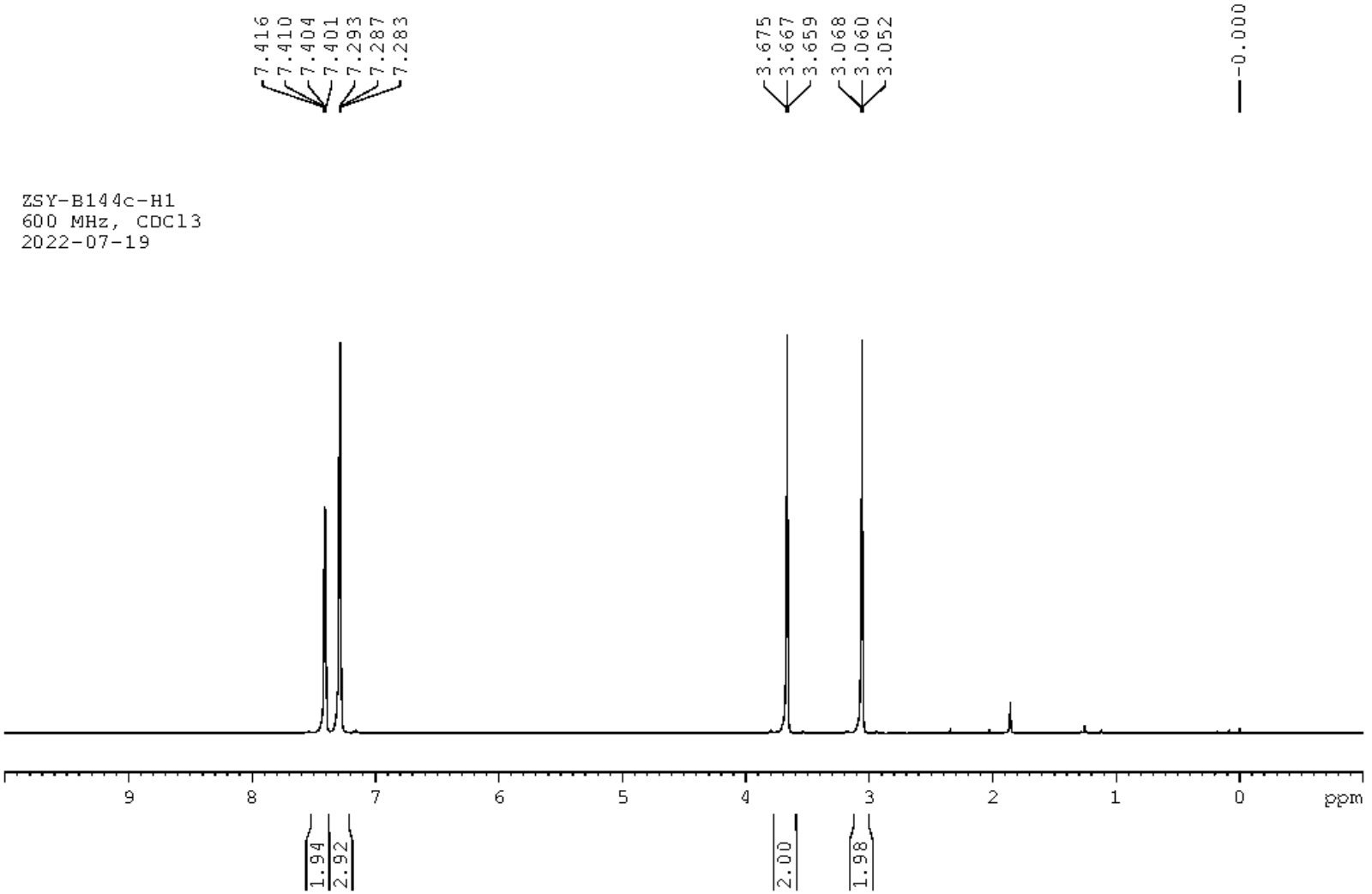

144.61
134.59
134.38
131.09
129.69
128.85
128.49
128.30
128.15
127.72
127.63
122.74
82.60
77.21
77.00
76.79
71.32
55.66
21.64
ZSY-B145-1-C13
150 MHz, CDCl3
2022-07-25
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

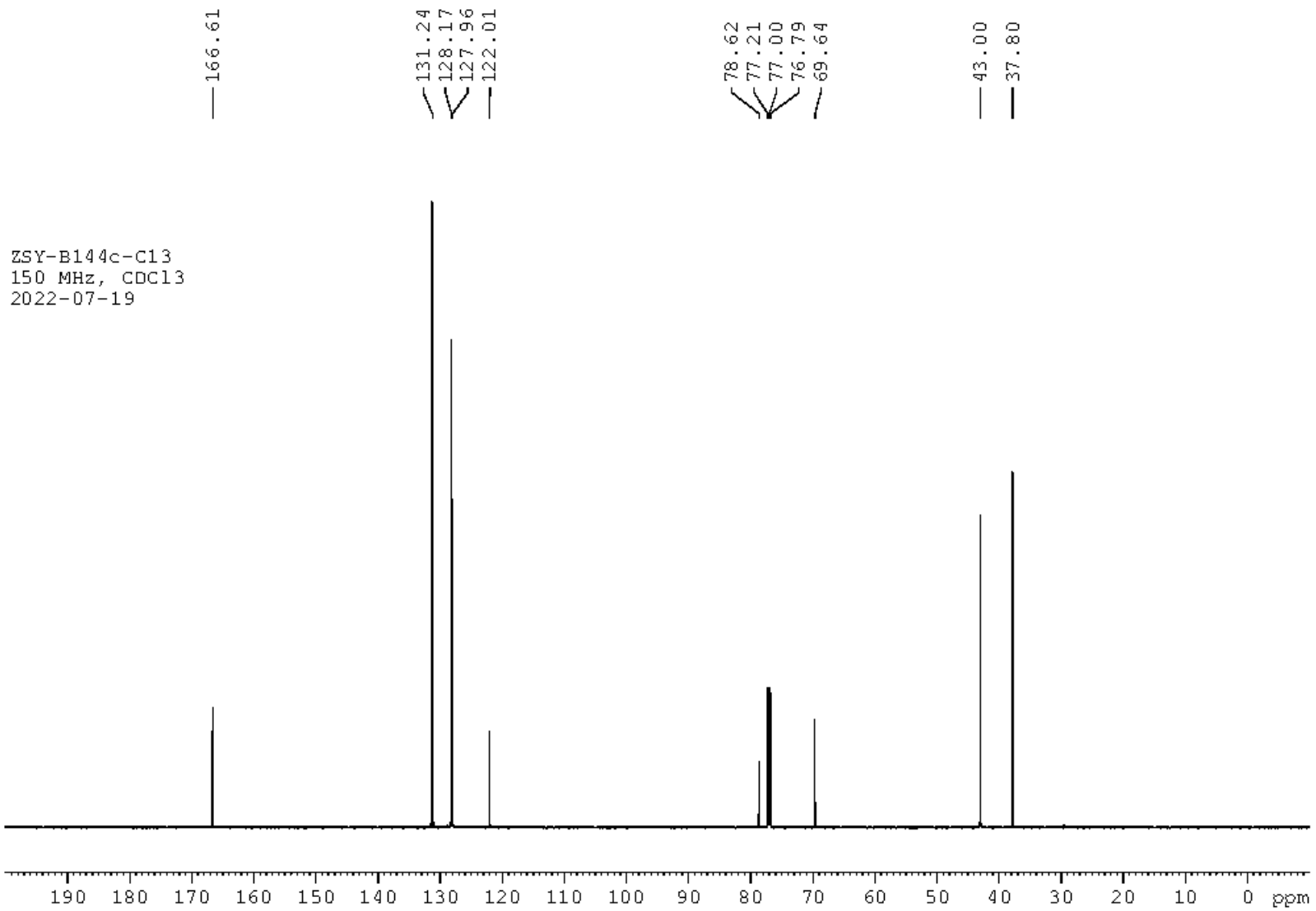

Ts
N
Ph
Ph
3fa
7.451
7.437
7.217
7.210
7.204
7.201
7.181
7.178
7.164
7.155
7.148
7.145
7.140
7.133
7.125
7.118
7.115
7.111
7.107
7.100
2.256
0.000
ZSY-B145-2-H1
600 MHz, CDCl3
2022-07-19
9
8
7
6
5
4
3
2
1
0
ppm
1.92
11.87
3.00

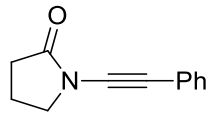

144.98
138.87
132.83
131.39
129.47
129.06
128.23
127.94
126.23
122.54
82.92
77.21
77.00
76.79
70.44
21.66
ZSY-B145-2-C13
150 MHz, CDCl3
2022-07-19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
Ph

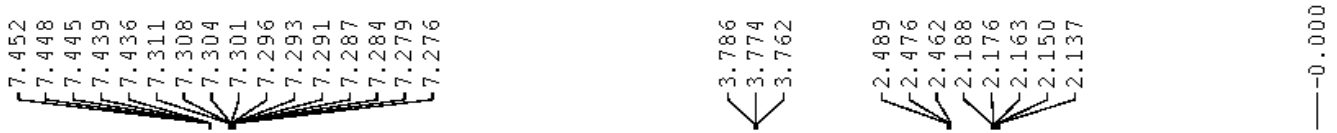
3ga

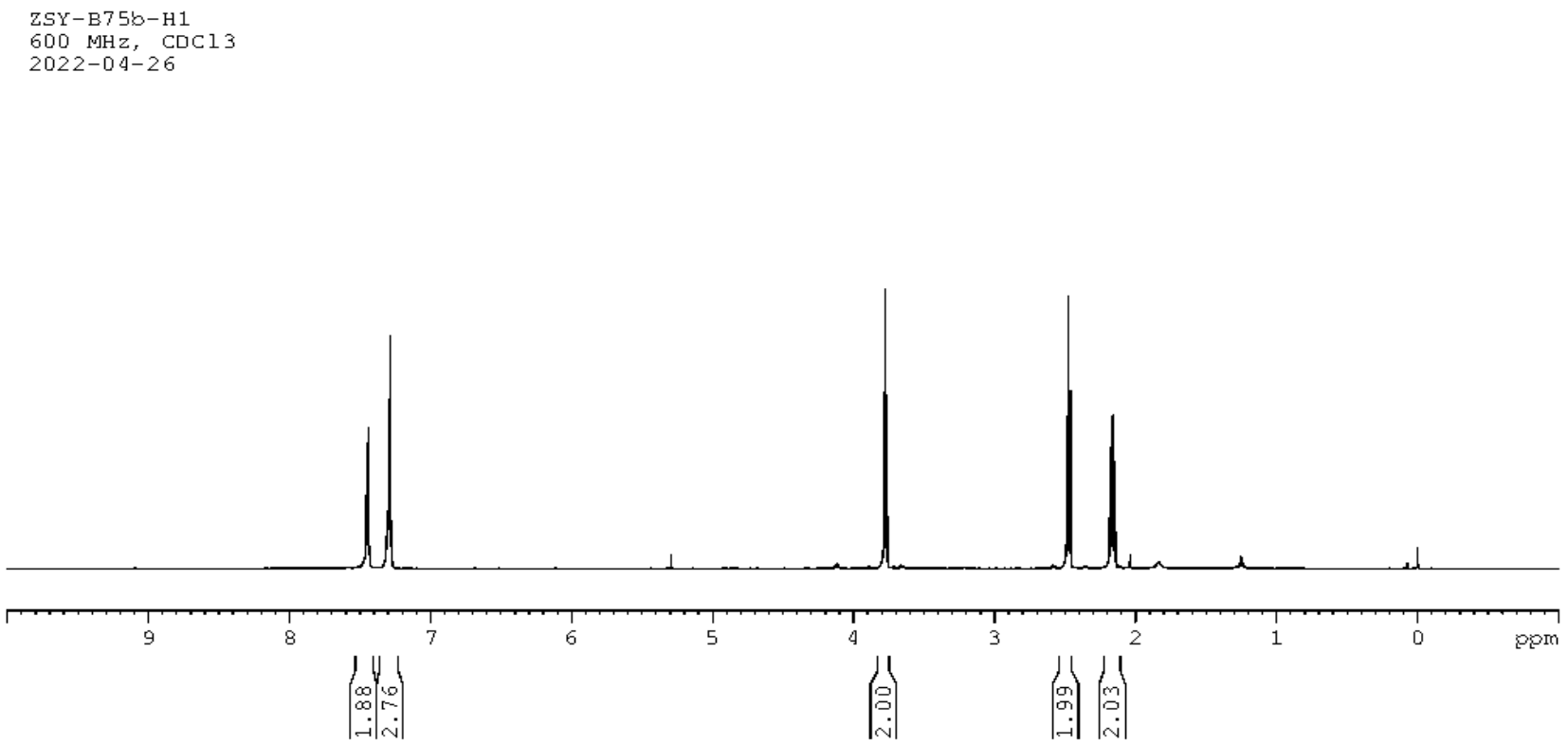

7.416
7.410
7.404
7.401
7.293
7.287
7.283
3.675
3.667
3.659
3.068
3.060
3.052
0.000
ZSY-B144c-H1
600 MHz, CDCl3
2022-07-19
9
8
7
6
5
4
3
2
1
0
ppm
1.94
2.92
2.00
1.98

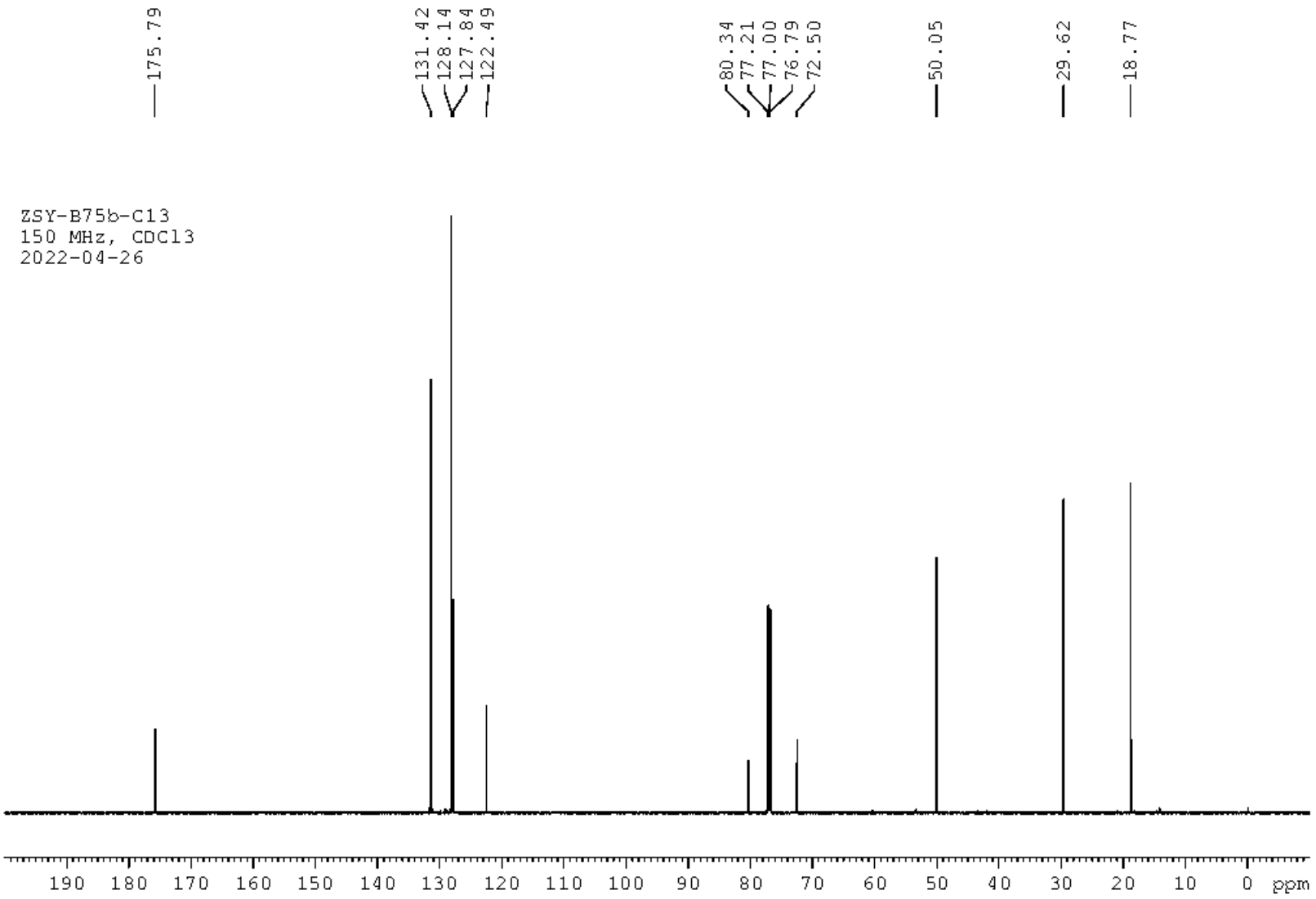

166.61
131.24
128.17
127.96
122.01
78.62
77.21
77.00
76.79
69.64
43.00
37.80
ZSY-B144c-C13
150 MHz, CDCl3
2022-07-19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

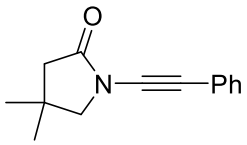

O
N
Ph

3ha

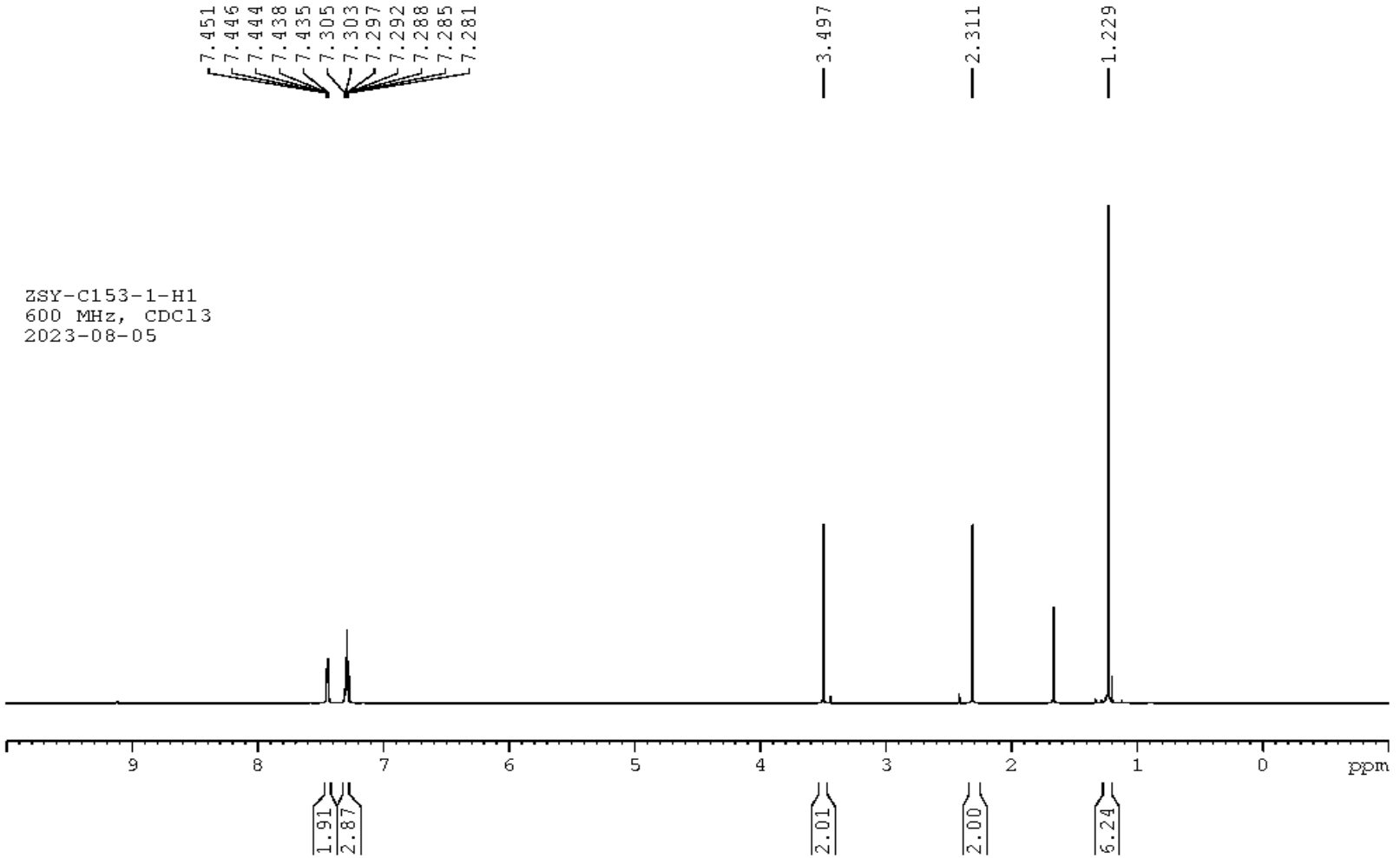

7.452
7.448
7.445
7.439
7.436
7.311
7.308
7.304
7.301
7.296
7.293
7.291
7.287
7.284
7.279
7.276
3.786
3.774
3.762
2.489
2.476
2.462
2.188
2.176
2.163
2.150
2.137
0.000

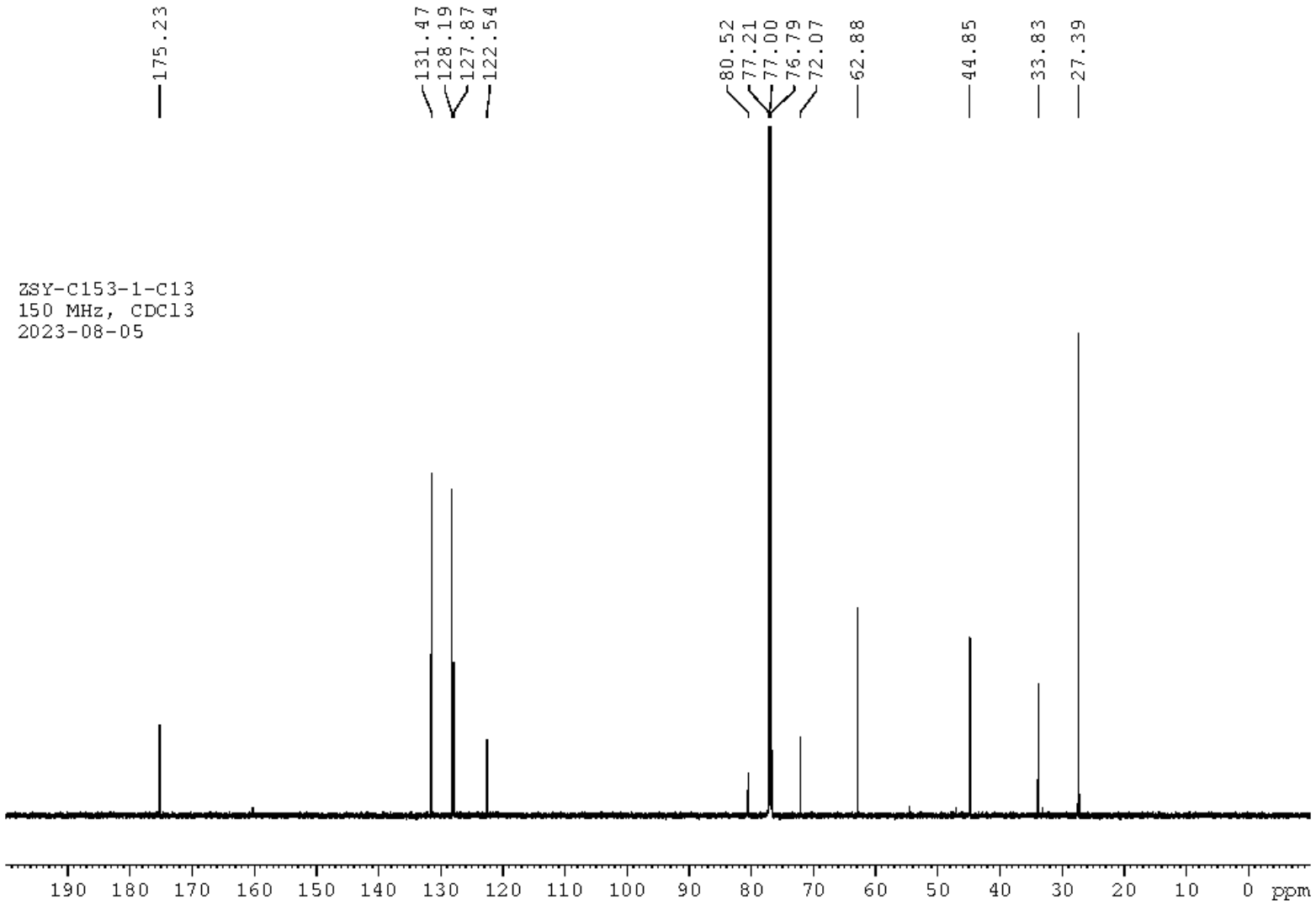

ZSY-B75b-H1
600 MHz, CDCl3
2022-04-26
9
8
7
6
5
4
3
2
1
0
ppm
1.88
2.76
2.00
1.99
2.03

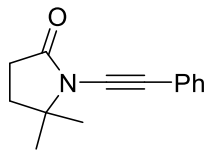

175.79
131.42
128.14
127.84
122.49
80.34
77.21
77.00
76.79
72.50
50.05
29.62
18.77
ZSY-B75b-C13
150 MHz, CDCl3
2022-04-26
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
Ph

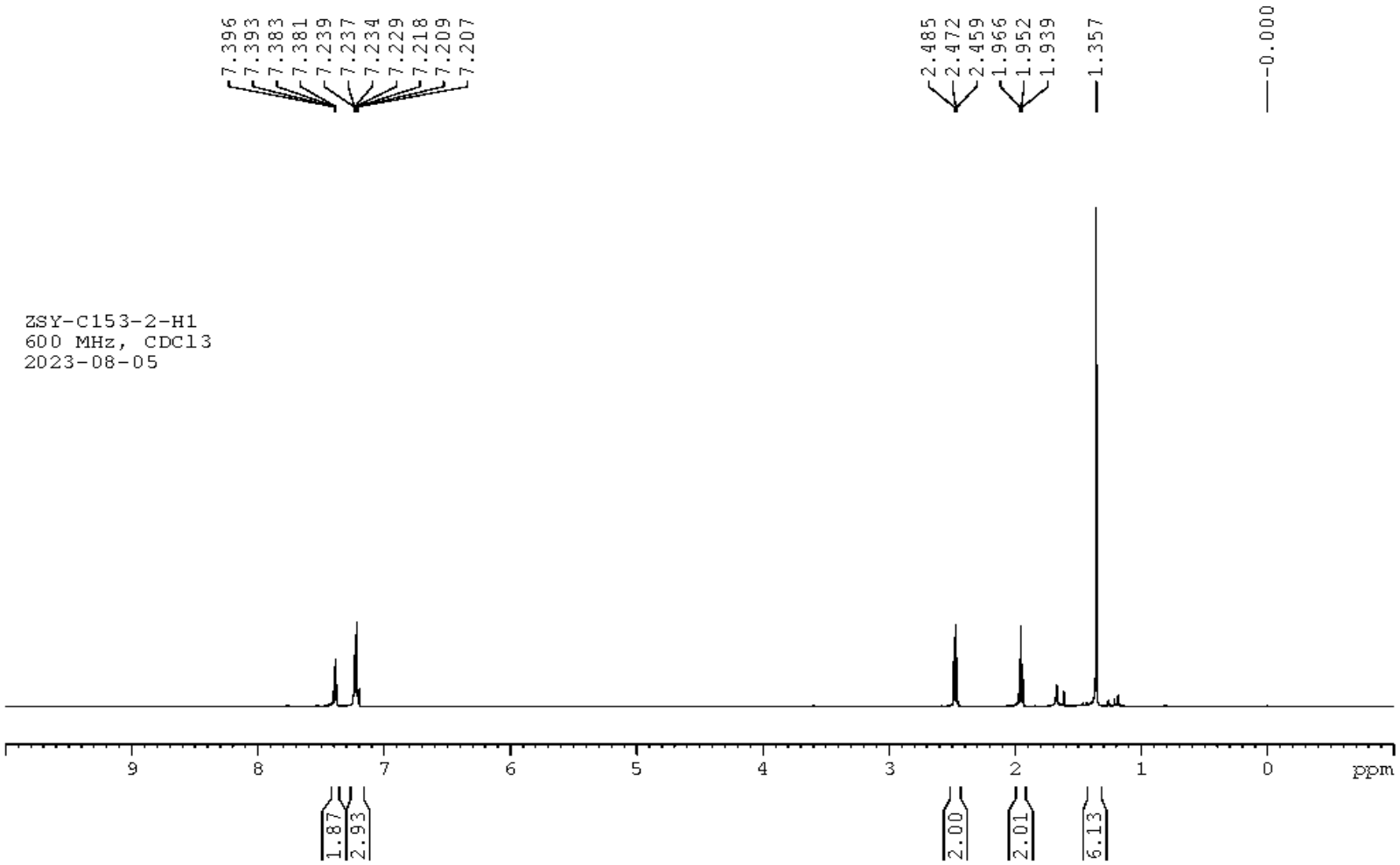
3ia

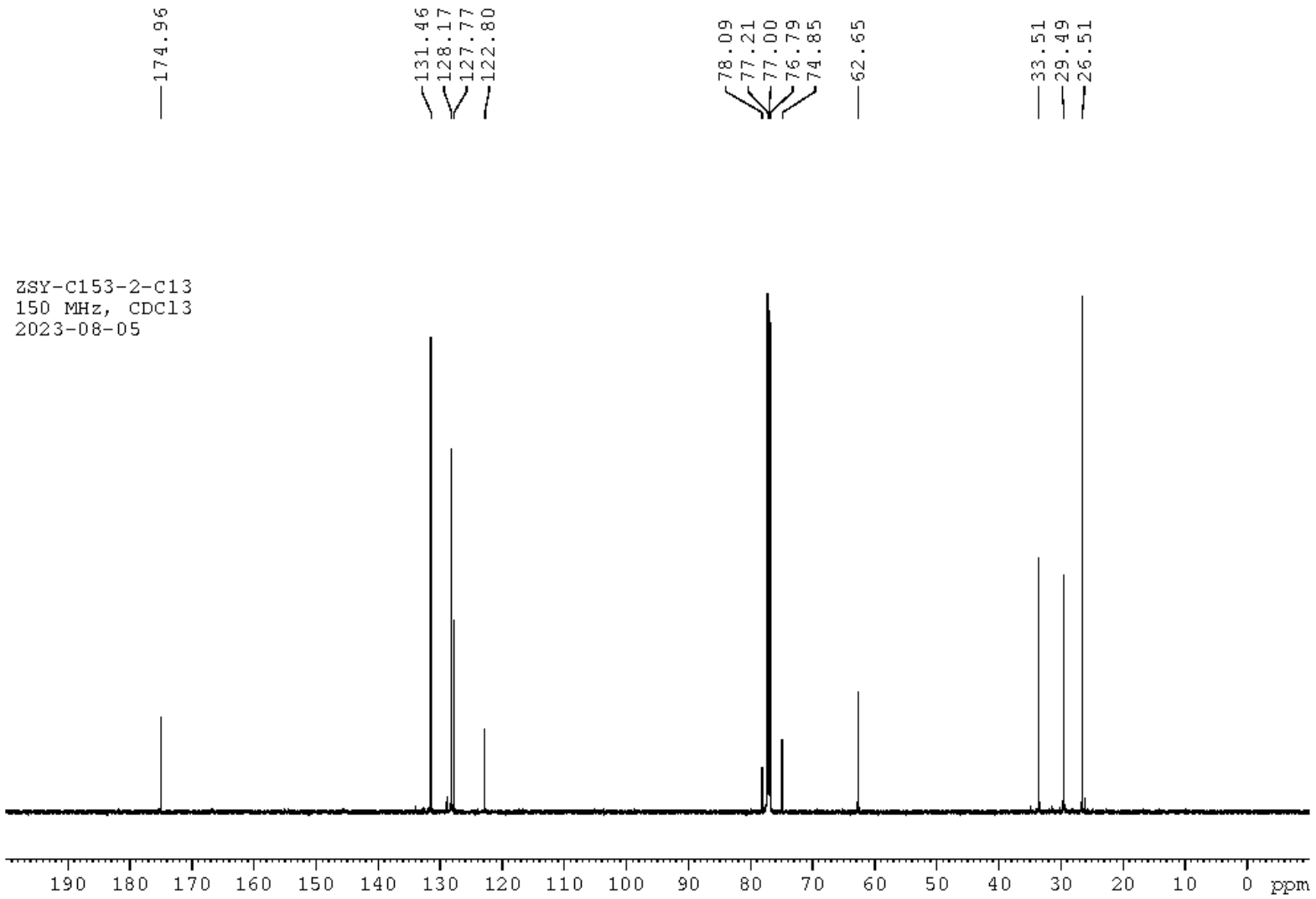

7.451
7.446
7.444
7.438
7.435
7.305
7.303
7.297
7.292
7.288
7.285
7.281
3.497
2.311
1.229
ZSY-C153-1-H1
600 MHz, CDCl3
2023-08-05
9
8
7
6
5
4
3
2
1
0
ppm
1.91
2.87
2.01
2.00
6.24

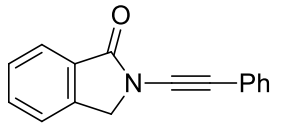

175.23
131.47
128.19
127.87
122.54
80.52
77.21
77.00
76.79
72.07
62.88
44.85
33.83
27.39
ZSY-C153-1-C13
150 MHz, CDCl3
2023-08-05
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
Ph

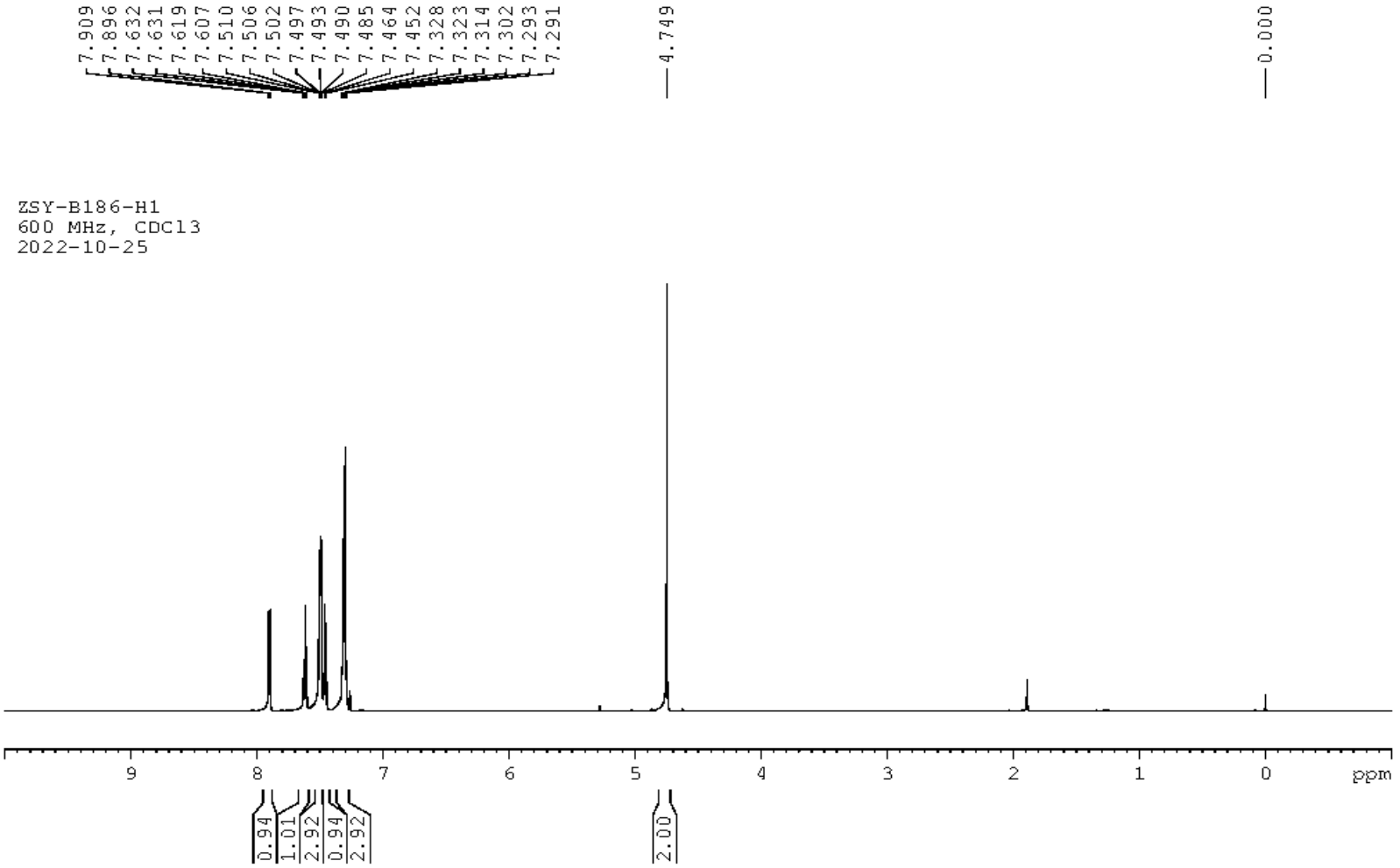
3ja

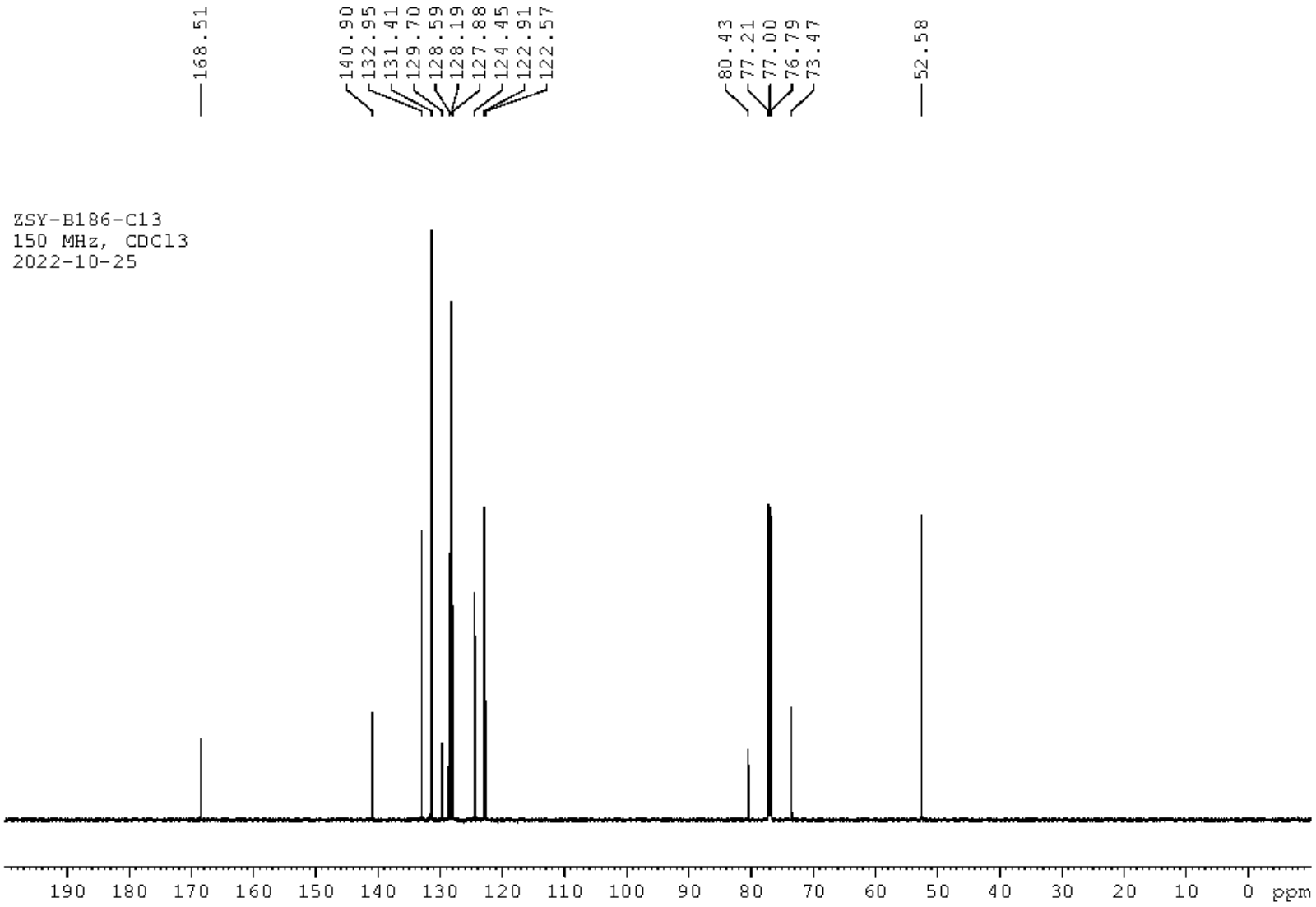

7.396
7.393
7.383
7.381
7.239
7.237
7.234
7.229
7.218
7.209
7.207
2.485
2.472
2.459
1.966
1.952
1.939
1.357
0.000
ZSY-C153-2-H1
600 MHz, CDCl3
2023-08-05
9
8
7
6
5
4
3
2
1
0
ppm
1.87
2.93
2.00
2.01
6.13

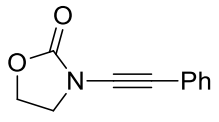

174.96
131.46
128.17
127.77
122.80
78.09
77.21
77.00
76.79
74.85
62.65
33.51
29.49
26.51
ZSY-C153-2-C13
150 MHz, CDCl3
2023-08-05
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
Ph

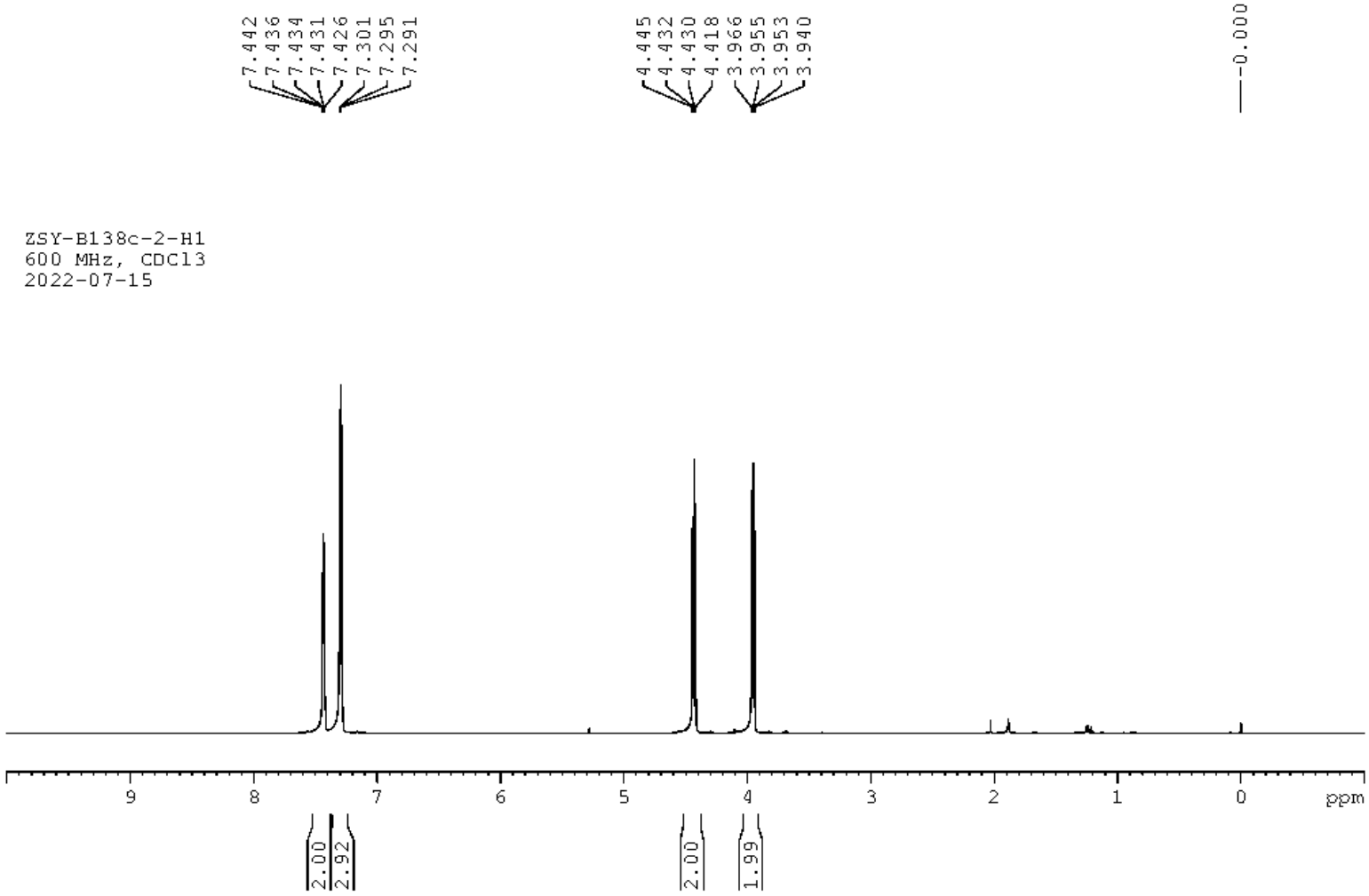
3ka

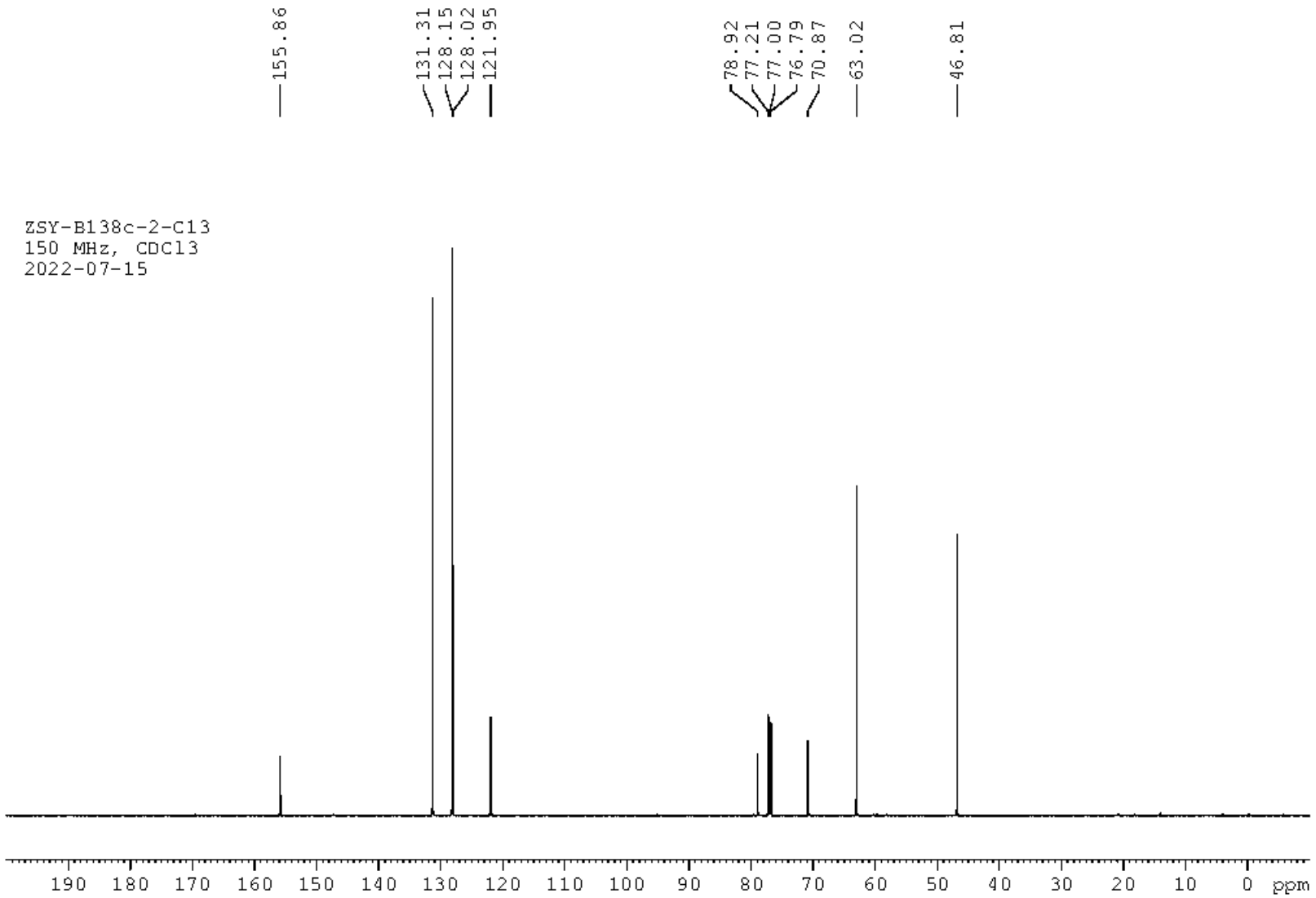

7.909
7.896
7.632
7.631
7.619
7.607
7.510
7.506
7.502
7.497
7.493
7.490
7.485
7.464
7.452
7.328
7.323
7.314
7.302
7.293
7.291
4.749
0.000
ZSY-B186-H1
600 MHz, CDCl3
2022-10-25
9
8
7
6
5
4
3
2
1
0
ppm
0.94
1.01
2.92
0.94
2.92
2.00

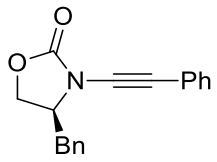

168.51
140.90
132.95
131.41
129.70
128.59
128.19
127.88
124.45
122.91
122.57
80.43
77.21
77.00
76.79
73.47
52.58
ZSY-B186-C13
150 MHz, CDCl3
2022-10-25
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
Ph

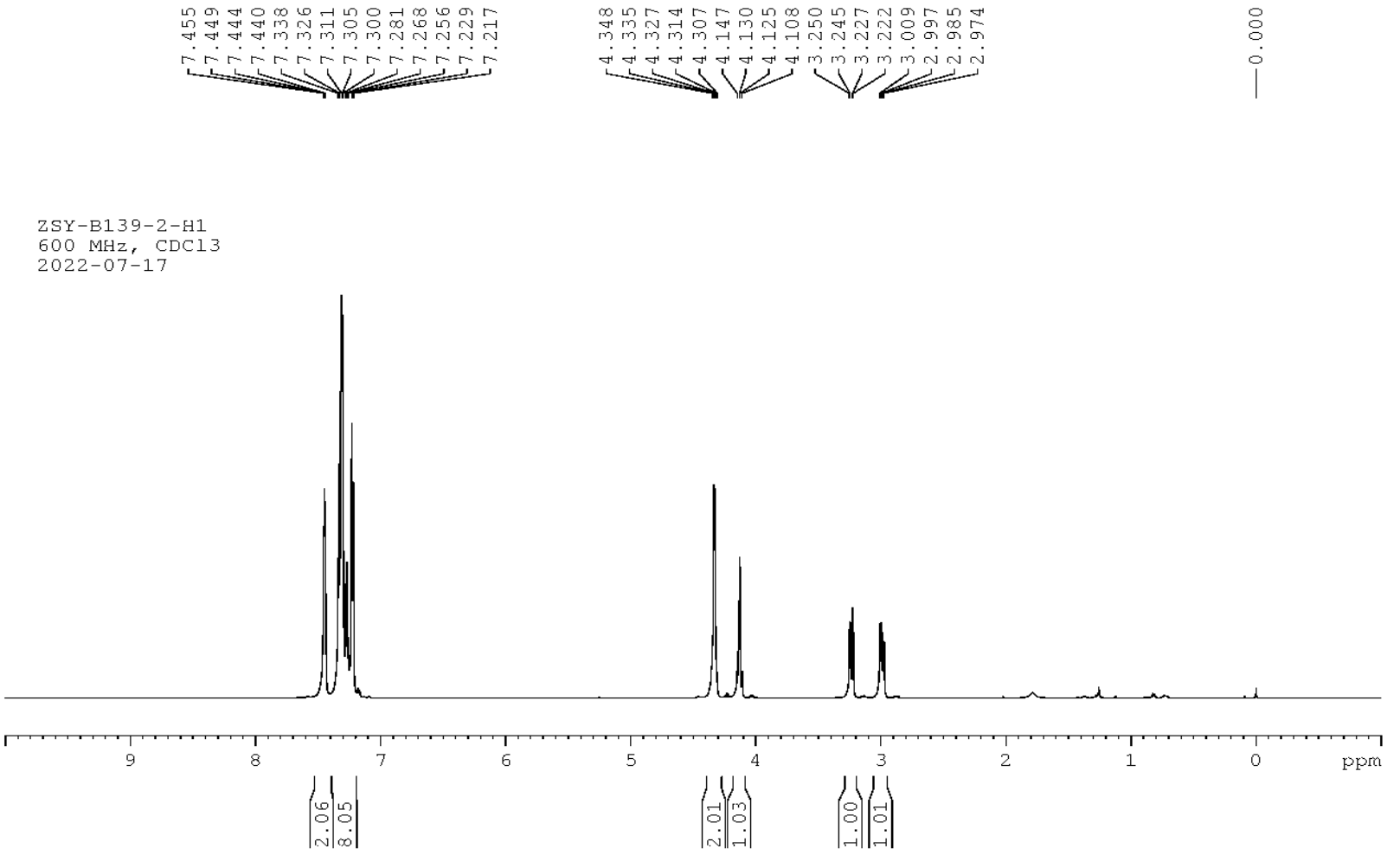
3la

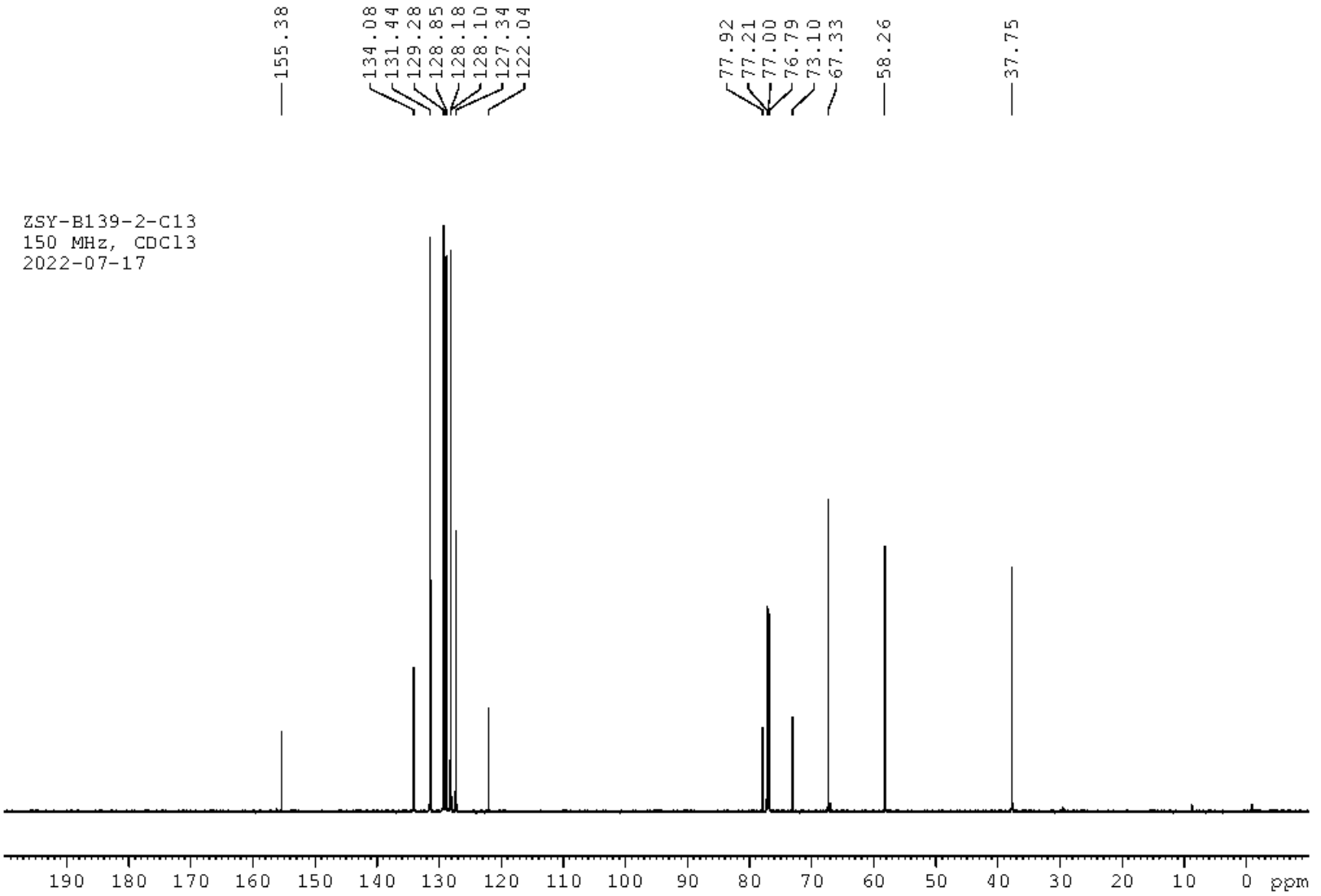

7.442
7.436
7.434
7.431
7.426
7.301
7.295
7.291
4.445
4.432
4.430
4.418
3.966
3.955
3.953
3.940
0.000
ZSY-B138c-2-H1
600 MHz, CDCl3
2022-07-15
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.92
2.00
1.99

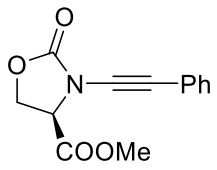

155.86
131.31
128.15
128.02
121.95
78.92
77.21
77.00
76.79
70.87
63.02
46.81
ZSY-B138c-2-C13
150 MHz, CDCl3
2022-07-15
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
Ph
Bn

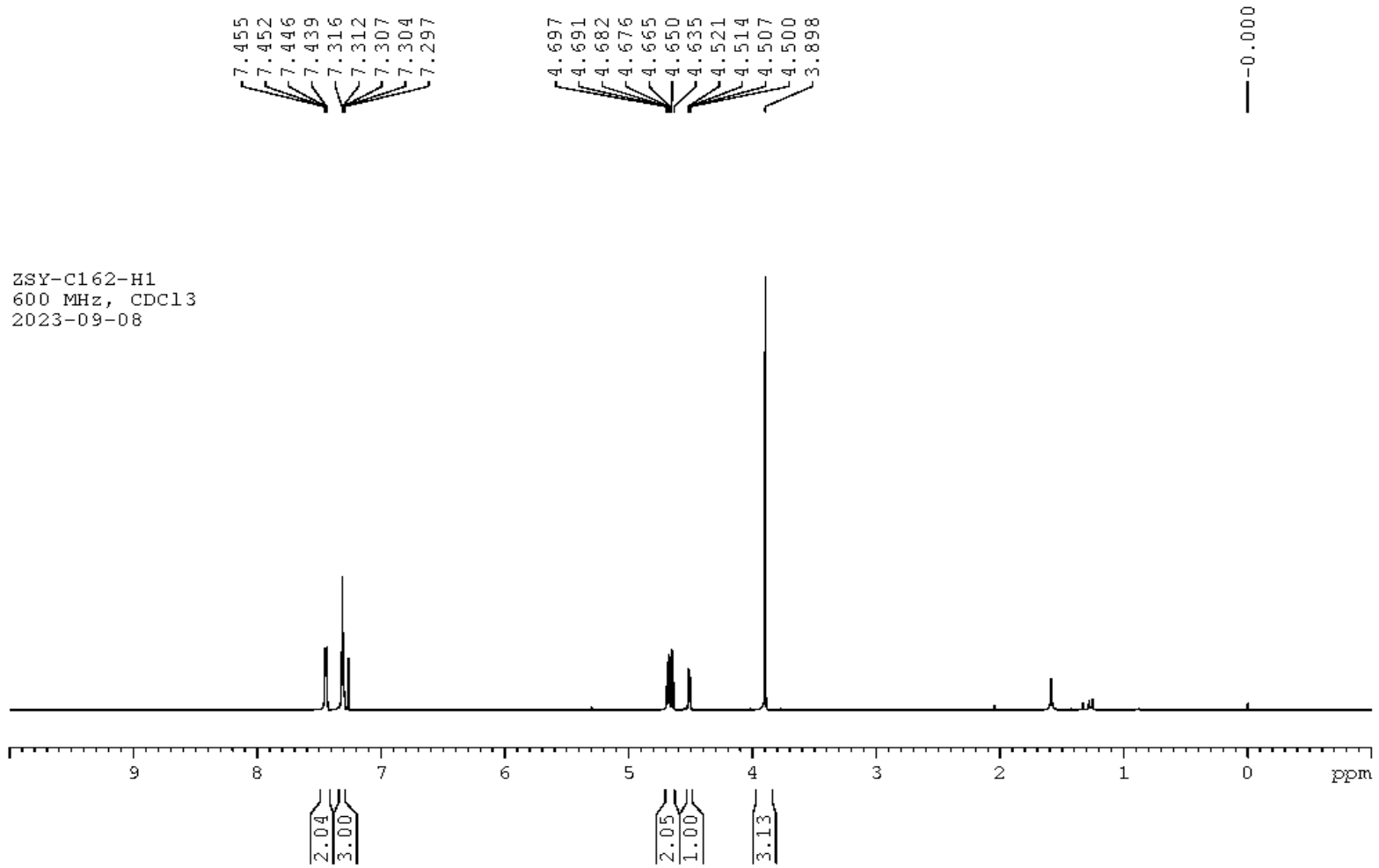
3ma

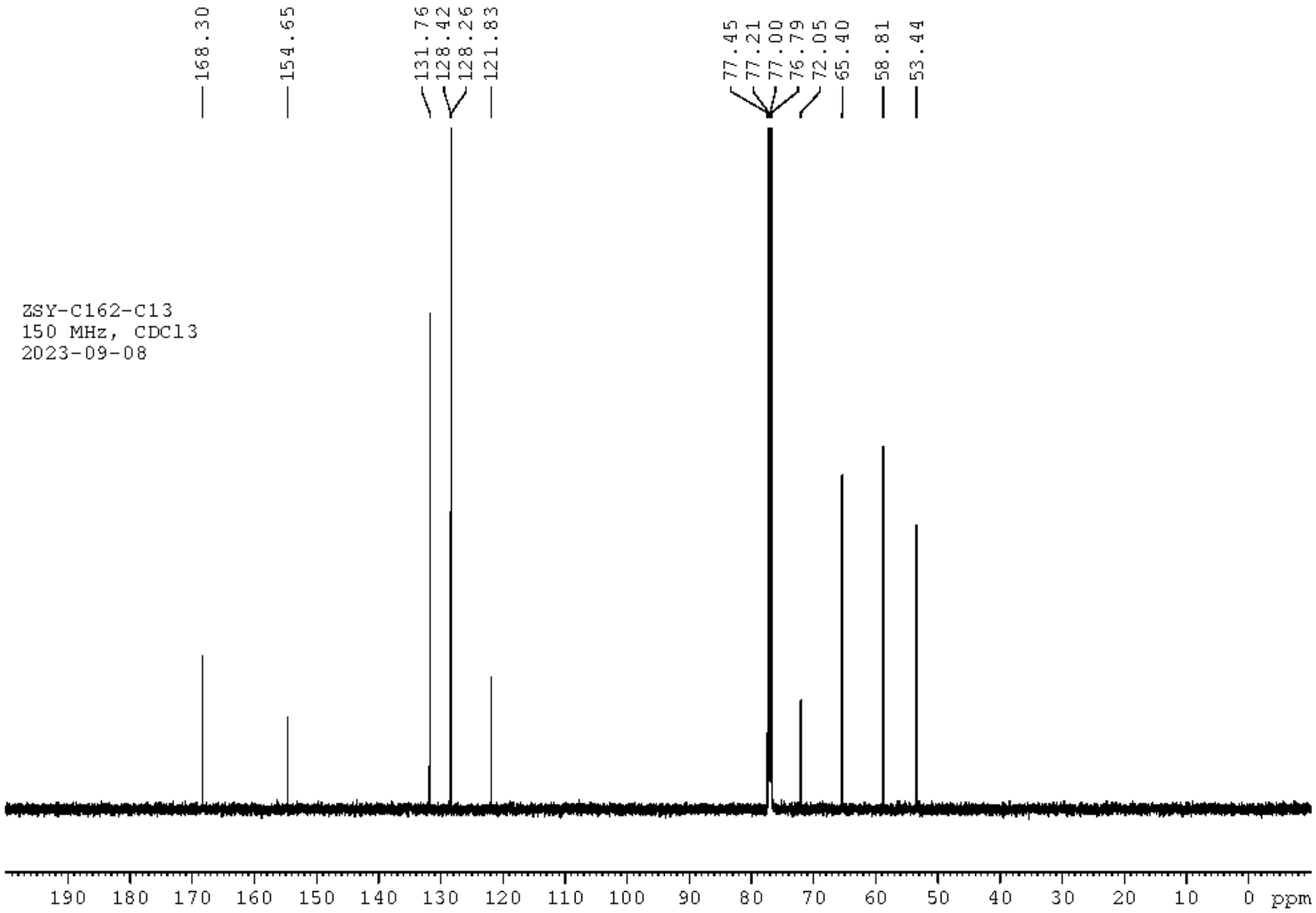

7.455
7.449
7.444
7.440
7.338
7.326
7.311
7.305
7.300
7.281
7.268
7.256
7.229
7.217
4.348
4.335
4.327
4.314
4.307
4.147
4.130
4.125
4.108
3.250
3.245
3.227
3.222
3.009
2.997
2.985
2.974
0.000
ZSY-B139-2-H1
600 MHz, CDCl3
2022-07-17
9
8
7
6
5
4
3
2
1
0
ppm
2.06
8.05
2.01
1.03
1.00
1.01

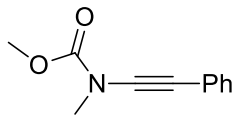

155.38
134.08
131.44
129.28
128.85
128.18
128.10
127.34
122.04
77.92
77.21
77.00
76.79
73.10
67.33
58.26
37.75
ZSY-B139-2-C13
150 MHz, CDCl3
2022-07-17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
Ph
COOMe

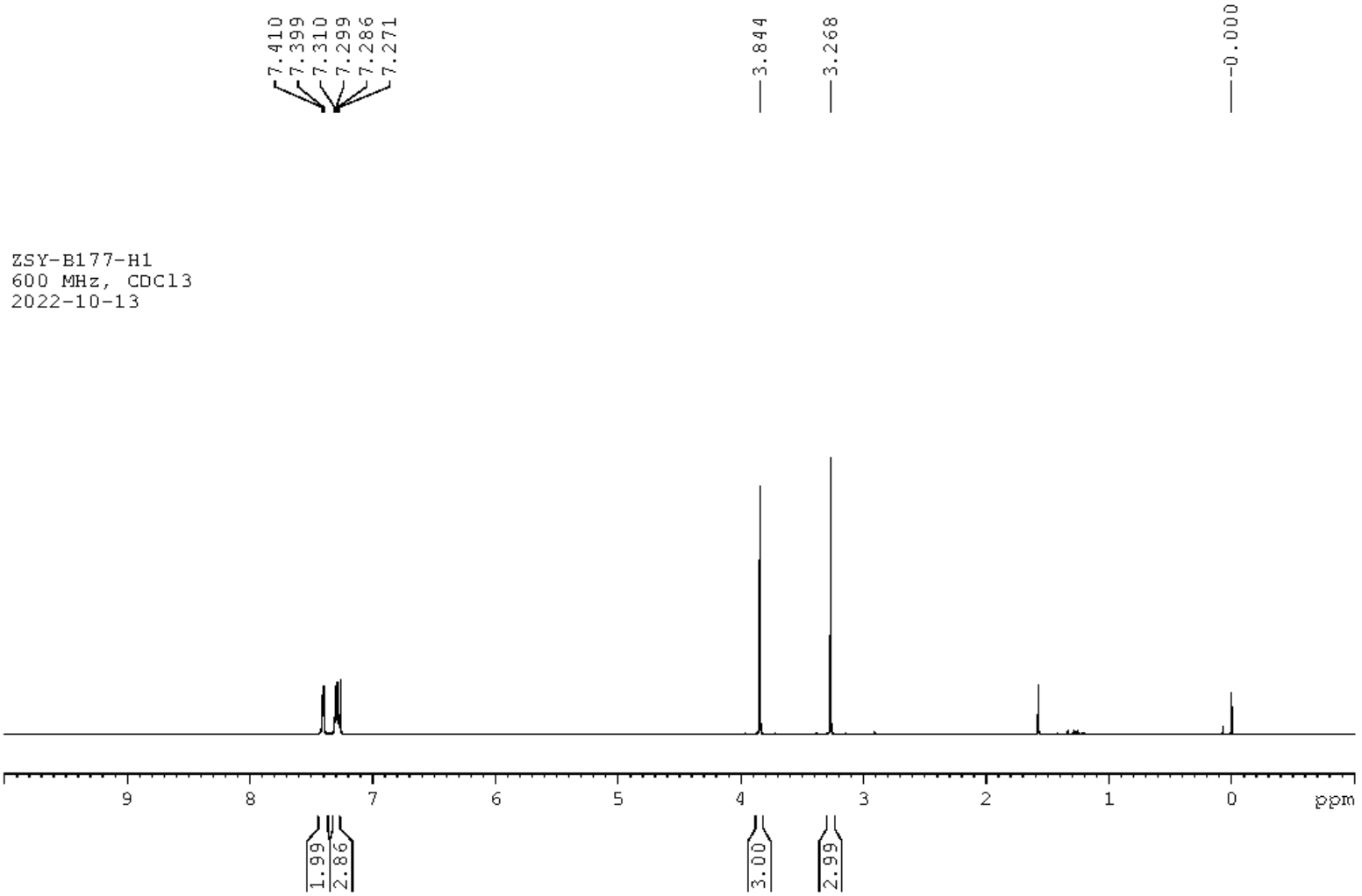
3na

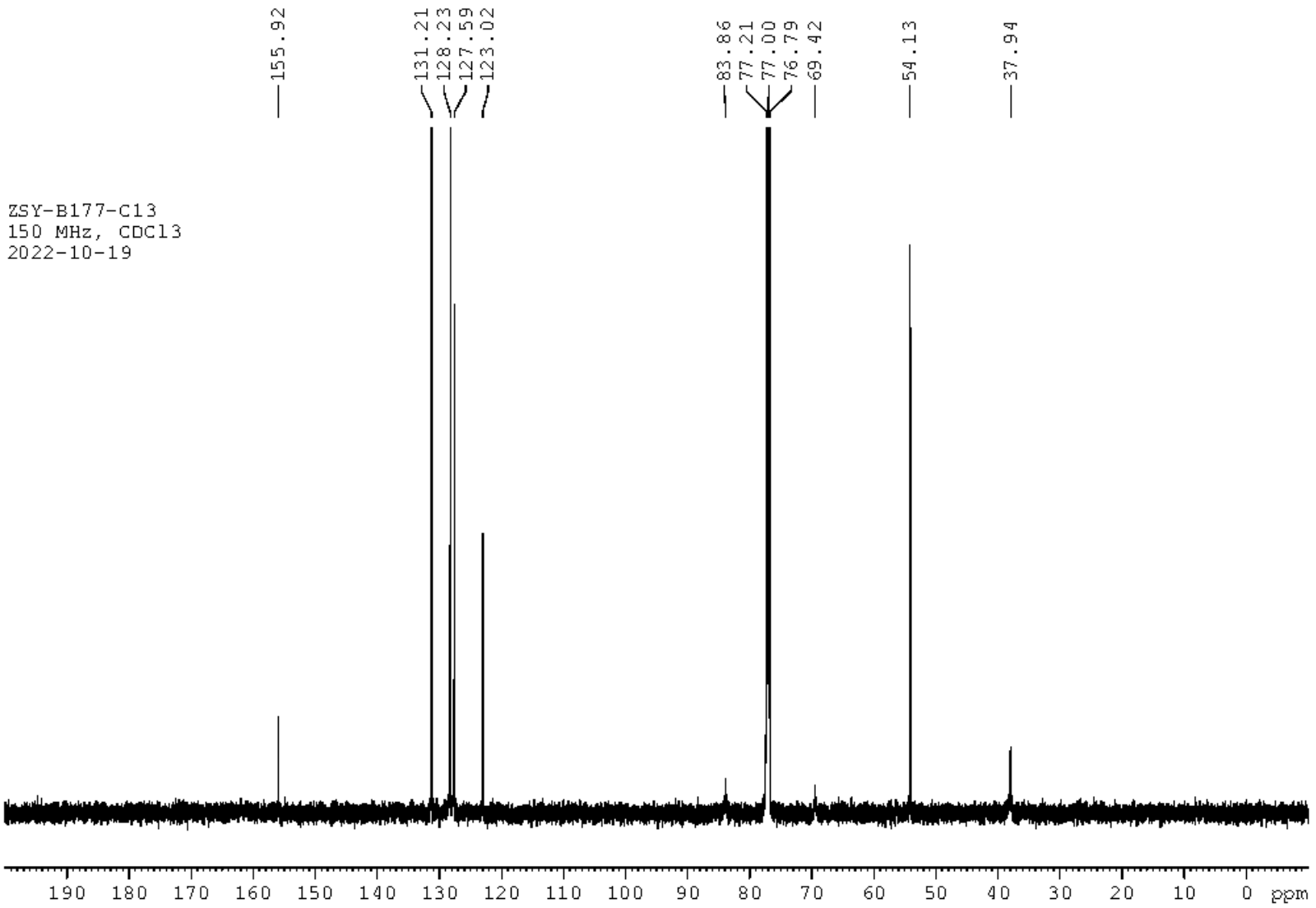

7.455
7.452
7.446
7.439
7.316
7.312
7.307
7.304
7.297
4.697
4.691
4.682
4.676
4.665
4.650
4.635
4.521
4.514
4.507
4.500
3.898
0.000
ZSY-C162-H1
600 MHz, CDCl3
2023-09-08
9
8
7
6
5
4
3
2
1
0
ppm
2.04
3.00
2.05
1.00
3.13

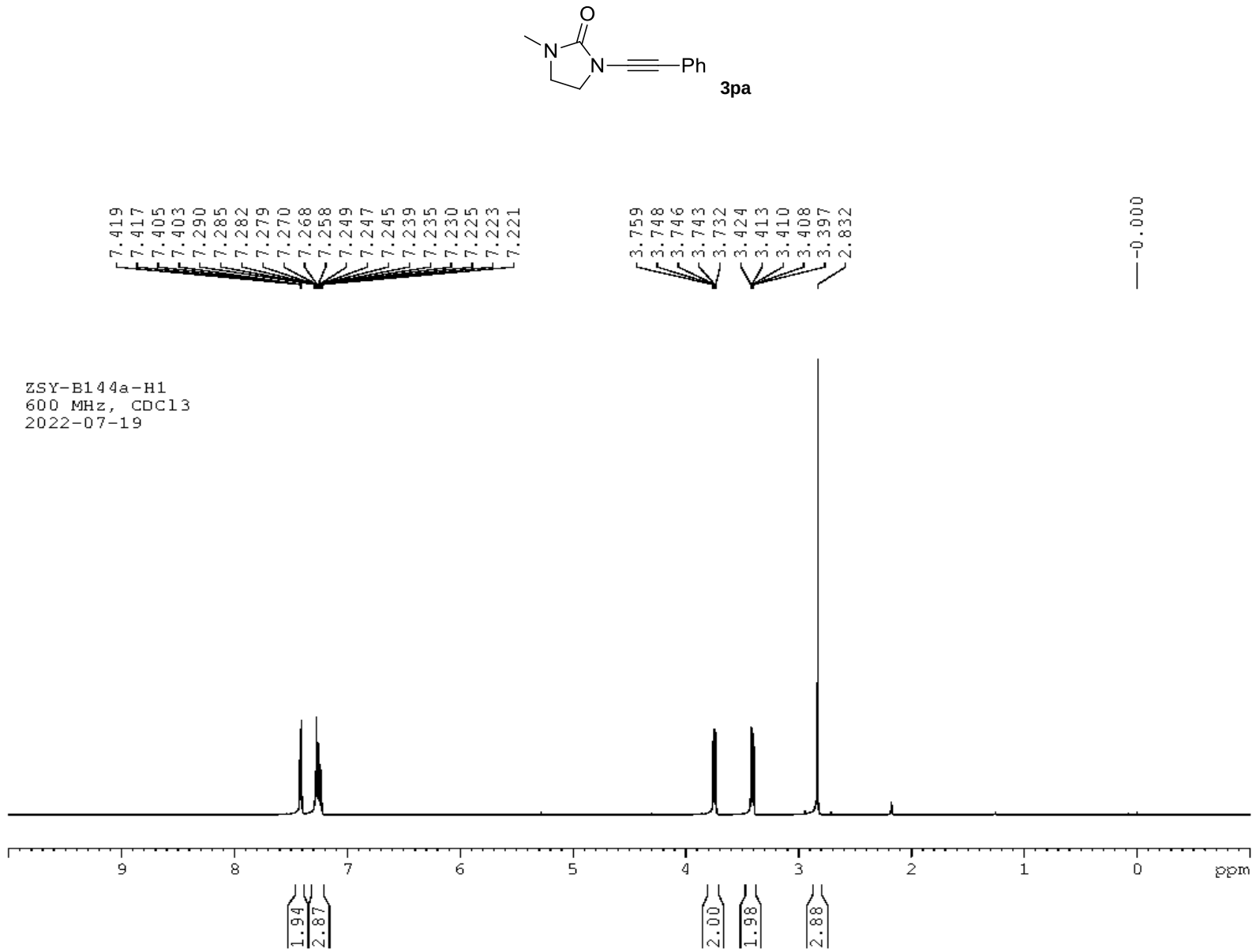

168.30
154.65
131.76
128.42
128.26
121.83
77.45
77.21
77.00
76.79
72.05
65.40
58.81
53.44
ZSY-C162-C13
150 MHz, CDCl3
2023-09-08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

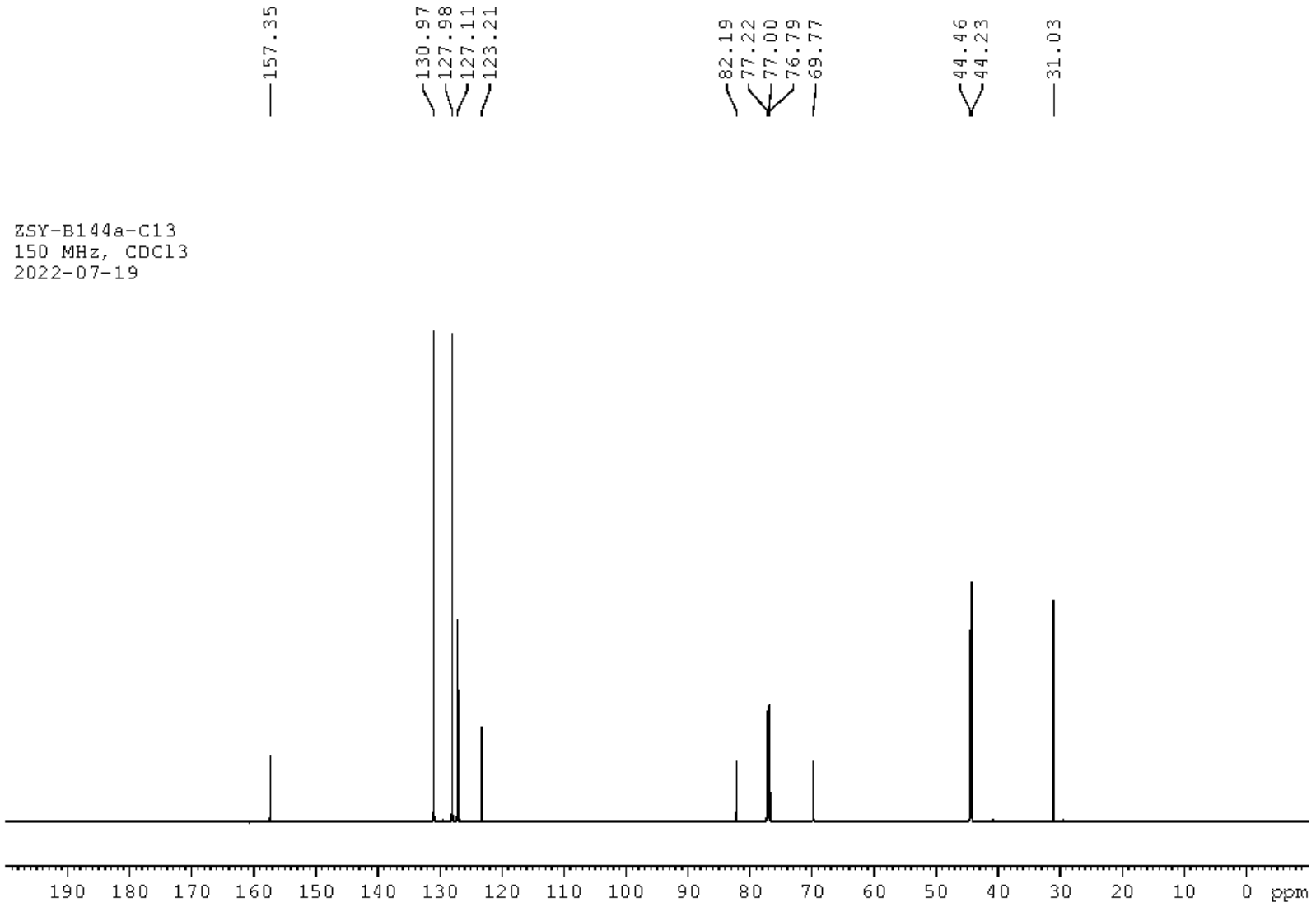

O
O
N
Ph

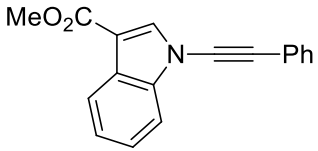
3oa


7.410
7.399
7.310
7.299
7.286
7.271
3.844
3.268
0.000
ZSY-B177-H1
600 MHz, CDCl3
2022-10-13
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.86
3.00
2.99

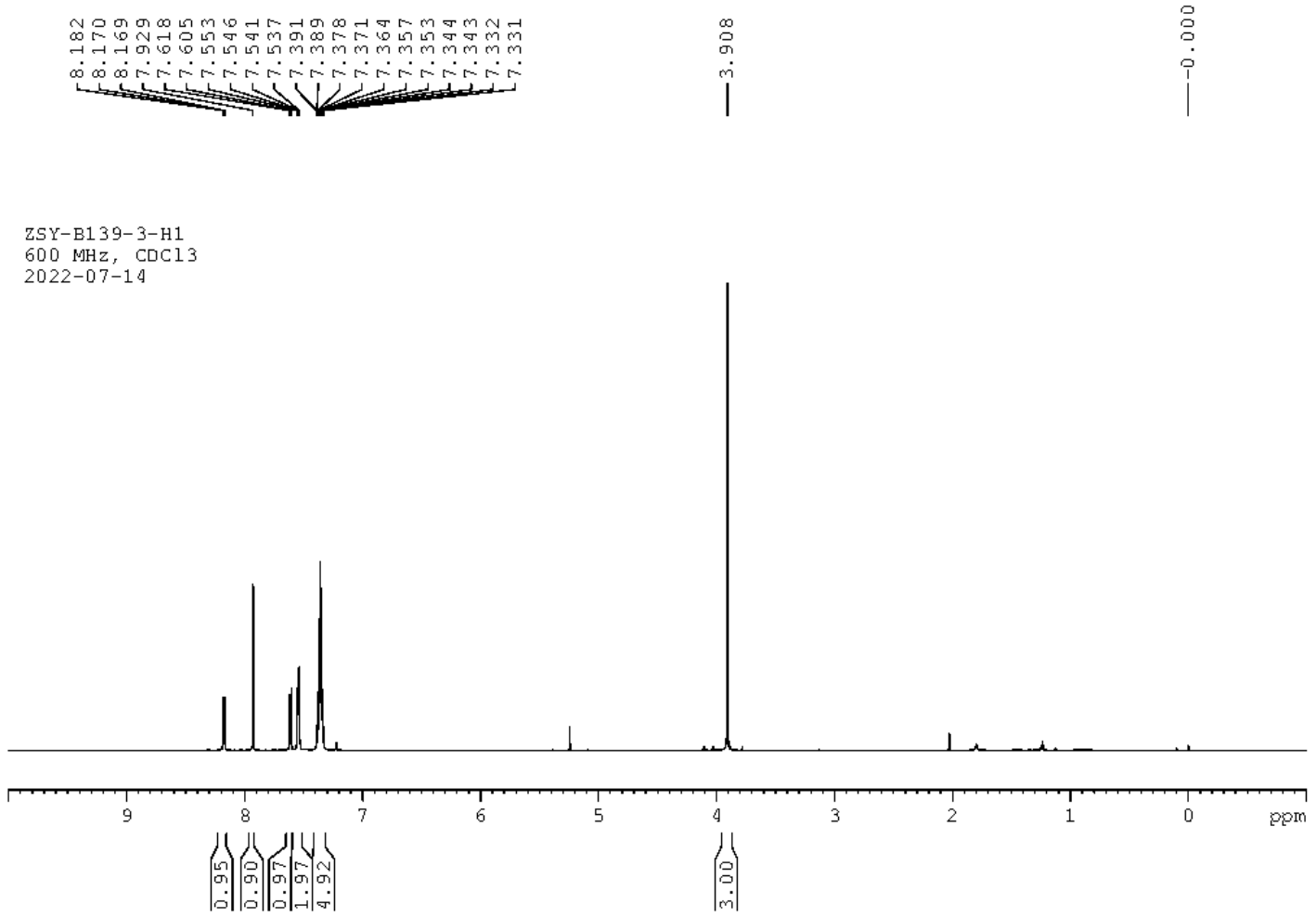

155.92
131.21
128.23
127.59
123.02
83.86
77.21
77.00
76.79
69.42
54.13
37.94
ZSY-B177-C13
150 MHz, CDCl3
2022-10-19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

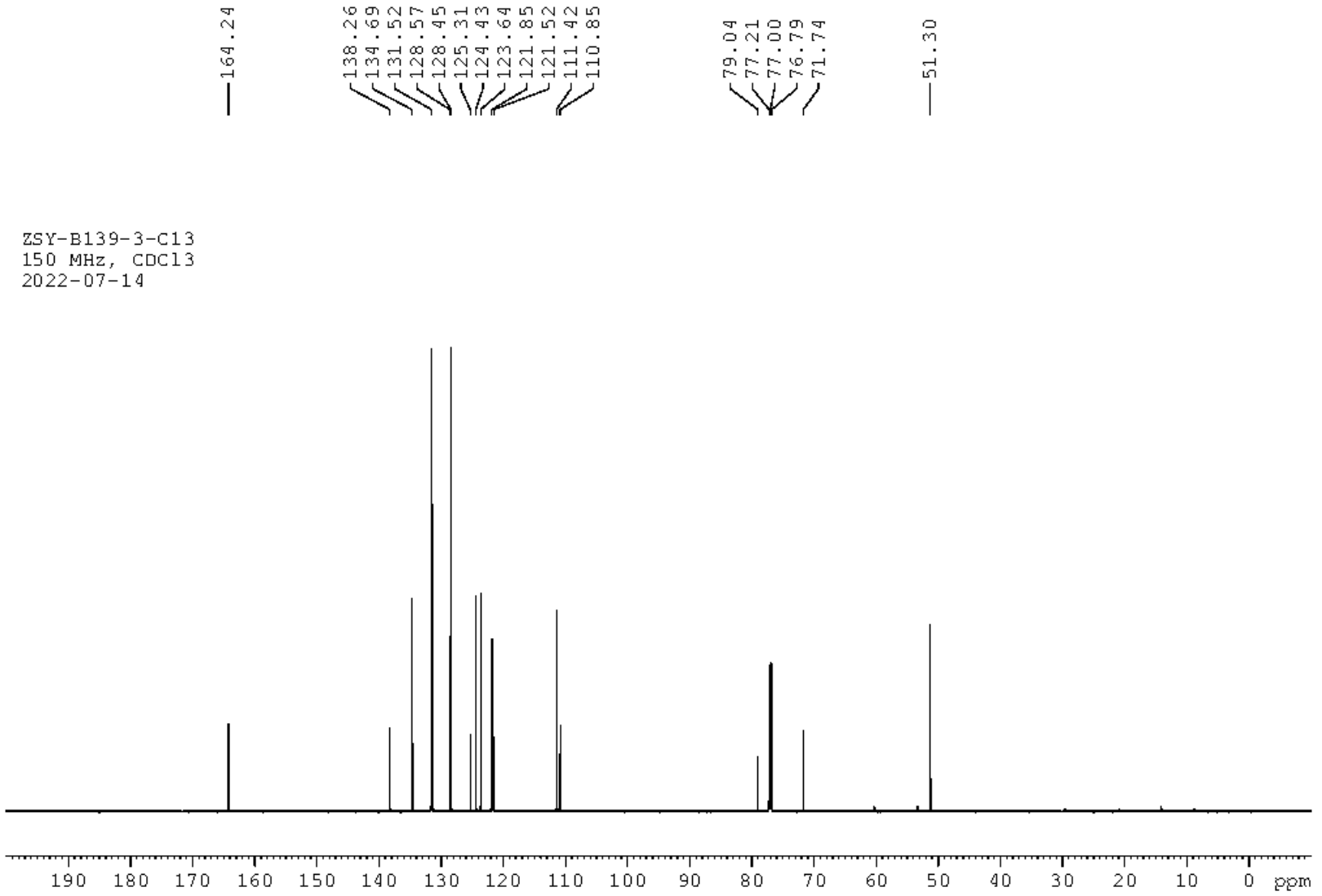

O
N
N
Ph
3pa
7.419
7.417
7.405
7.403
7.290
7.285
7.282
7.279
7.270
7.268
7.258
7.249
7.247
7.245
7.239
7.235
7.230
7.225
7.223
7.221
3.759
3.748
3.746
3.743
3.732
3.424
3.413
3.410
3.408
3.397
2.832
0.000
ZSY-B144a-H1
600 MHz, CDCl3
2022-07-19
9
8
7
6
5
4
3
2
1
0
ppm
1.94
2.87
2.00
1.98
2.88

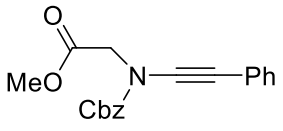

157.35
130.97
127.98
127.11
123.21
82.19
77.22
77.00
76.79
69.77
44.46
44.23
31.03
ZSY-B144a-C13
150 MHz, CDCl3
2022-07-19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


MeO2C
N
Ph

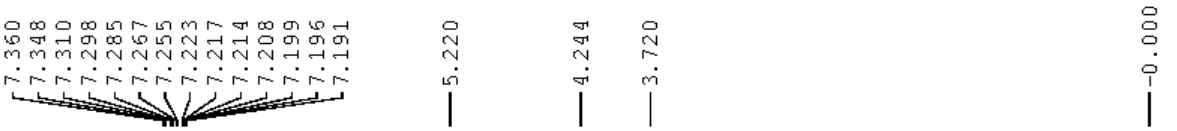
3qa


8.182
8.170
8.169
7.929
7.618
7.605
7.553
7.546
7.541
7.537
7.391
7.389
7.378
7.371
7.364
7.357
7.353
7.344
7.343
7.332
7.331
3.908
0.000
ZSY-B139-3-H1
600 MHz, CDCl3
2022-07-14
9
8
7
6
5
4
3
2
1
0
ppm
0.95
0.90
0.97
1.97
4.92
3.00

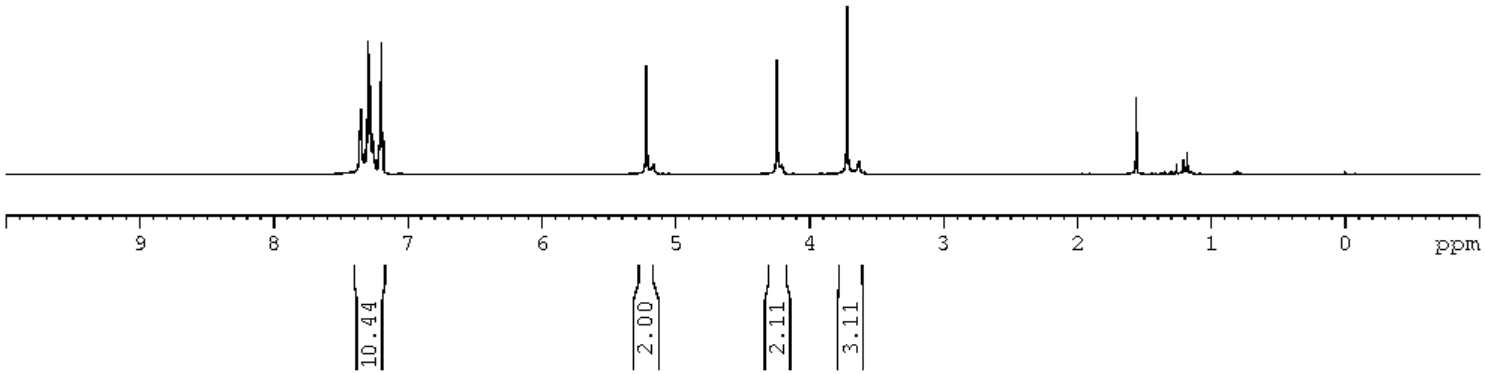

164.24
138.26
134.69
131.52
128.57
128.45
125.31
124.43
123.64
121.85
121.52
111.42
110.85
79.04
77.21
77.00
76.79
71.74
51.30
ZSY-B139-3-C13
150 MHz, CDCl3
2022-07-14
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

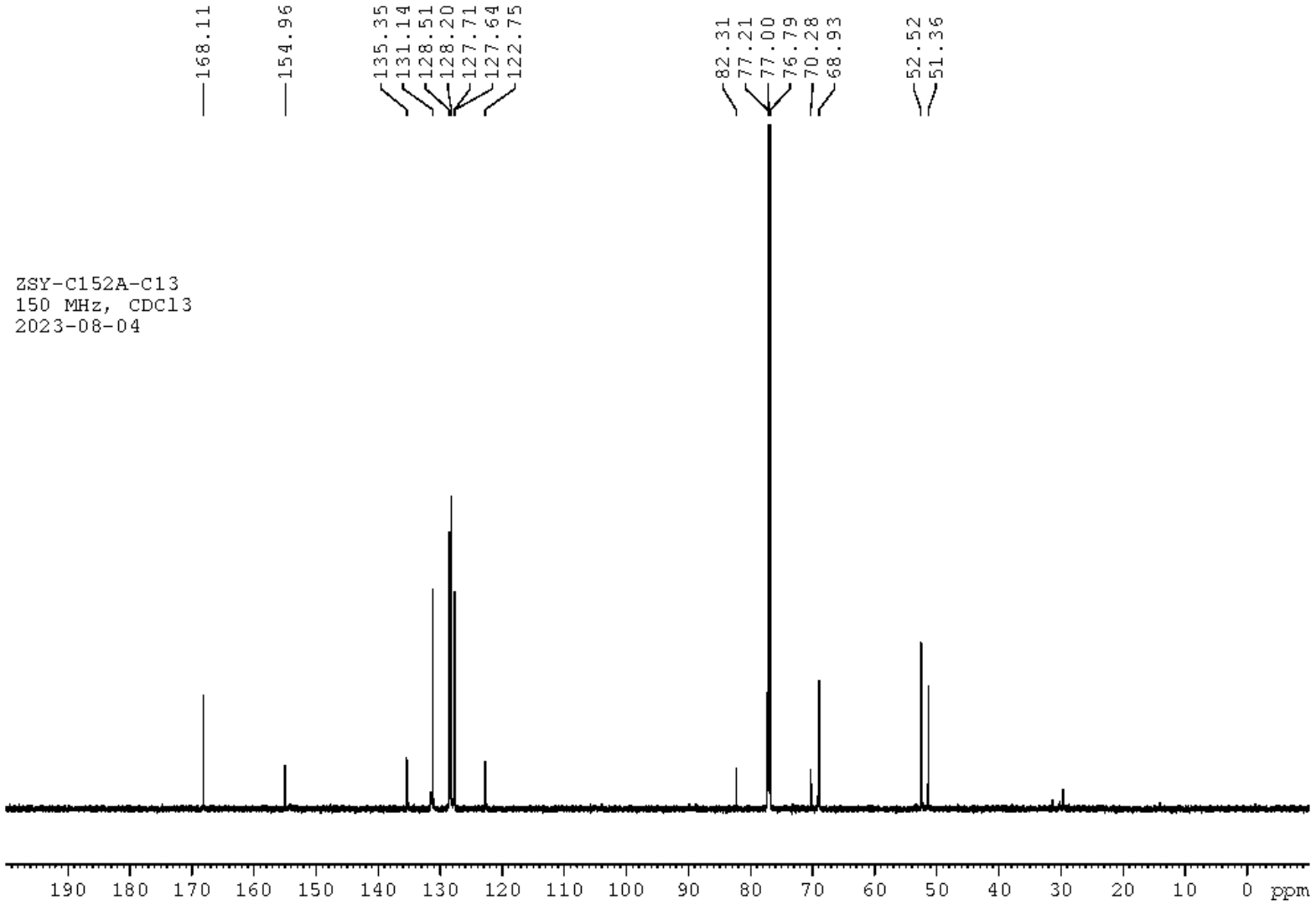


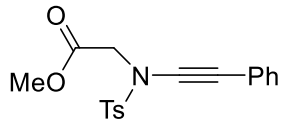
3ra



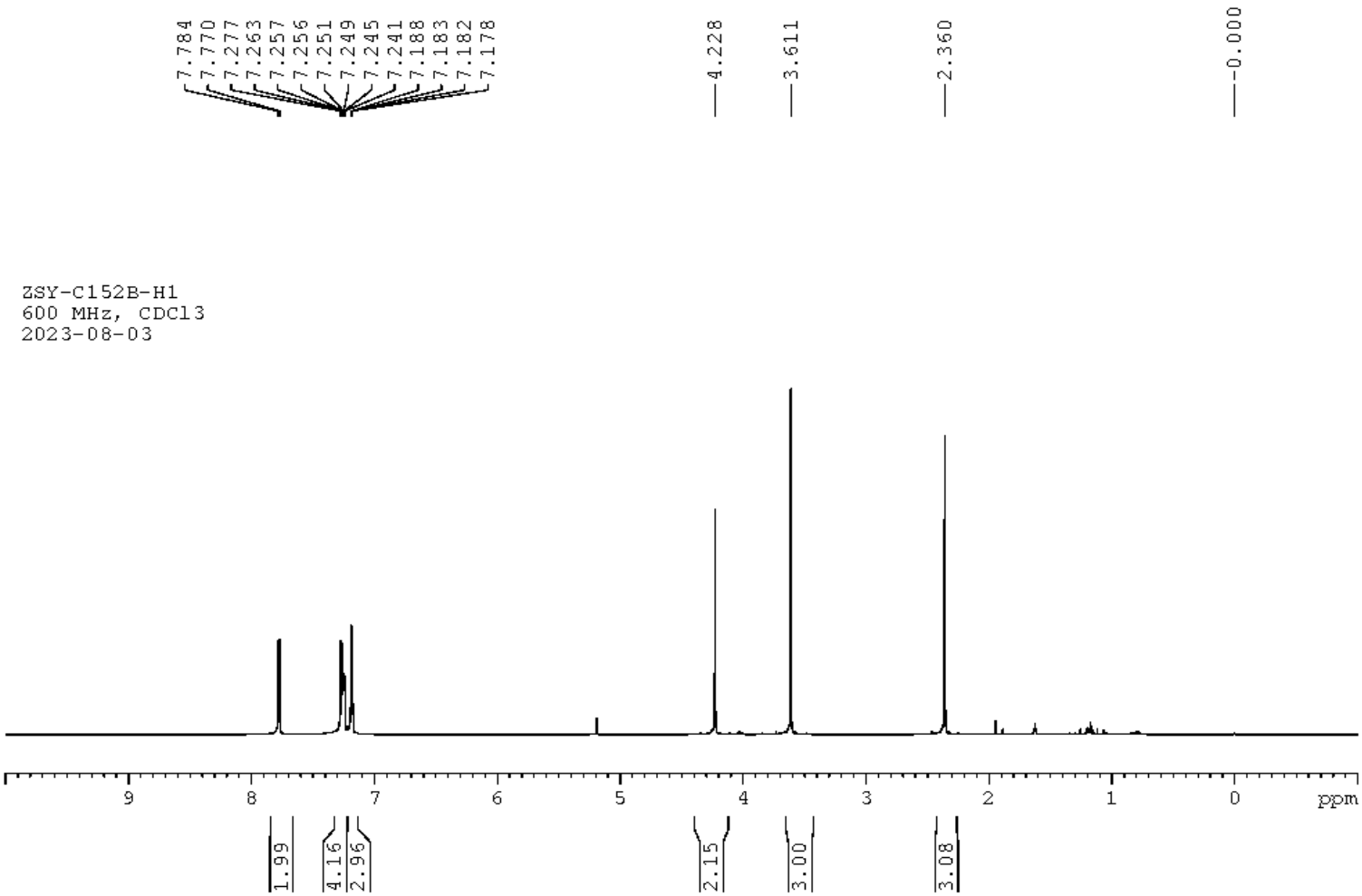
ZSY-C152A-H1
600 MHz, CDCl3
2023-08-04

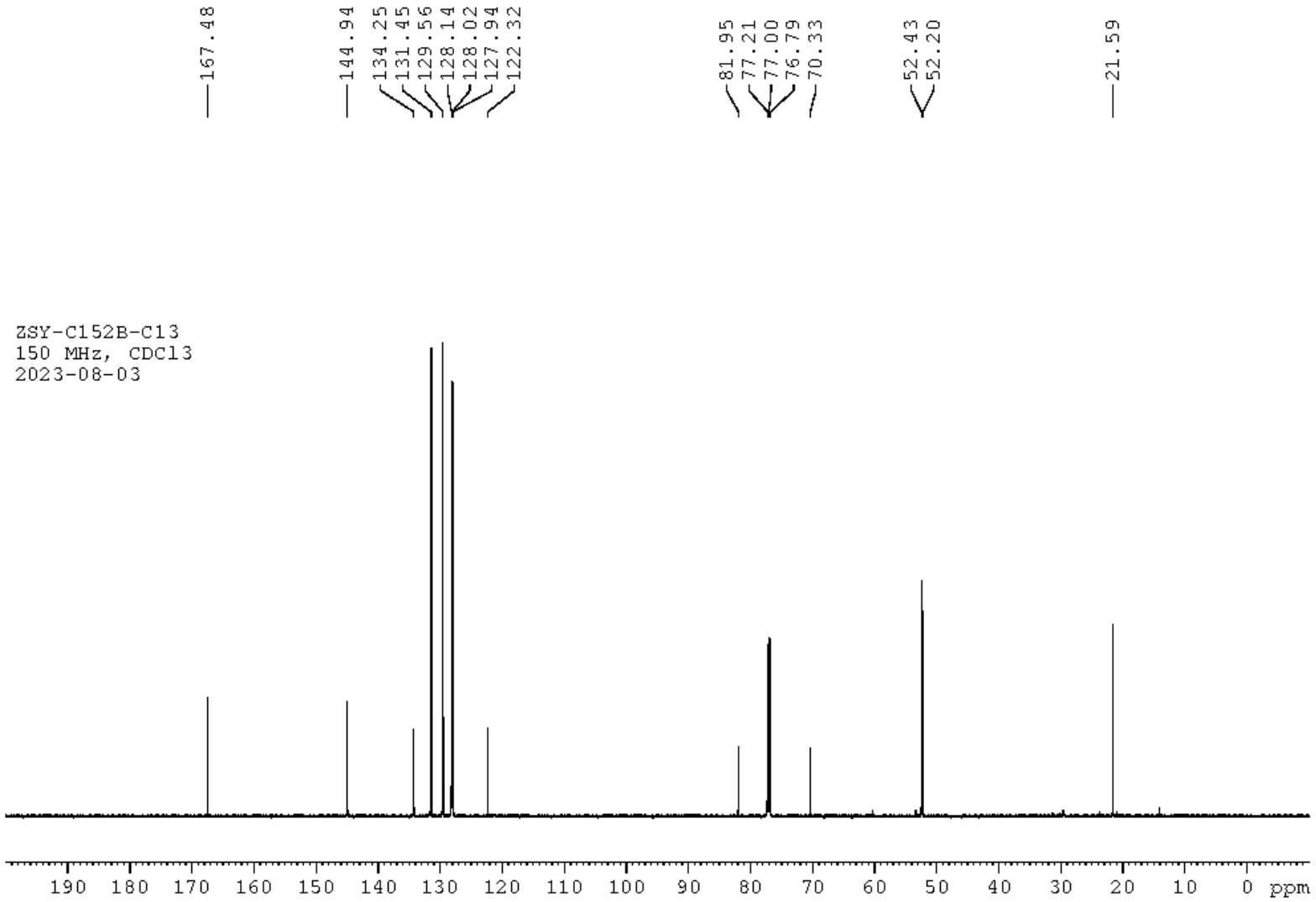


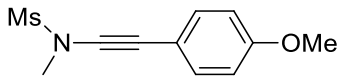

168.11
154.96
135.35
131.14
128.51
128.20
127.71
127.64
122.75
82.31
77.21
77.00
76.79
70.28
68.93
52.52
51.36
ZSY-C152A-C13
150 MHz, CDCl3
2023-08-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
MeO
N
Ph
Ts

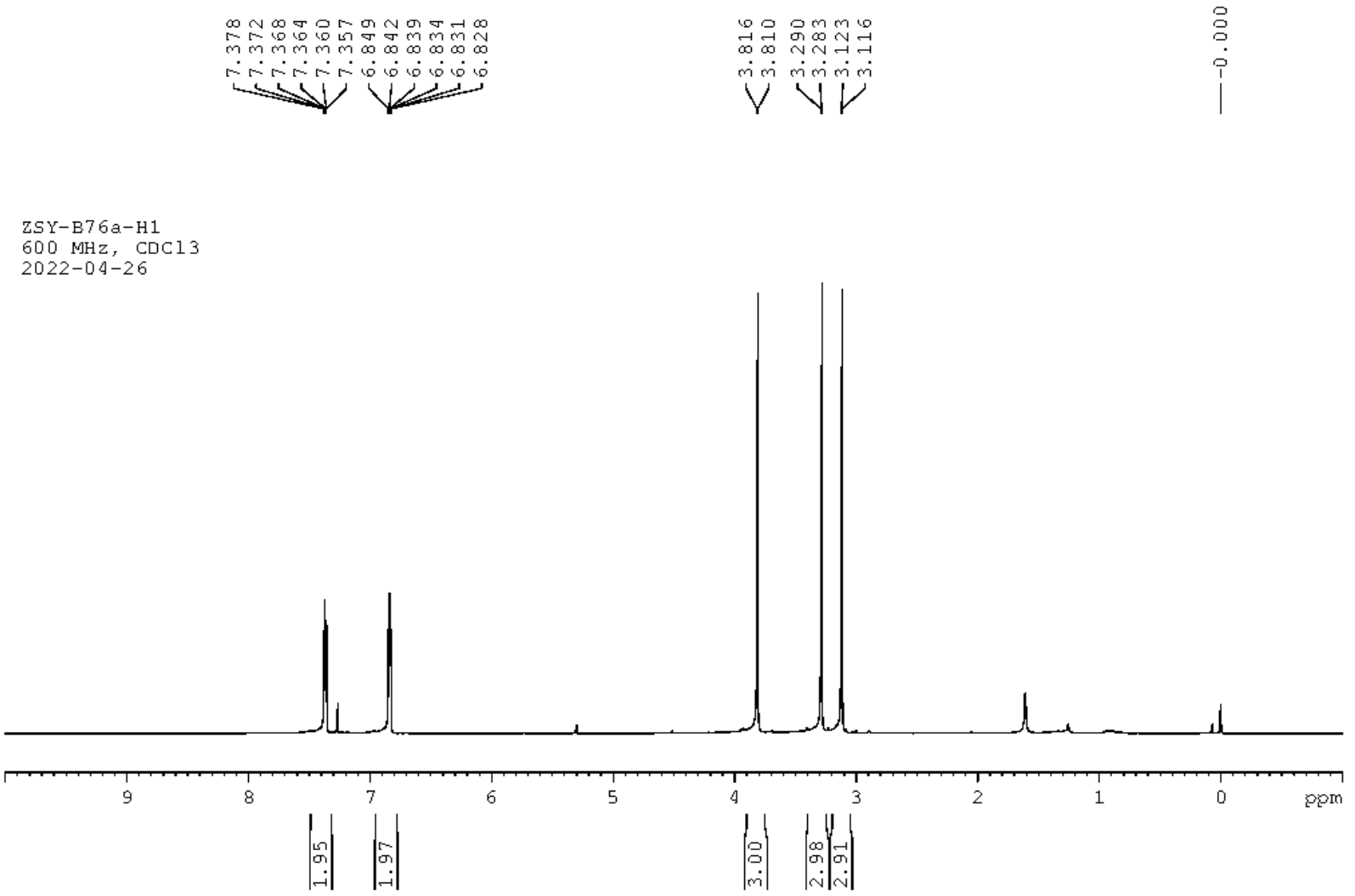
3sa

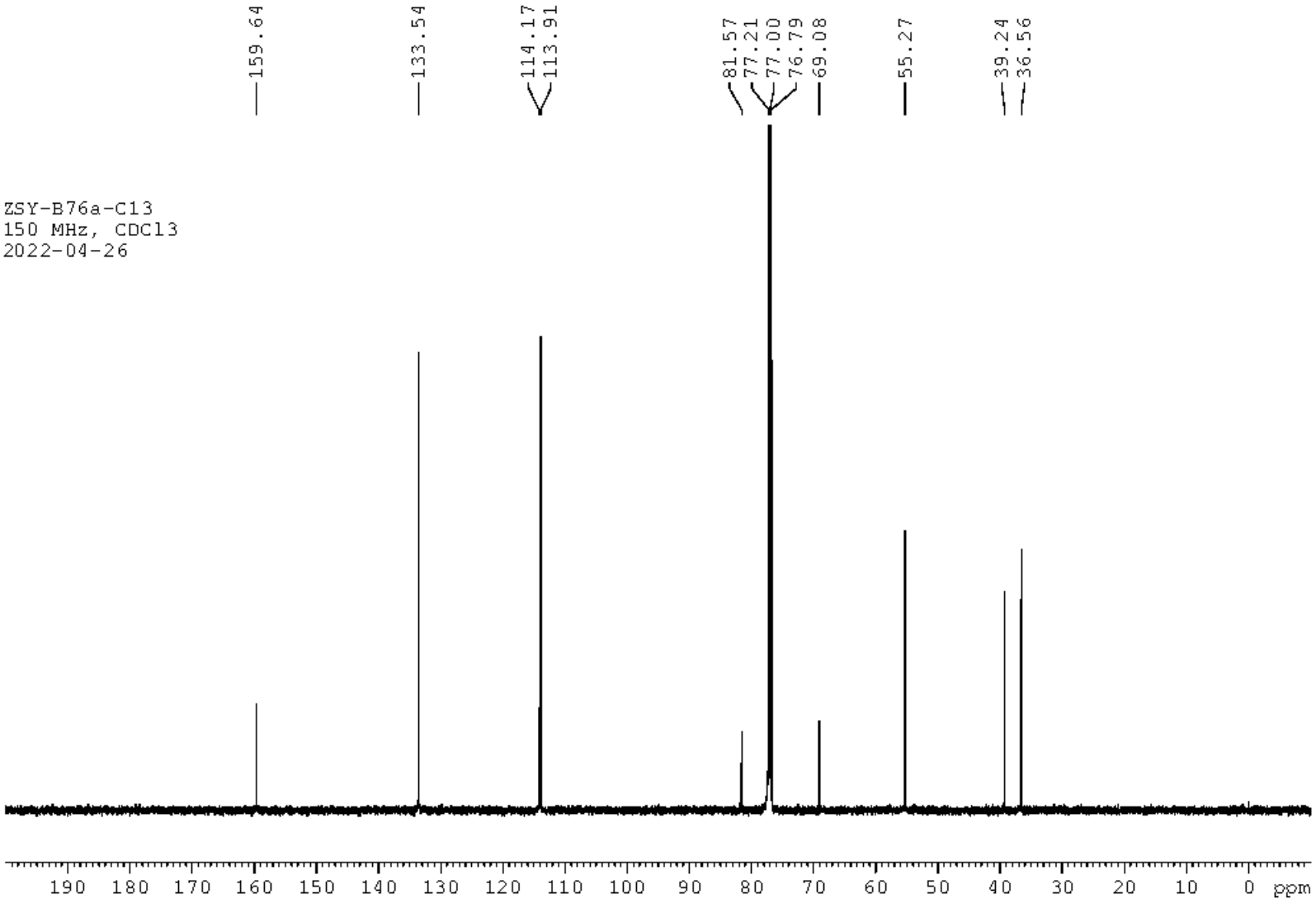

7.784
7.770
7.277
7.263
7.257
7.256
7.251
7.249
7.245
7.241
7.188
7.183
7.182
7.178
4.228
3.611
2.360
0.000
ZSY-C152B-H1
600 MHz, CDCl3
2023-08-03
9
8
7
6
5
4
3
2
1
0
ppm
1.99
4.16
2.96
2.15
3.00
3.08

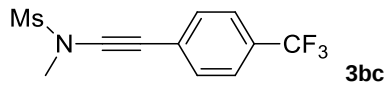

167.48
144.94
134.25
131.45
129.56
128.14
128.02
127.94
122.32
81.95
77.21
77.00
76.79
70.33
52.43
52.20
21.59
ZSY-C152B-C13
150 MHz, CDCl3
2023-08-03
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ms
N
OMe

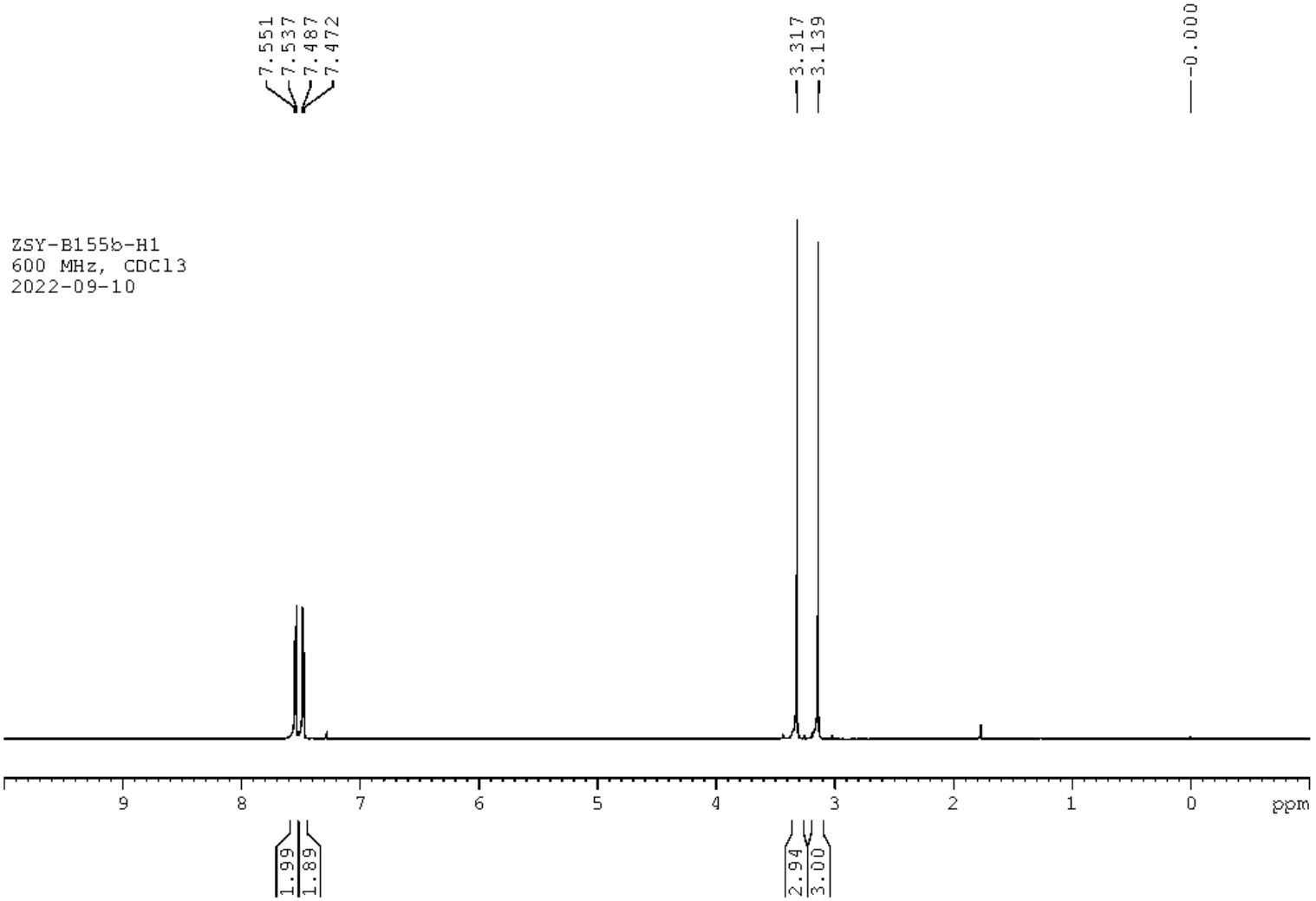
3bb

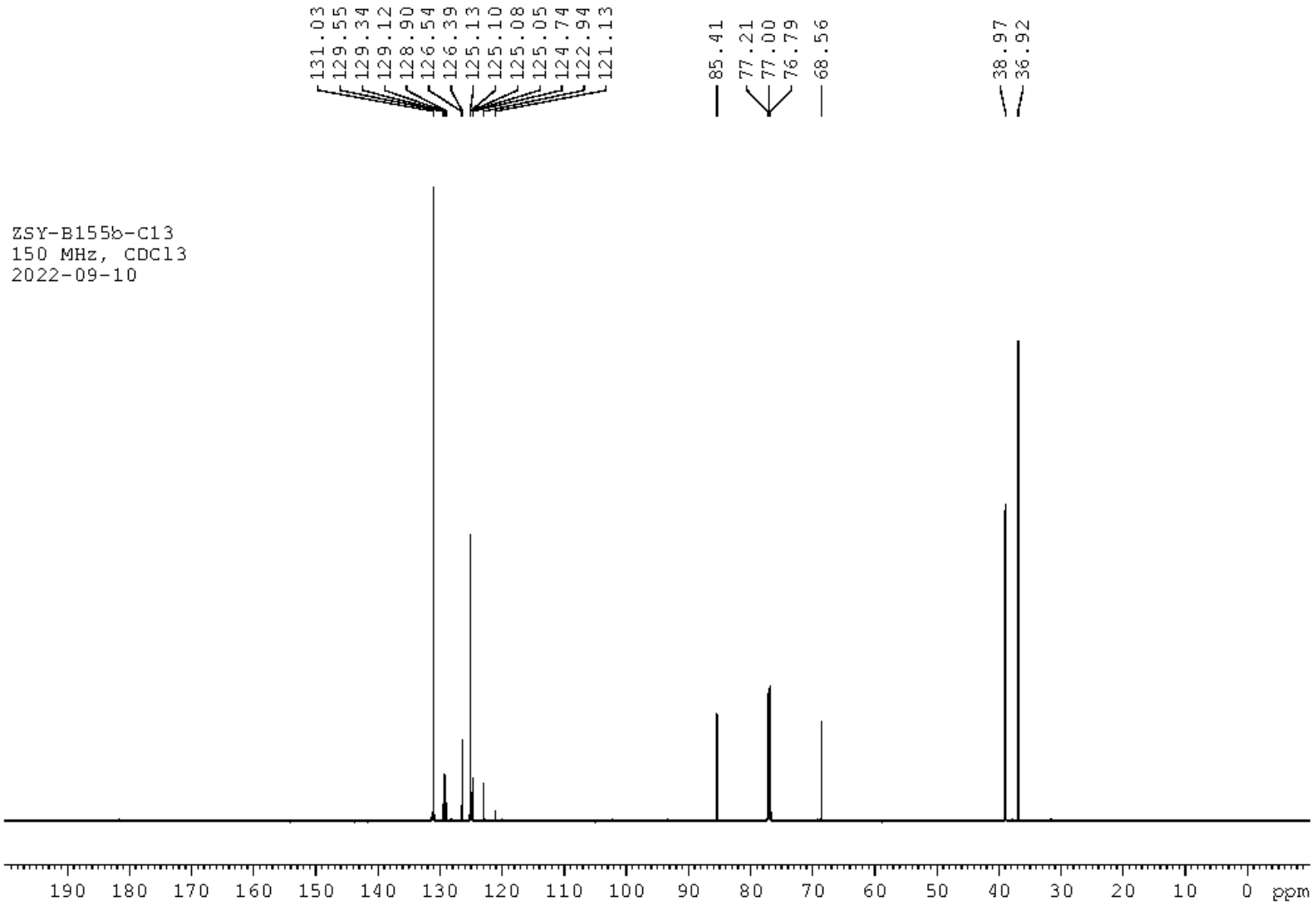

7.378
7.372
7.368
7.364
7.360
7.357
6.849
6.842
6.839
6.834
6.831
6.828
3.816
3.810
3.290
3.283
3.123
3.116
0.000
ZSY-B76a-H1
600 MHz, CDCl3
2022-04-26
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.97
3.00
2.98
2.91

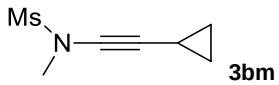

159.64
133.54
114.17
113.91
81.57
77.21
77.00
76.79
69.08
55.27
39.24
36.56
ZSY-B76a-C13
150 MHz, CDCl3
2022-04-26
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ms
N
CF3

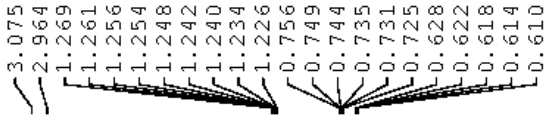
3bc


7.551
7.537
7.487
7.472
3.317
3.139
0.000
ZSY-B155b-H1
600 MHz, CDCl3
2022-09-10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
1.89
2.94
3.00

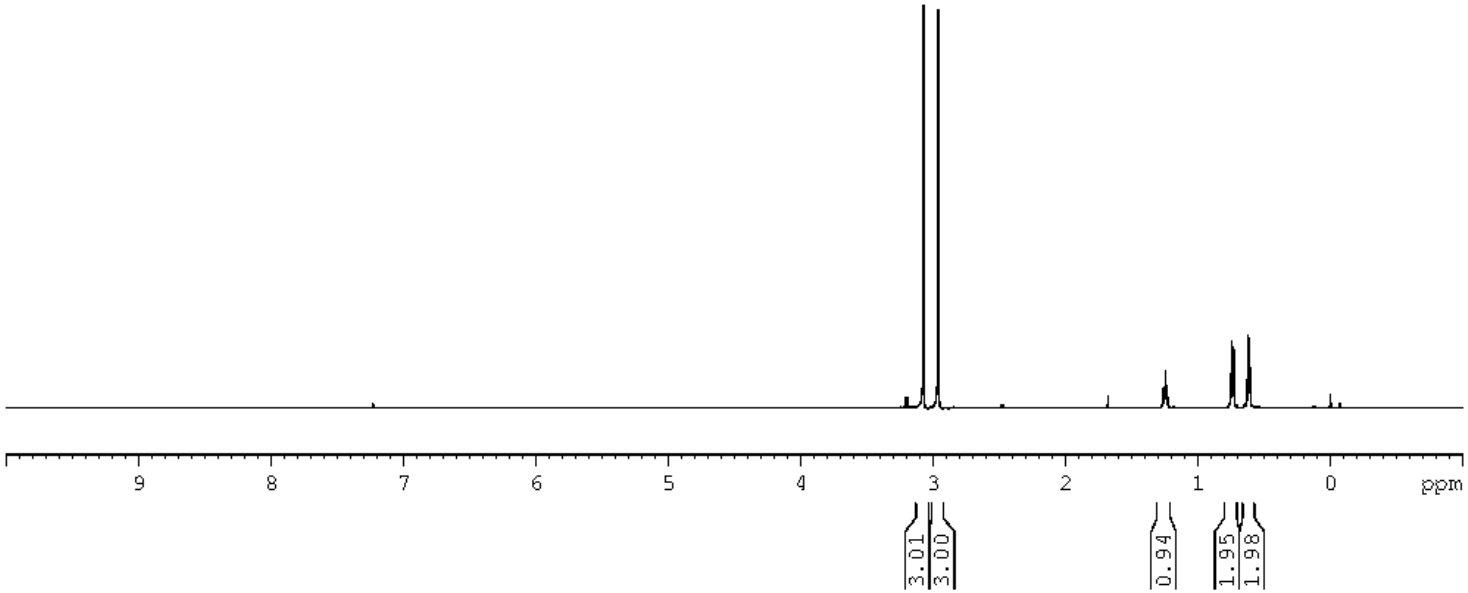

131.03
129.55
129.34
129.12
128.90
126.54
126.39
125.13
125.10
125.08
125.05
124.74
122.94
121.13
85.41
77.21
77.00
76.79
68.56
38.97
36.92
ZSY-B155b-C13
150 MHz, CDCl3
2022-09-10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

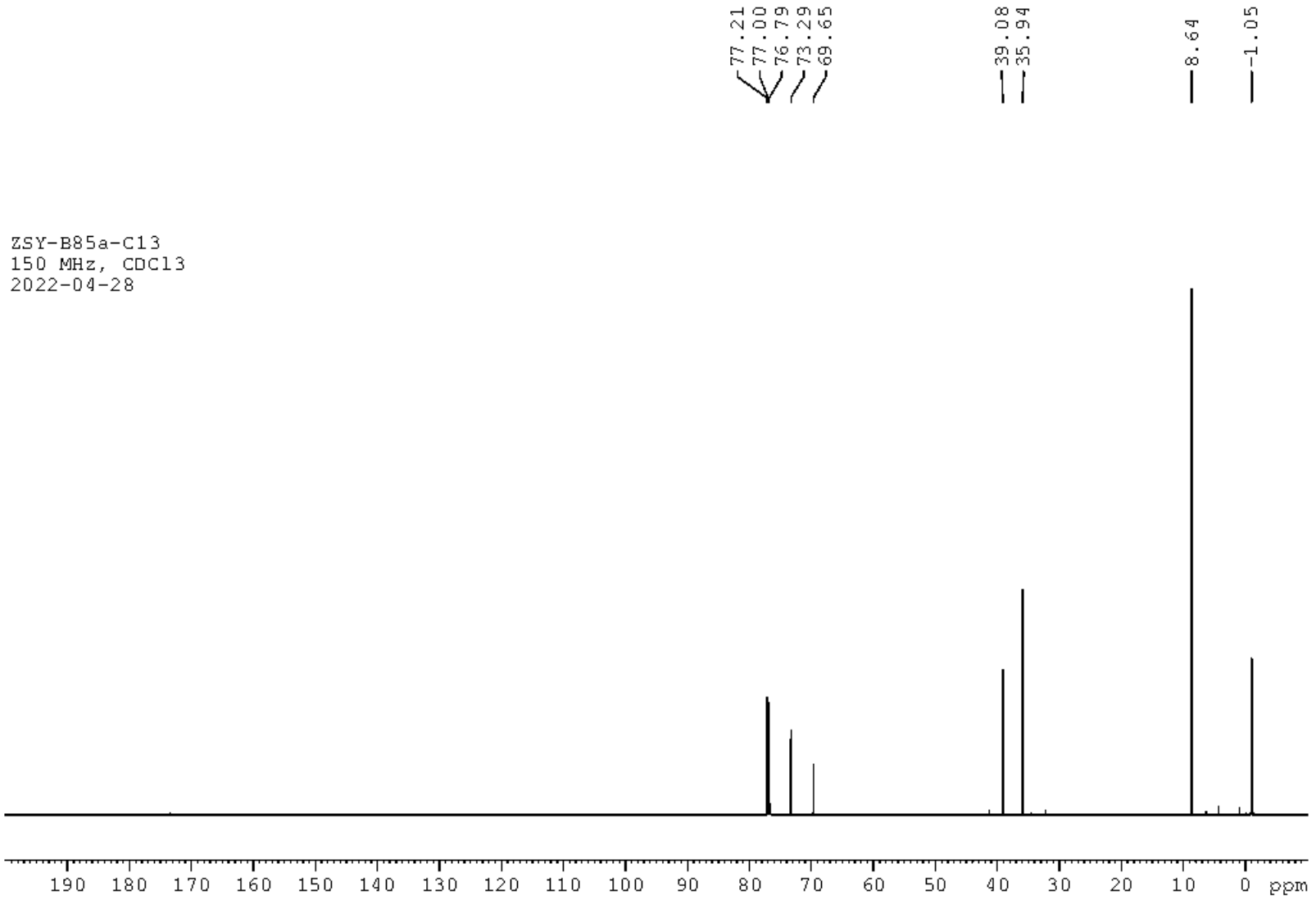


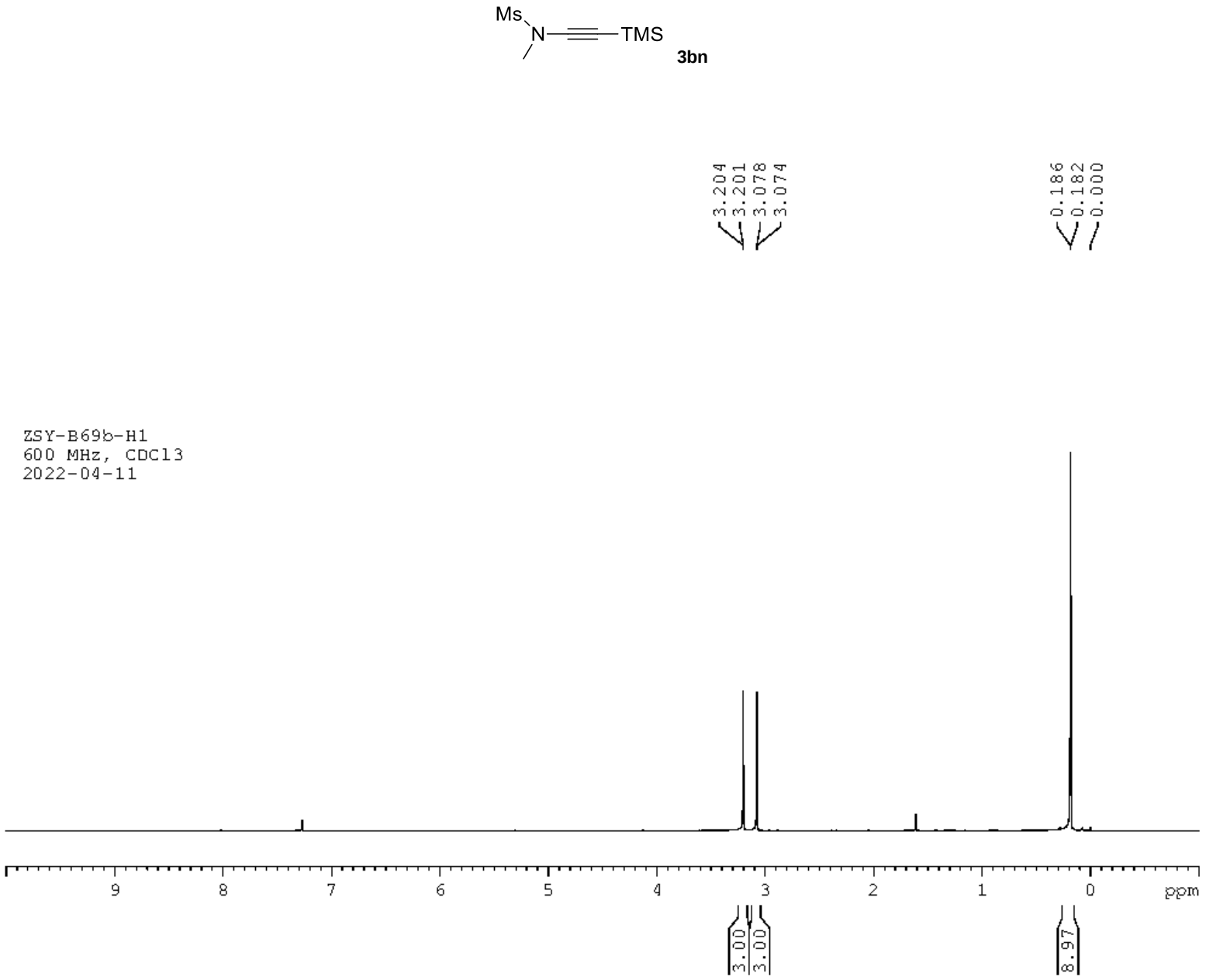
3bm

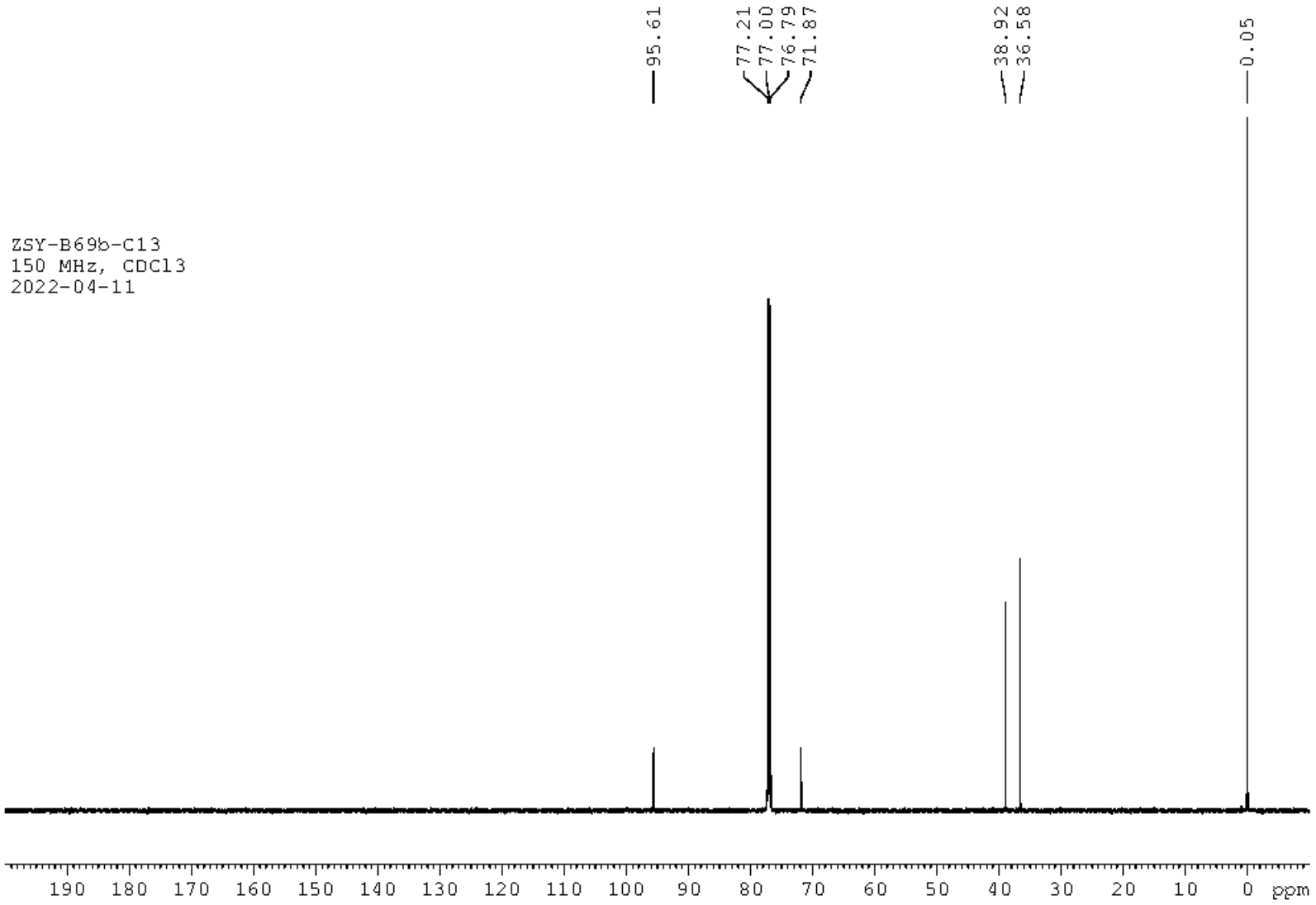


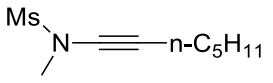
ZSY-B85a-H1
600 MHz, CDCl3
2022-04-28



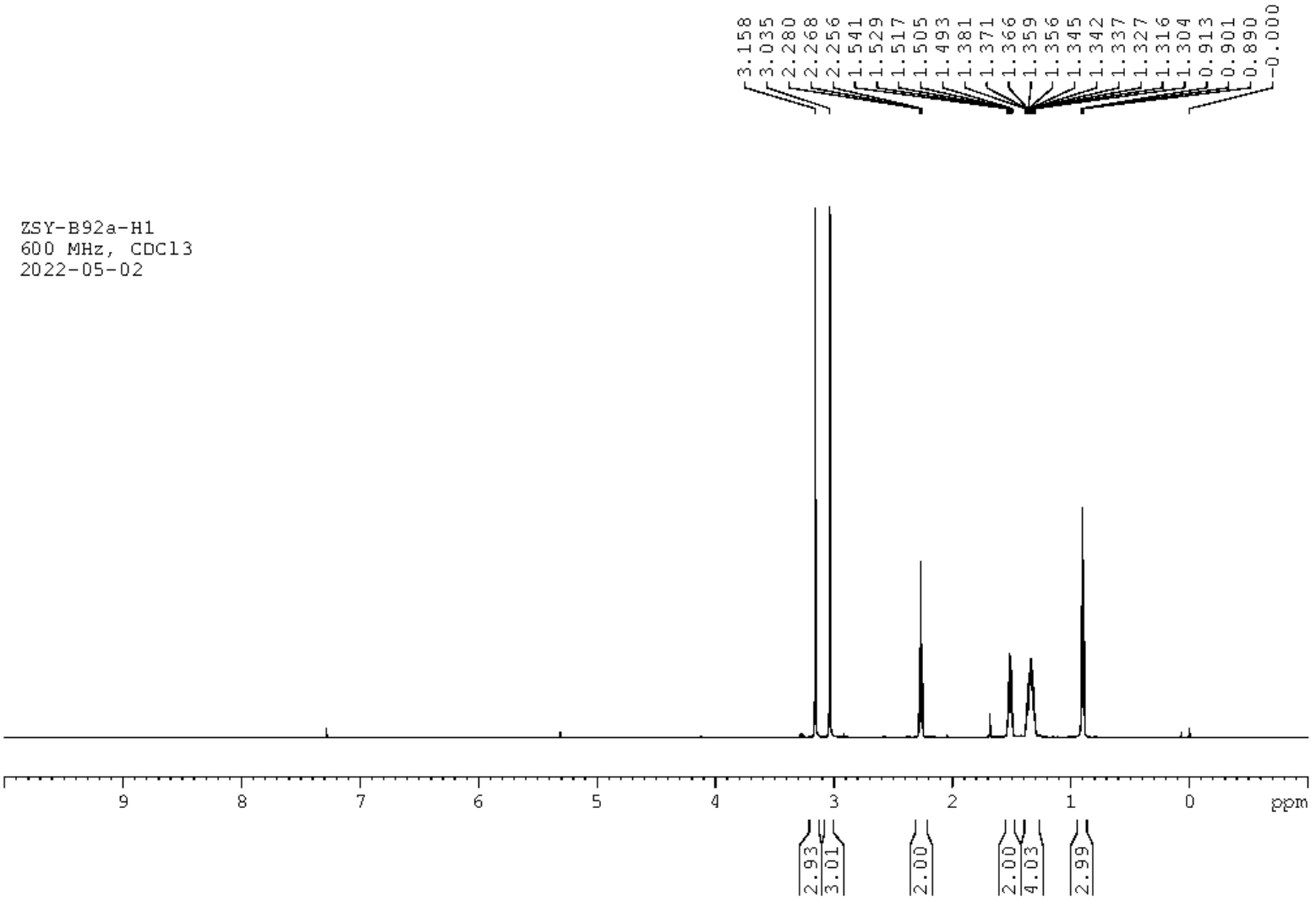

77.21
77.00
76.79
73.29
69.65
39.08
35.94
8.64
-1.05
ZSY-B85a-C13
150 MHz, CDCl3
2022-04-28
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

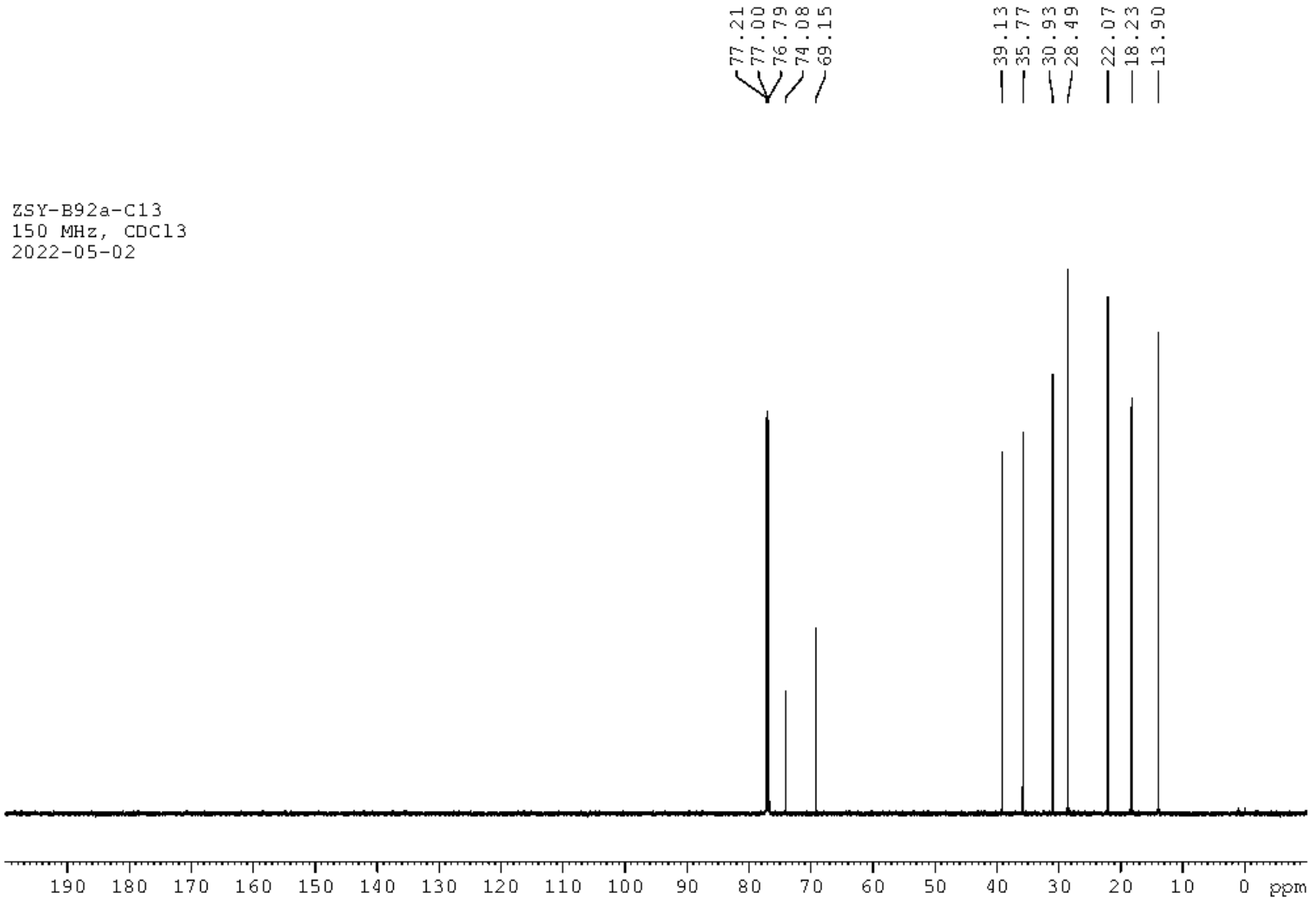

Ms
N
TMS
3bn
3.204
3.201
3.078
3.074
0.186
0.182
0.000
ZSY-B69b-H1
600 MHz, CDCl3
2022-04-11
9
8
7
6
5
4
3
2
1
0
ppm
3.00
3.00
8.97

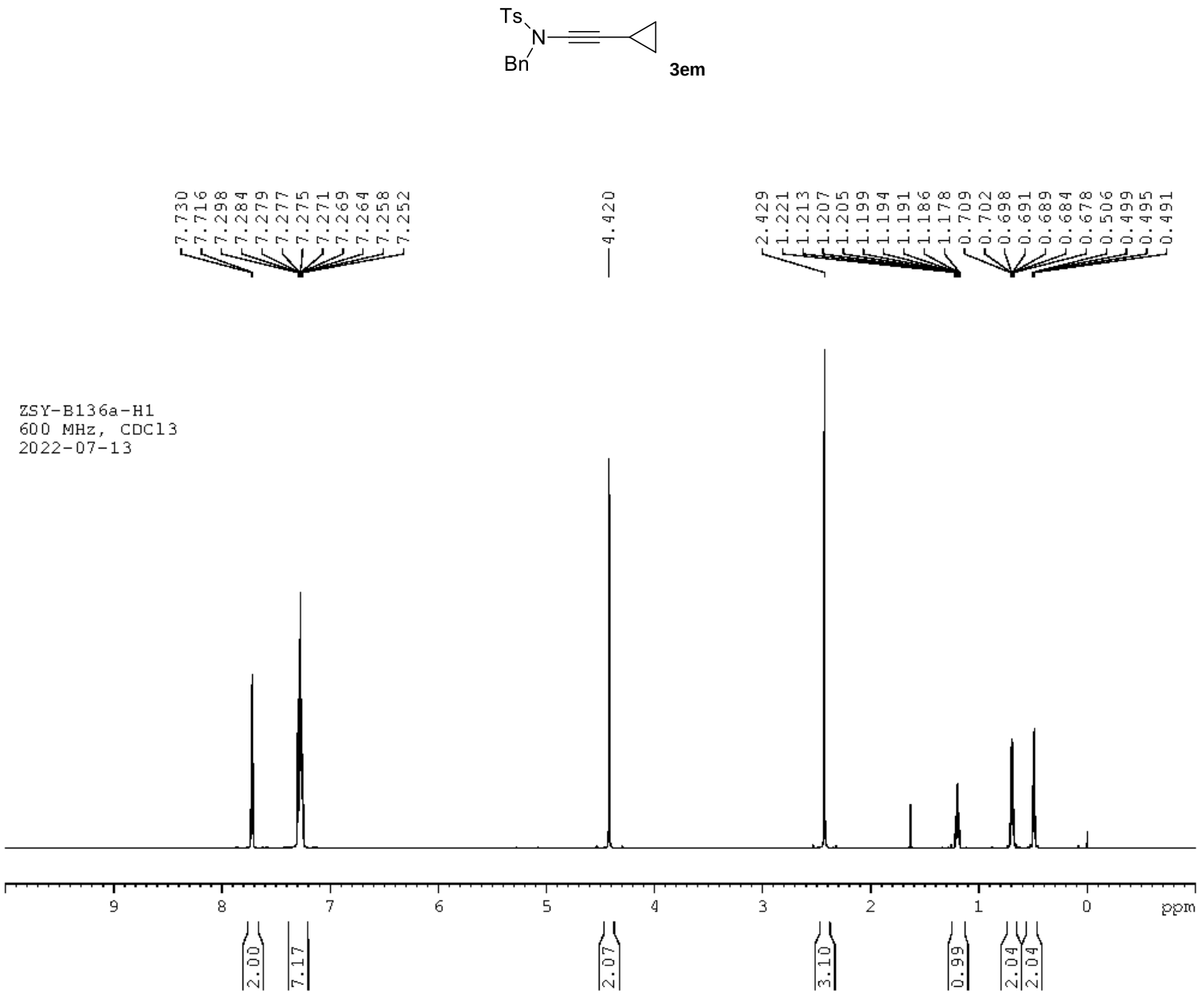

95.61
77.21
77.00
76.79
71.87
38.92
36.58
0.05
ZSY-B69b-C13
150 MHz, CDCl3
2022-04-11
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

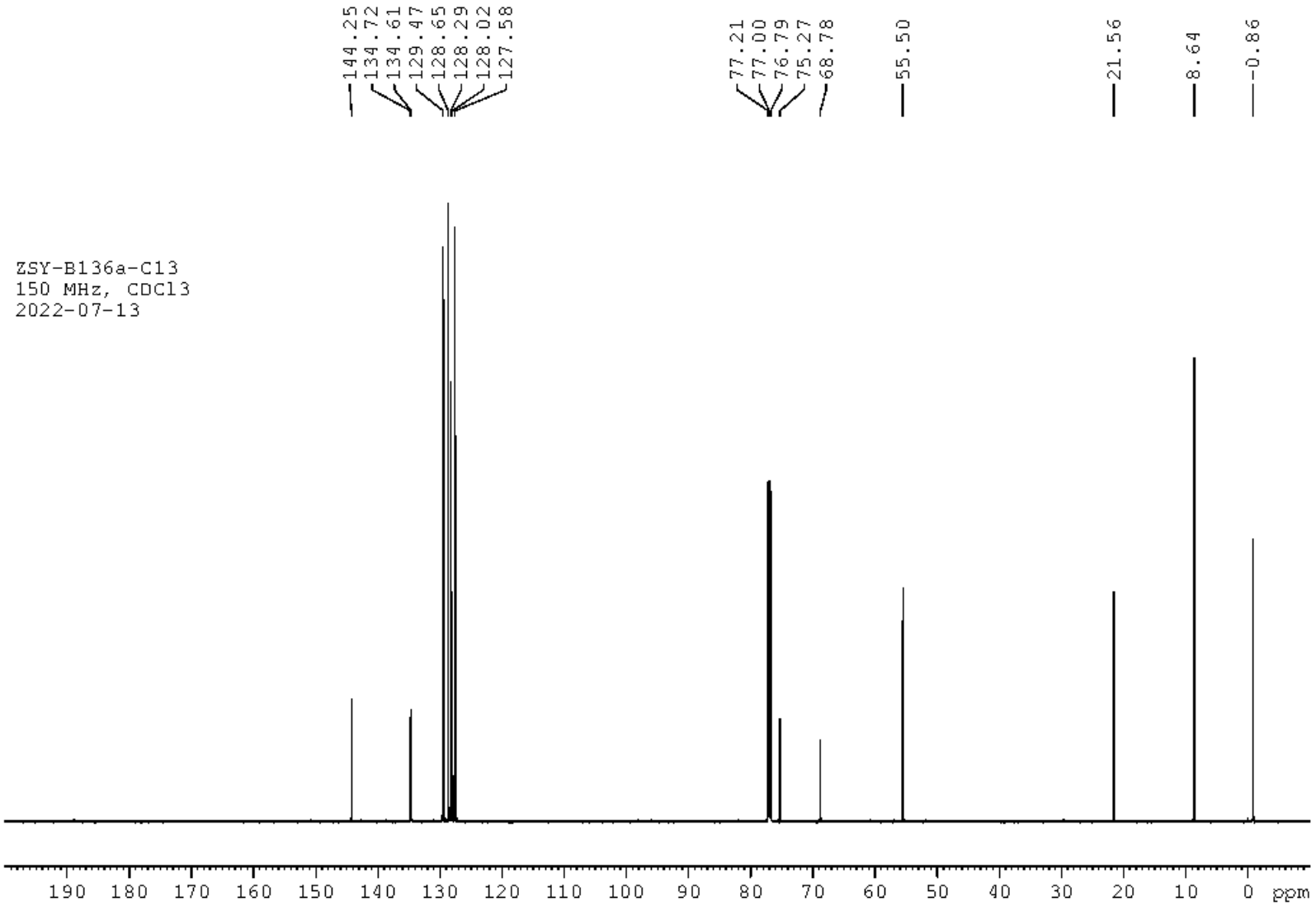

Ms
N
n-C5H11

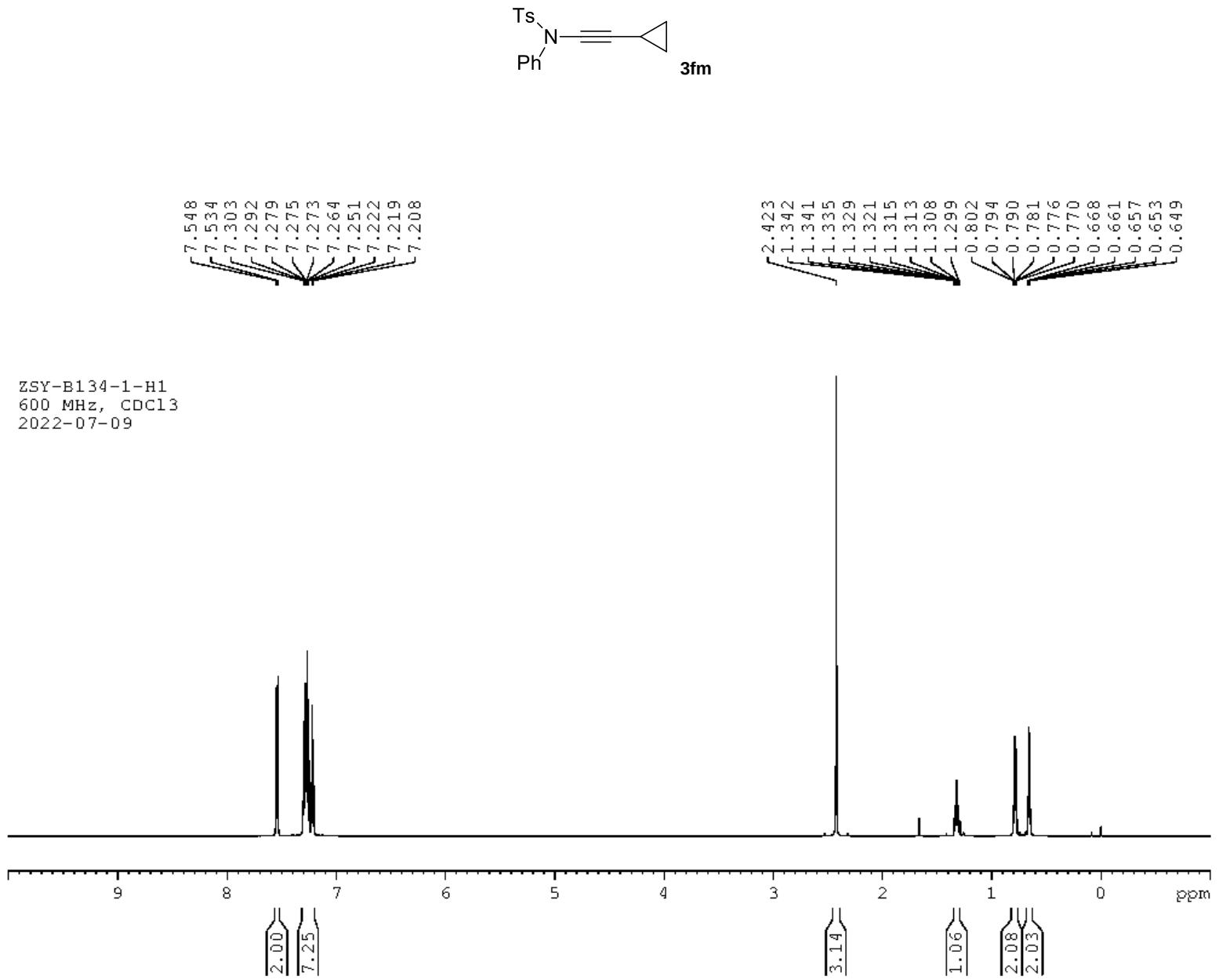
3br

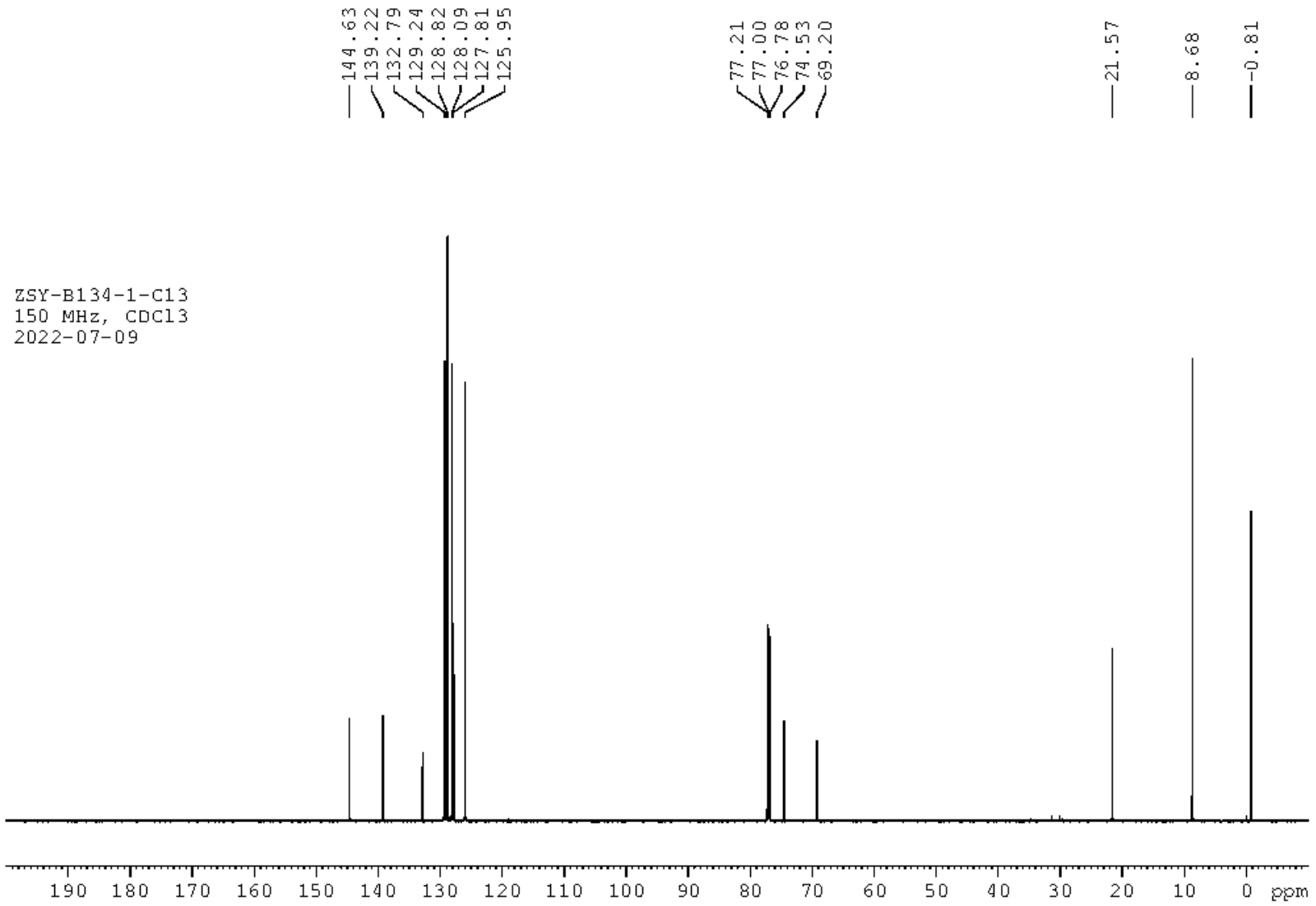

3.158
3.035
2.280
2.268
2.256
1.541
1.529
1.517
1.505
1.493
1.381
1.371
1.366
1.359
1.356
1.345
1.342
1.337
1.327
1.316
1.304
0.913
0.901
0.890
0.000
ZSY-B92a-H1
600 MHz, CDCl3
2022-05-02
9
8
7
6
5
4
3
2
1
0
ppm
2.93
3.01
2.00
2.00
4.03
2.99

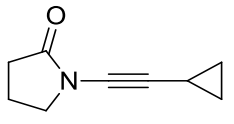

77.21
77.00
76.79
74.08
69.15
39.13
35.77
30.93
28.49
22.07
18.23
13.90
ZSY-B92a-C13
150 MHz, CDCl3
2022-05-02
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ts
N
Bn
3em
7.730
7.716
7.298
7.284
7.279
7.277
7.275
7.271
7.269
7.264
7.258
7.252
4.420
2.429
1.221
1.213
1.207
1.205
1.199
1.194
1.191
1.186
1.178
0.709
0.702
0.698
0.691
0.689
0.684
0.678
0.506
0.499
0.495
0.491
ZSY-B136a-H1
600 MHz, CDCl3
2022-07-13
9
8
7
6
5
4
3
2
1
0
ppm
2.00
7.17
2.07
3.10
0.99
2.04
2.04

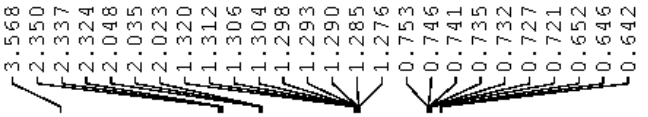

144.25
134.72
134.61
129.47
128.65
128.29
128.02
127.58
77.21
77.00
76.79
75.27
68.78
55.50
21.56
8.64
0.86
ZSY-B136a-C13
150 MHz, CDCl3
2022-07-13
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

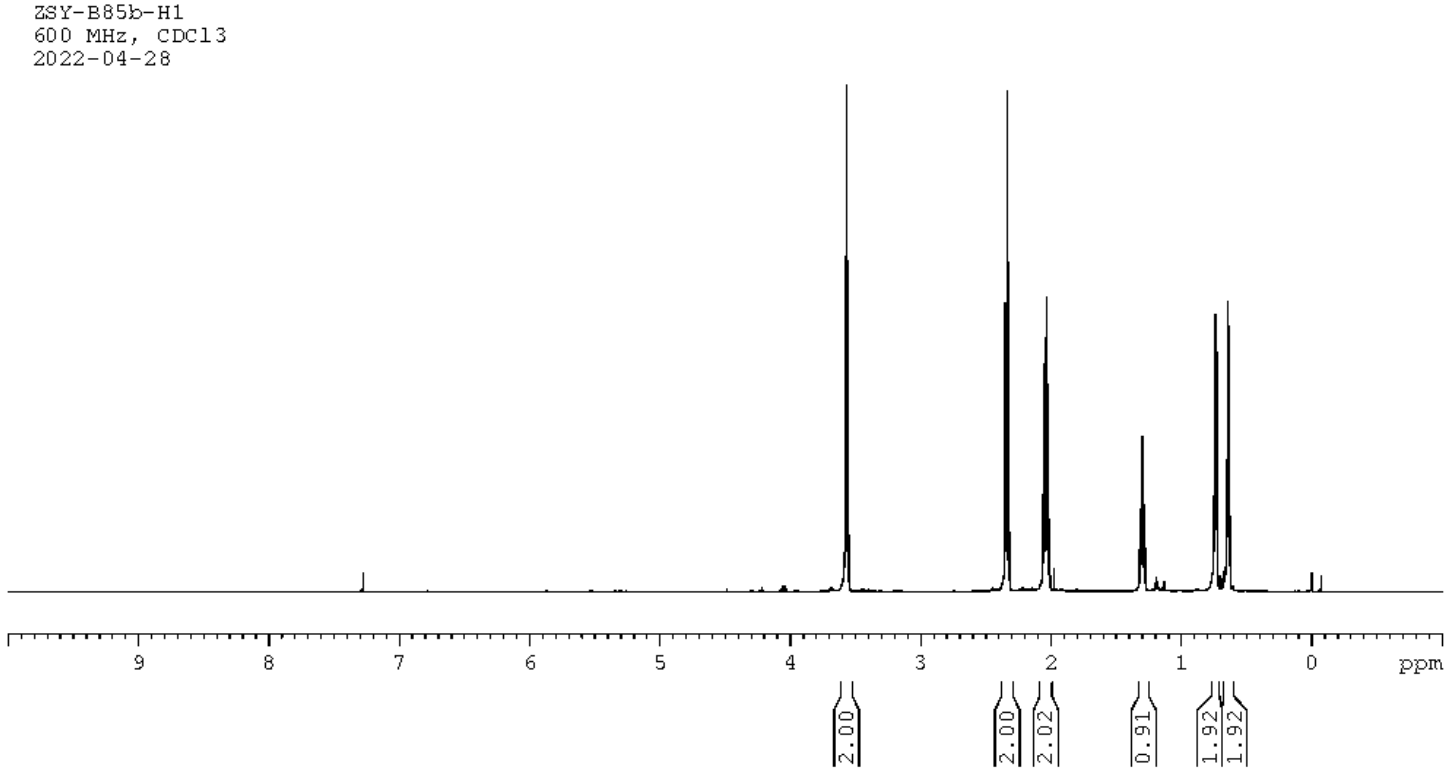

Ts
N
Ph
3fm
7.548
7.534
7.303
7.292
7.279
7.275
7.273
7.264
7.251
7.222
7.219
7.208
2.423
1.342
1.341
1.335
1.329
1.321
1.315
1.313
1.308
1.299
0.802
0.794
0.790
0.781
0.776
0.770
0.668
0.661
0.657
0.653
0.649
ZSY-B134-1-H1
600 MHz, CDCl3
2022-07-09
9
8
7
6
5
4
3
2
1
0
ppm
2.00
7.25
3.14
1.06
2.08
2.03

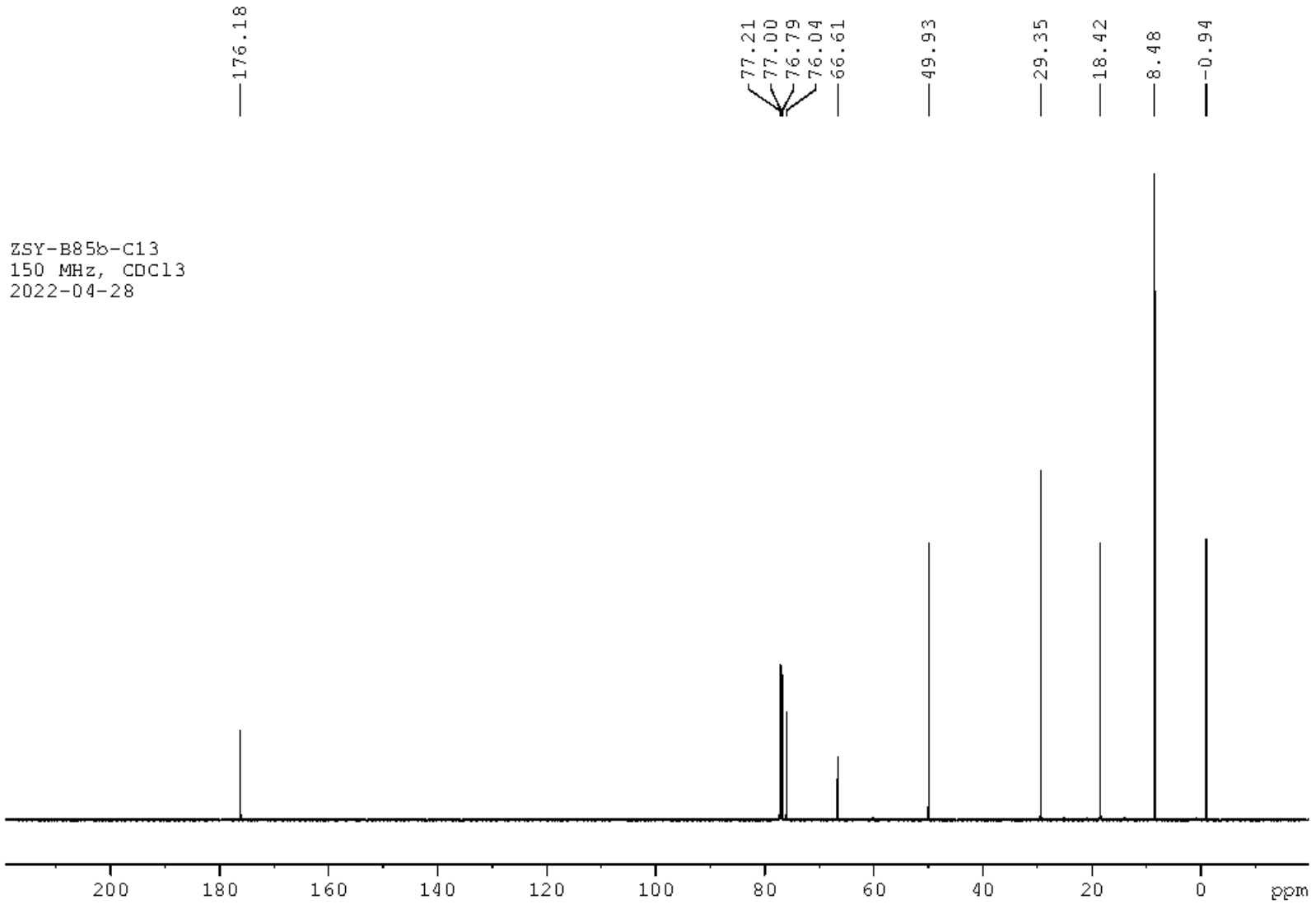

144.63
139.22
132.79
129.24
128.82
128.09
127.81
125.95
77.21
77.00
76.78
74.53
69.20
21.57
8.68
-0.81
ZSY-B134-1-C13
150 MHz, CDCl3
2022-07-09
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

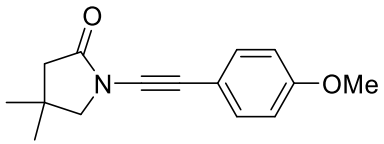

O
N

3hm

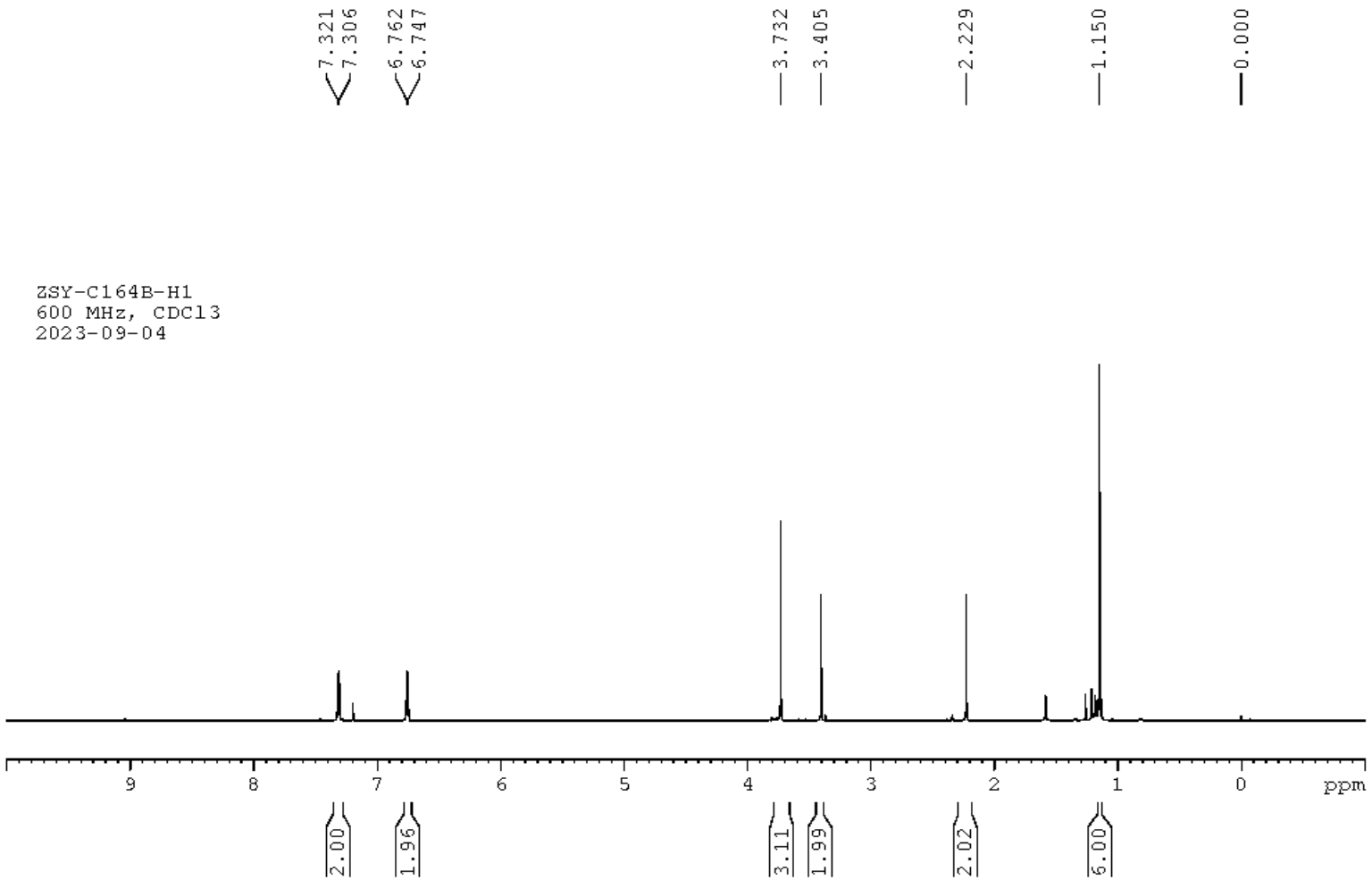

3.568
2.350
2.337
2.324
2.048
2.035
2.023
1.320
1.312
1.306
1.304
1.298
1.293
1.290
1.285
1.276
0.753
0.746
0.741
0.735
0.732
0.727
0.721
0.652
0.646
0.642

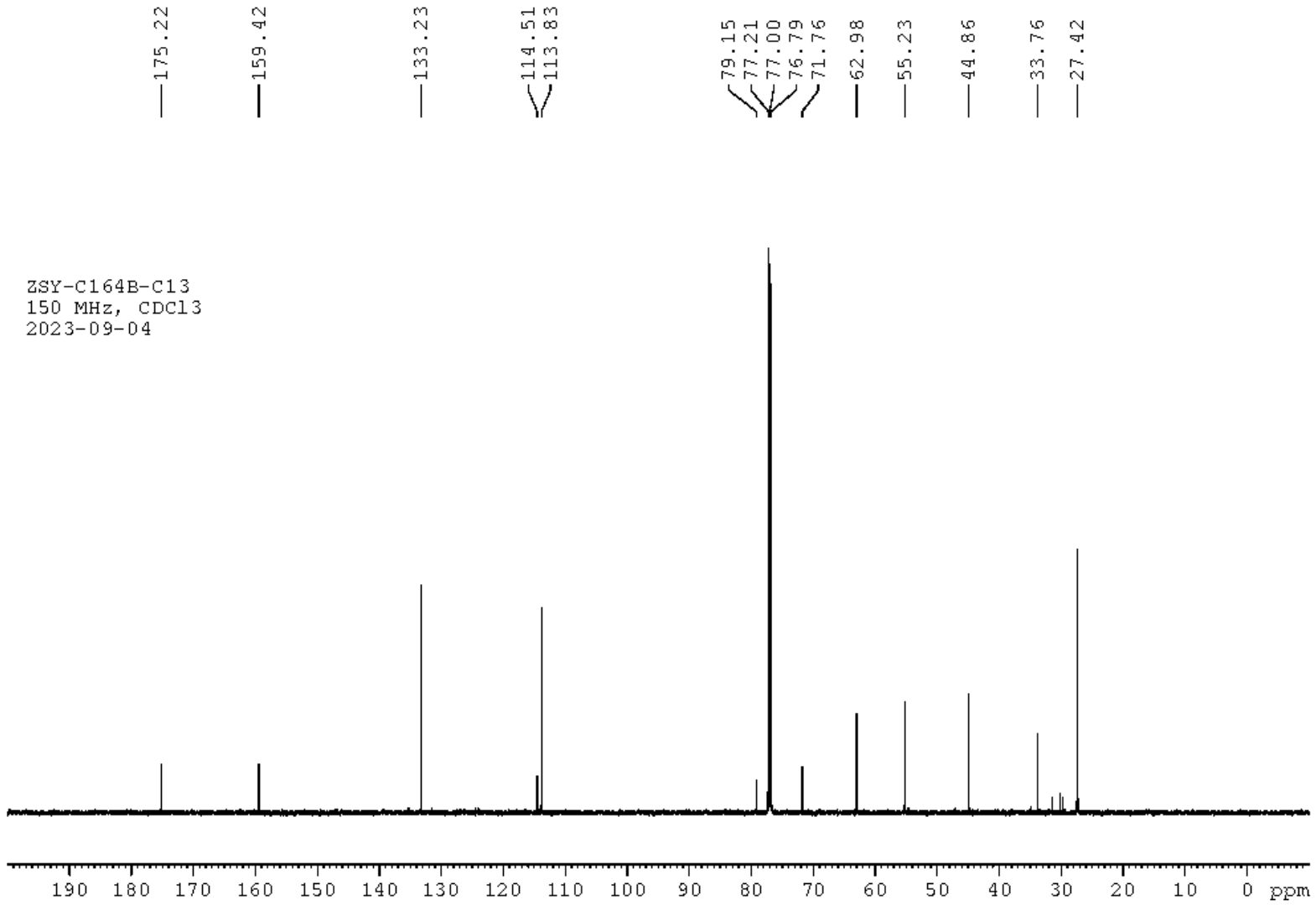

ZSY-B85b-H1
600 MHz, CDCl3
2022-04-28
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.00
2.02
0.91
1.92
1.92

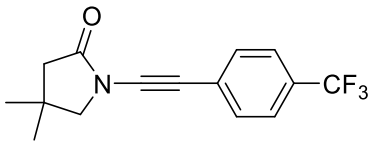

176.18
77.21
77.00
76.79
76.04
66.61
49.93
29.35
18.42
8.48
-0.94
ZSY-B85b-C13
150 MHz, CDCl3
2022-04-28
200
180
160
140
120
100
80
60
40
20
0
ppm


O
N
OMe

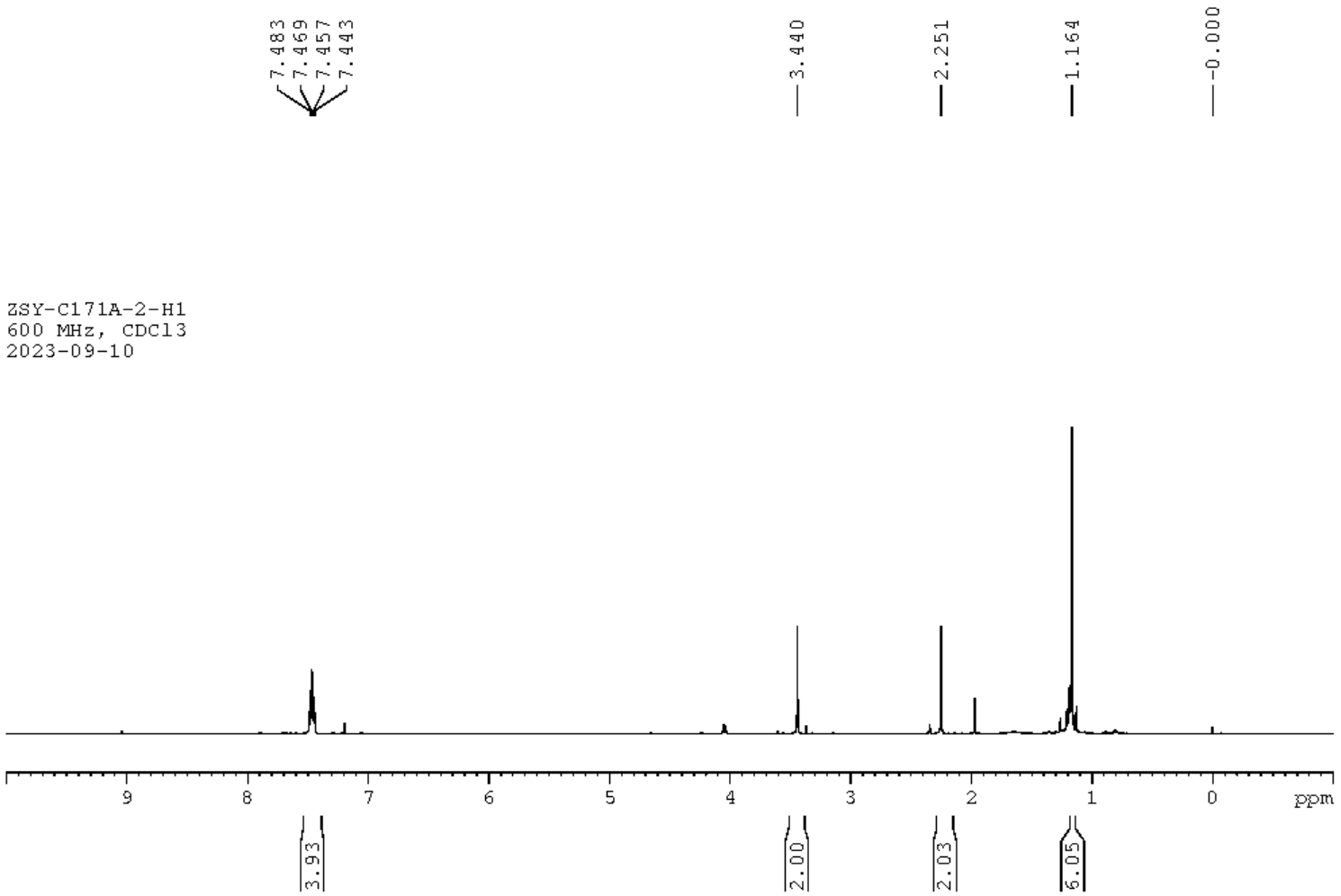
3ib

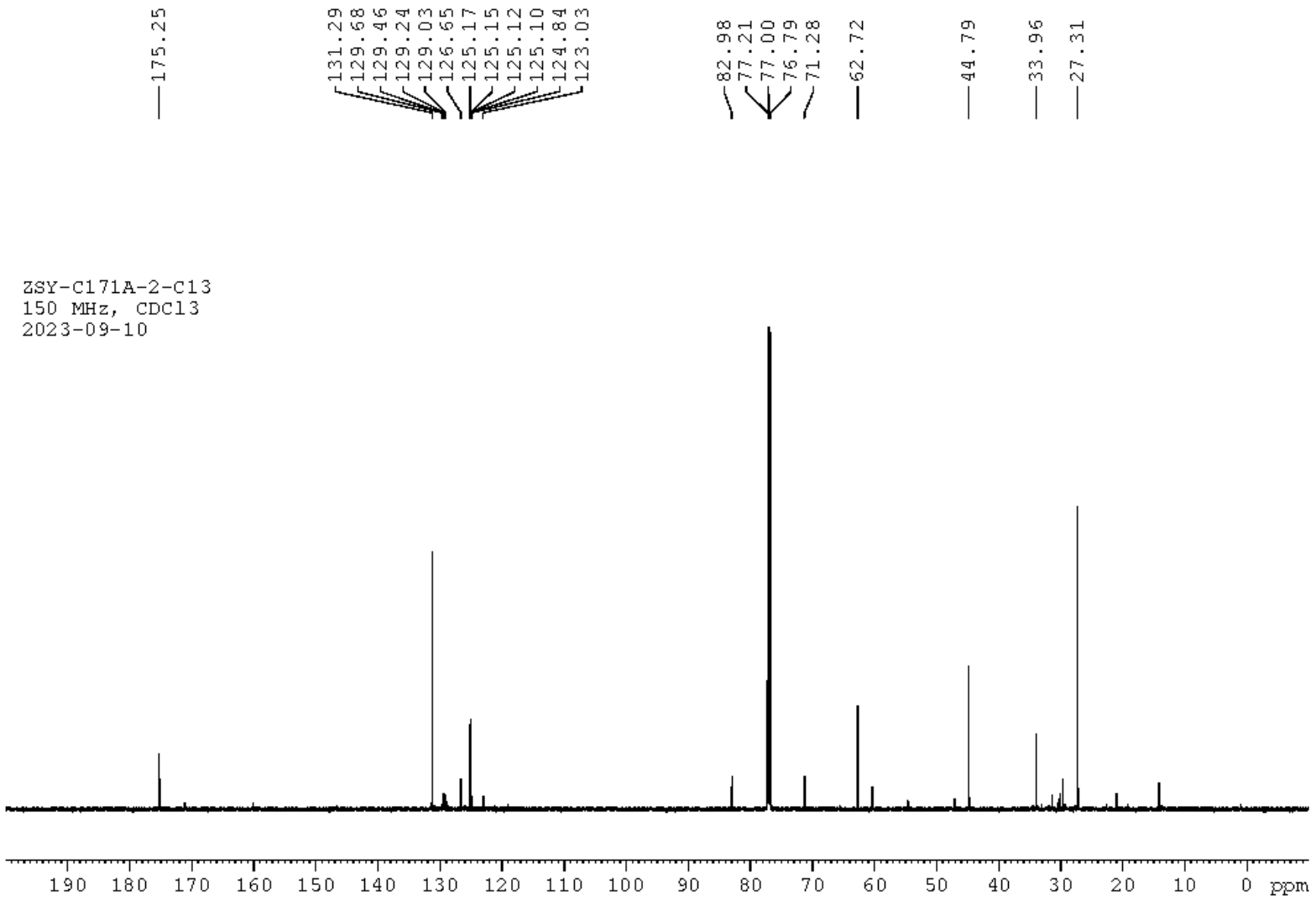

7.321
7.306
6.762
6.747
3.732
3.405
2.229
1.150
0.000
ZSY-C164B-H1
600 MHz, CDCl3
2023-09-04
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.96
3.11
1.99
2.02
6.00

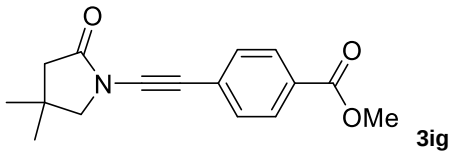

175.22
159.42
133.23
114.51
113.83
79.15
77.21
77.00
76.79
71.76
62.98
55.23
44.86
33.76
27.42
ZSY-C164B-C13
150 MHz, CDCl3
2023-09-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
CF3

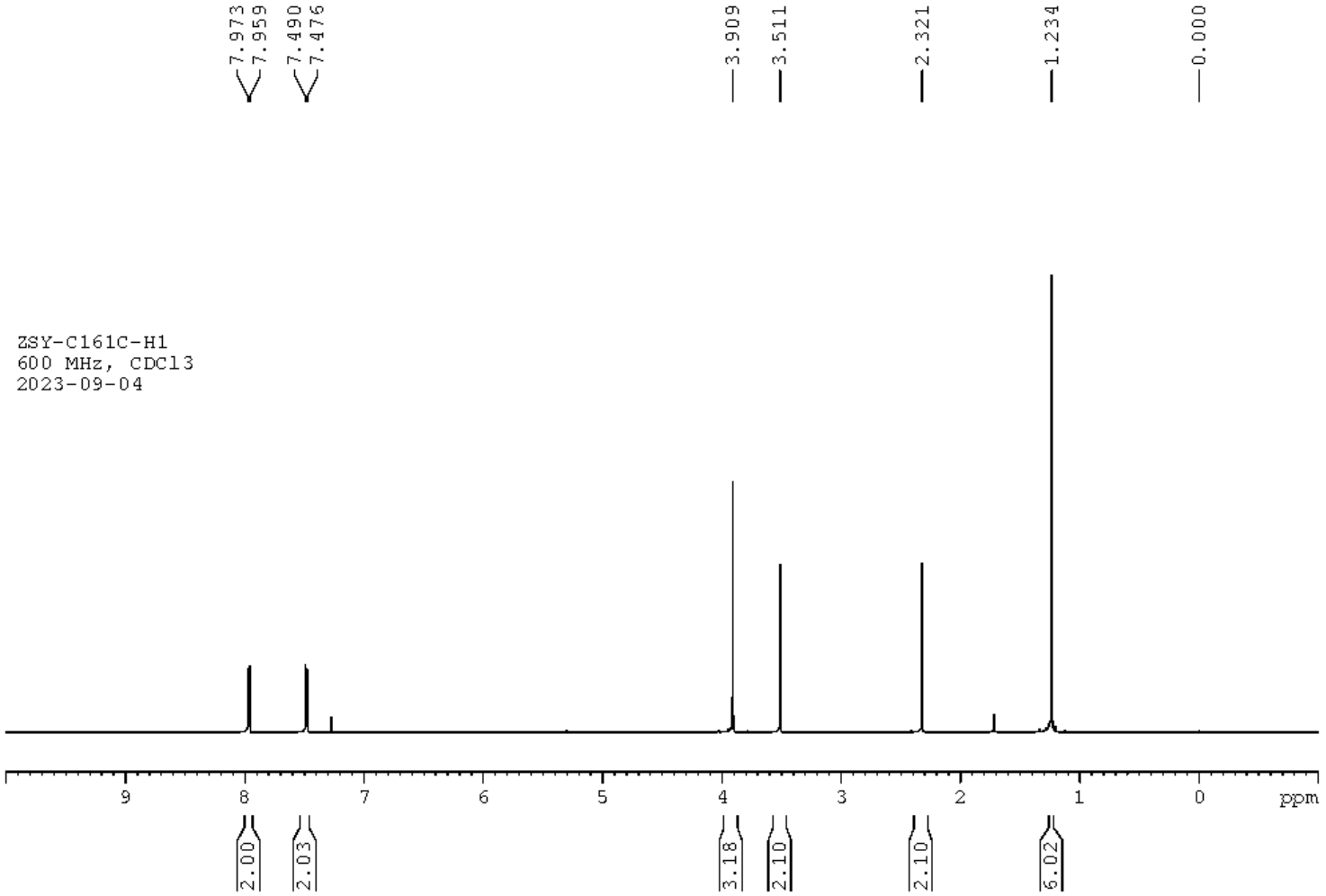
3ic

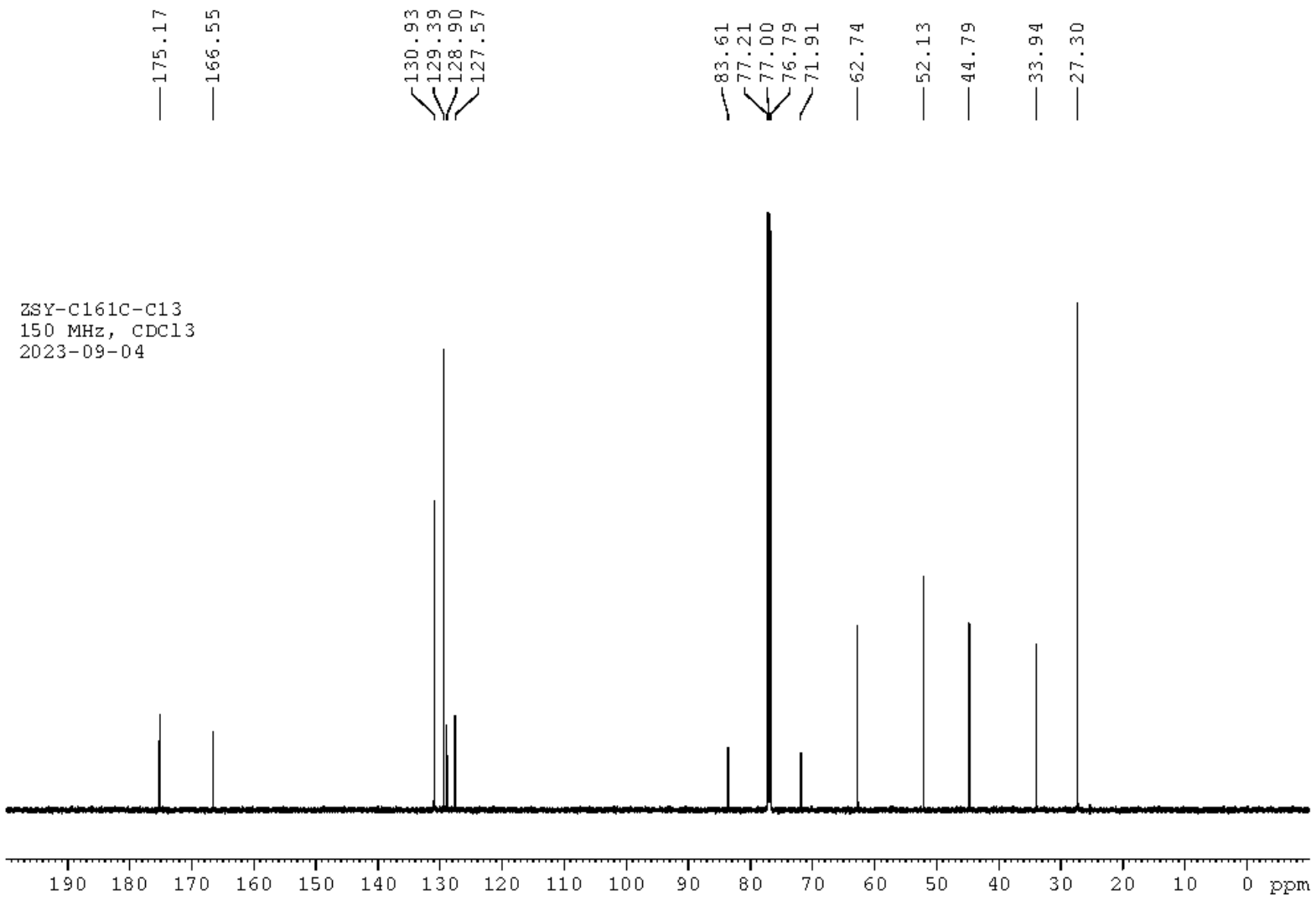

7.483
7.469
7.457
7.443
3.440
2.251
1.164
0.000
ZSY-C171A-2-H1
600 MHz, CDCl3
2023-09-10
9
8
7
6
5
4
3
2
1
0
ppm
3.93
2.00
2.03
6.05

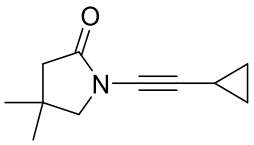

175.25
131.29
129.68
129.46
129.24
129.03
126.65
125.17
125.15
125.12
125.10
124.84
123.03
82.98
77.21
77.00
76.79
71.28
62.72
44.79
33.96
27.31
ZSY-C171A-2-C13
150 MHz, CDCl3
2023-09-10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
N
O
OMe

3ig

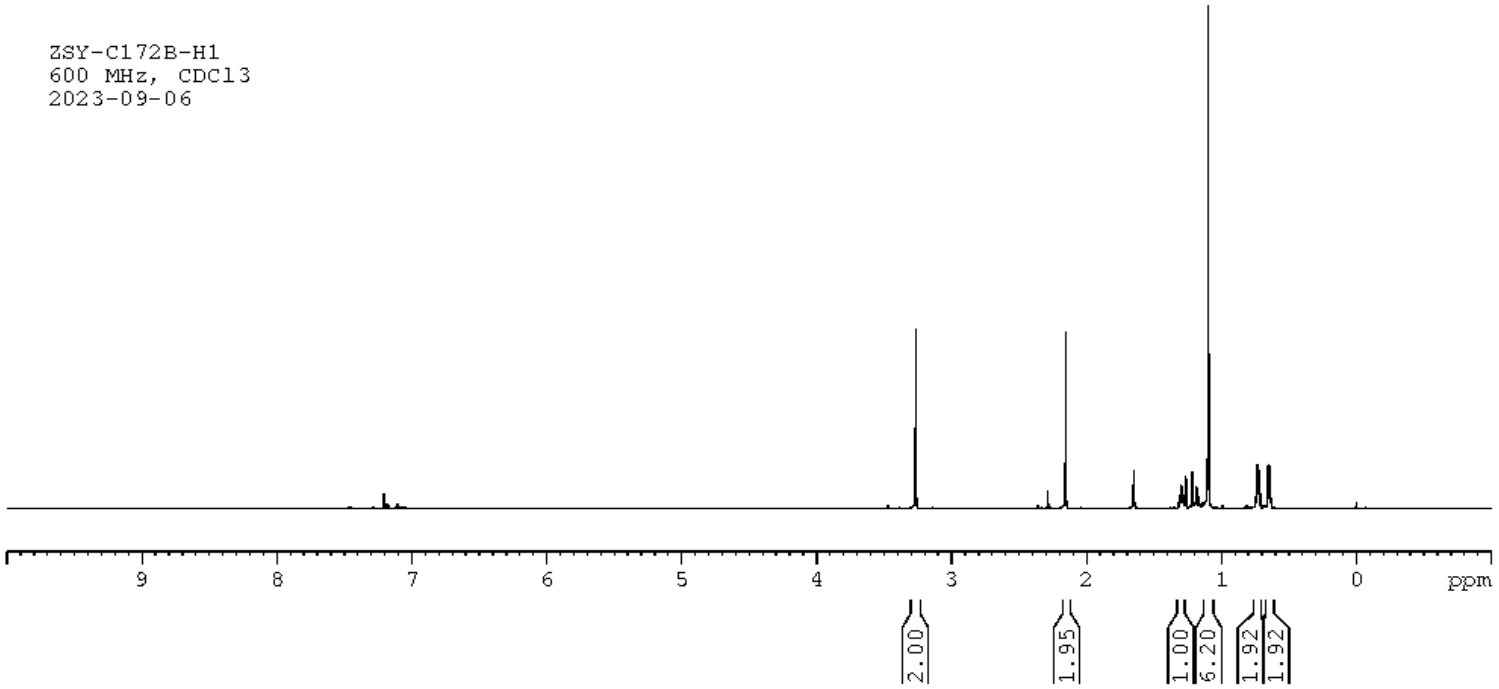

7.973
7.959
7.490
7.476
3.909
3.511
2.321
1.234
0.000
ZSY-C161C-H1
600 MHz, CDCl3
2023-09-04
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.03
3.18
2.10
2.10
6.02

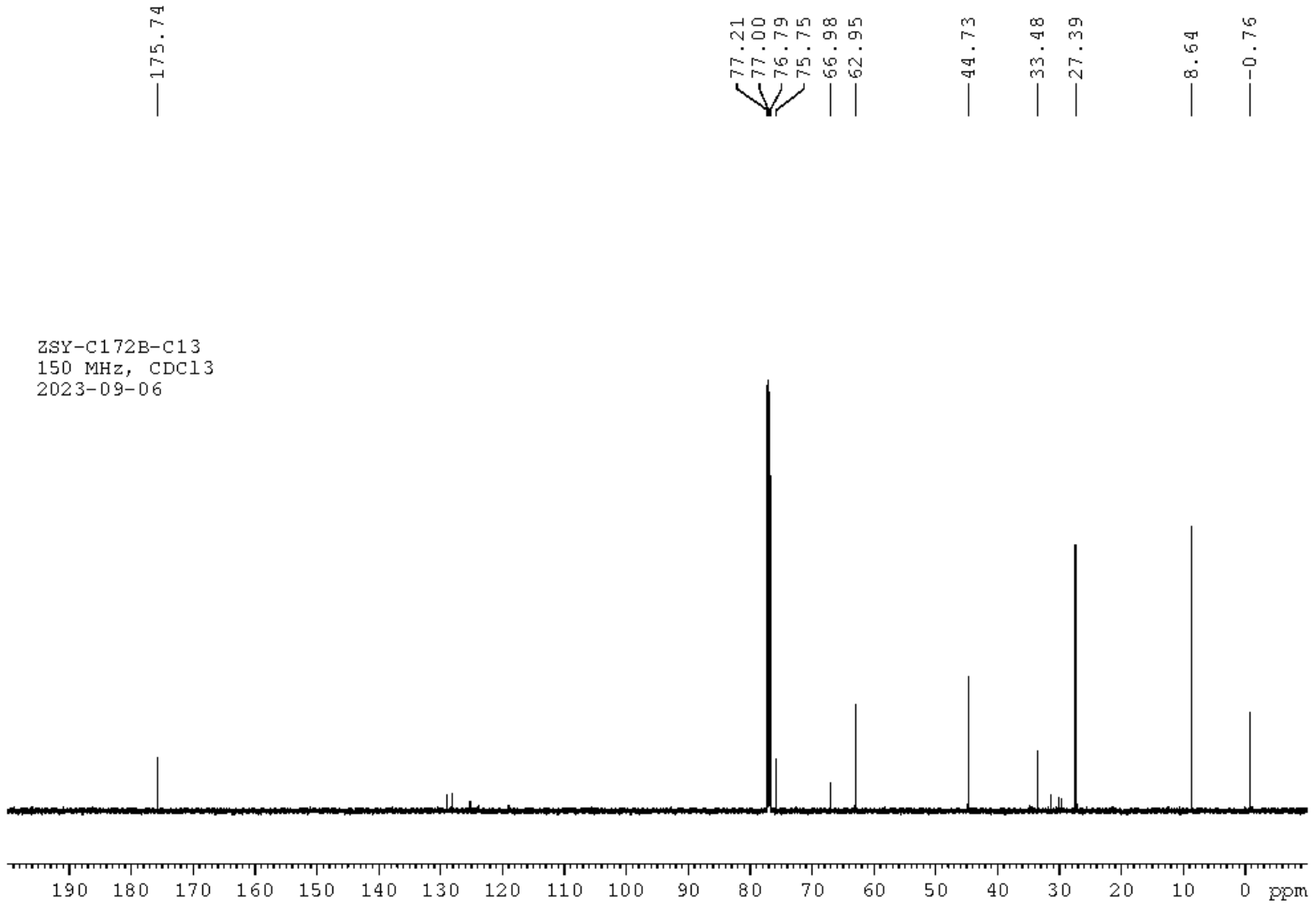

175.17
166.55
130.93
129.39
128.90
127.57
83.61
77.21
77.00
76.79
71.91
62.74
52.13
44.79
33.94
27.30
ZSY-C161C-C13
150 MHz, CDCl3
2023-09-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

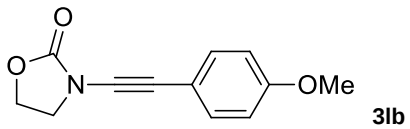


3im

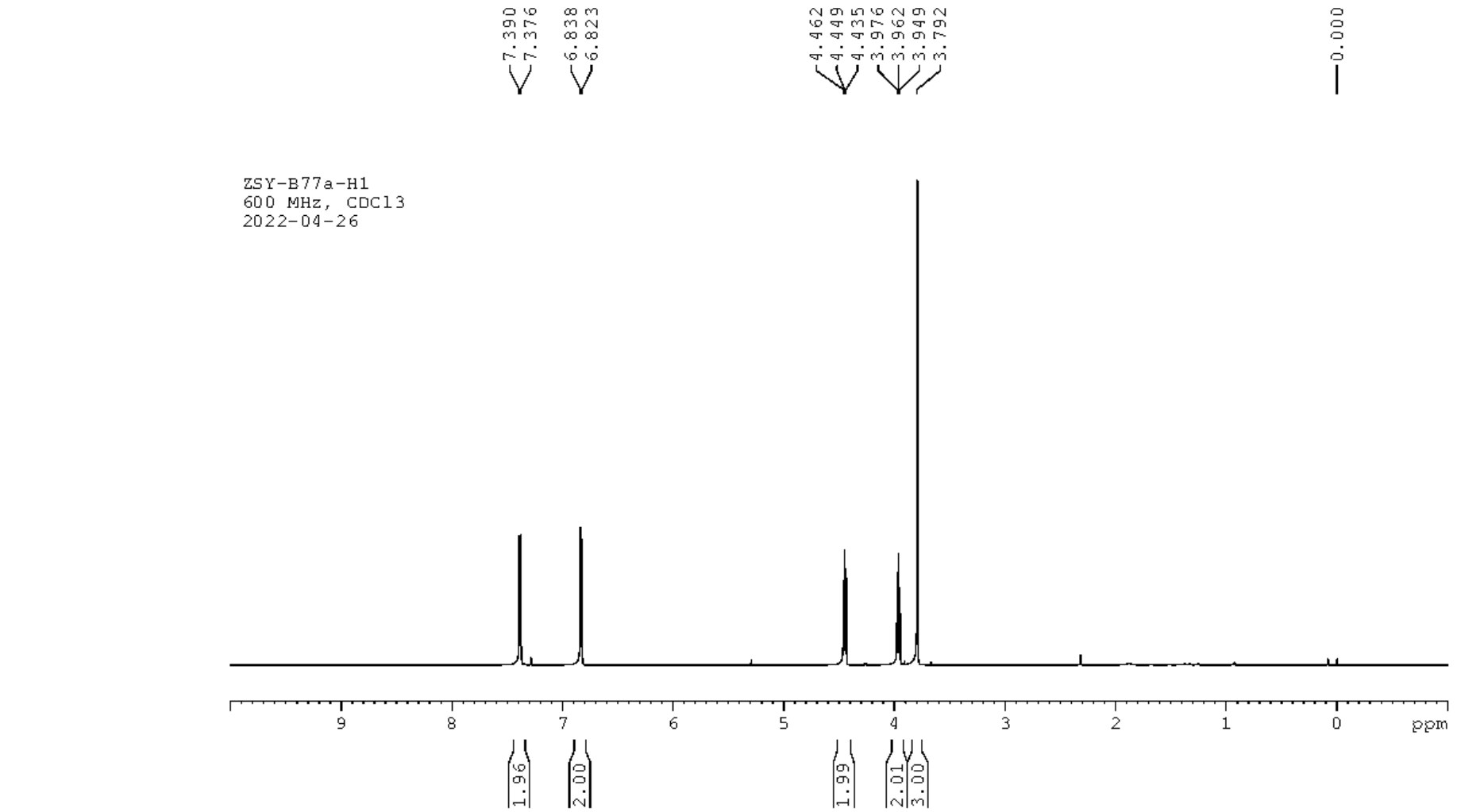

3.265
2.154
1.317
1.309
1.303
1.295
1.287
1.282
1.273
1.263
1.096
0.745
0.737
0.733
0.724
0.720
0.713
0.658
0.652
0.648
0.644
0.640

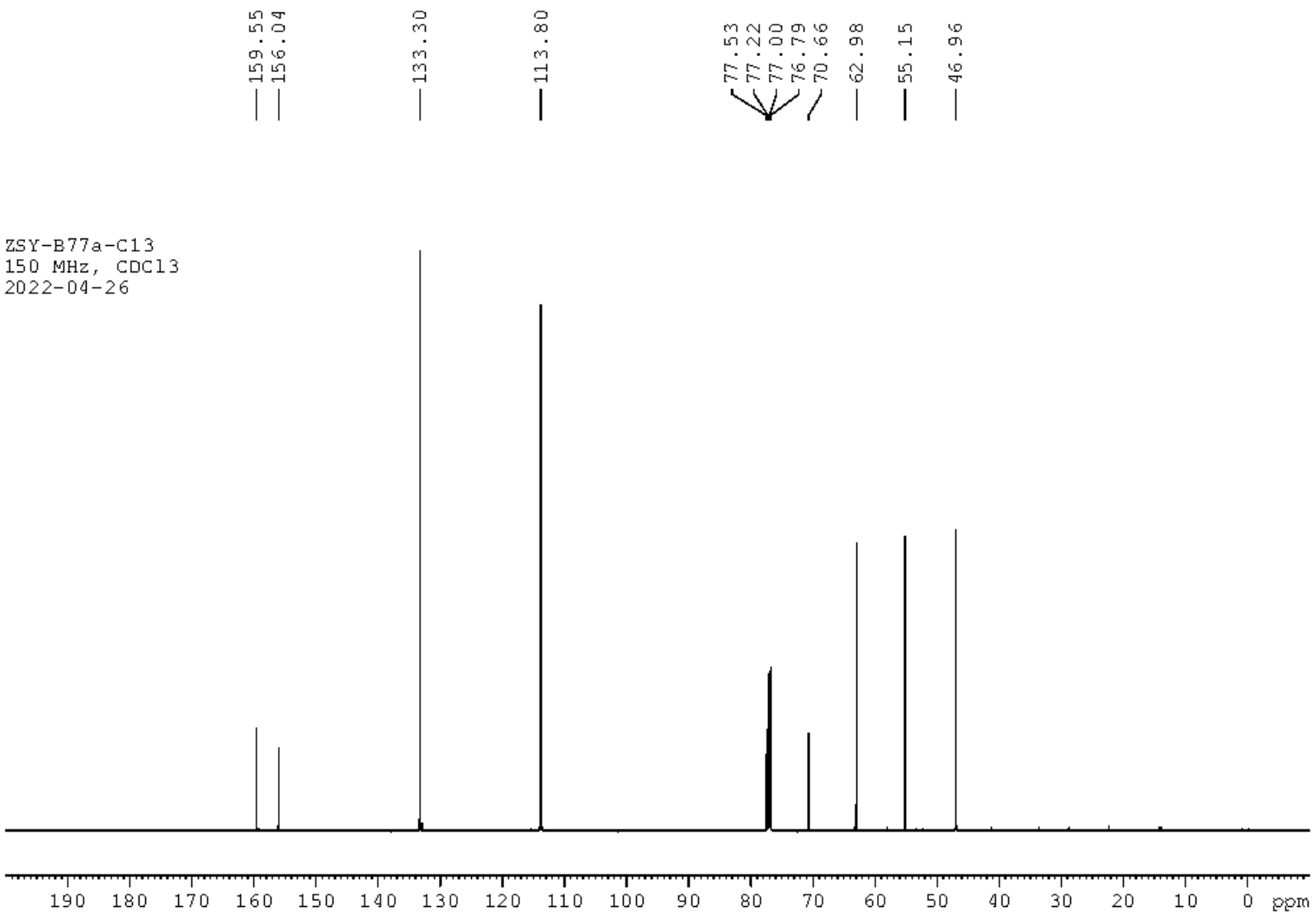

ZSY-C172B-H1
600 MHz, CDCl3
2023-09-06
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.95
1.00
6.20
1.92
1.92

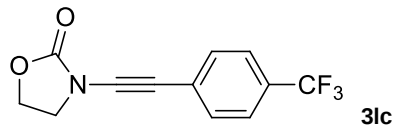

175.74
77.21
77.00
76.79
75.75
66.98
62.95
44.73
33.48
27.39
8.64
-0.76
ZSY-C172B-C13
150 MHz, CDCl3
2023-09-06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
OMe

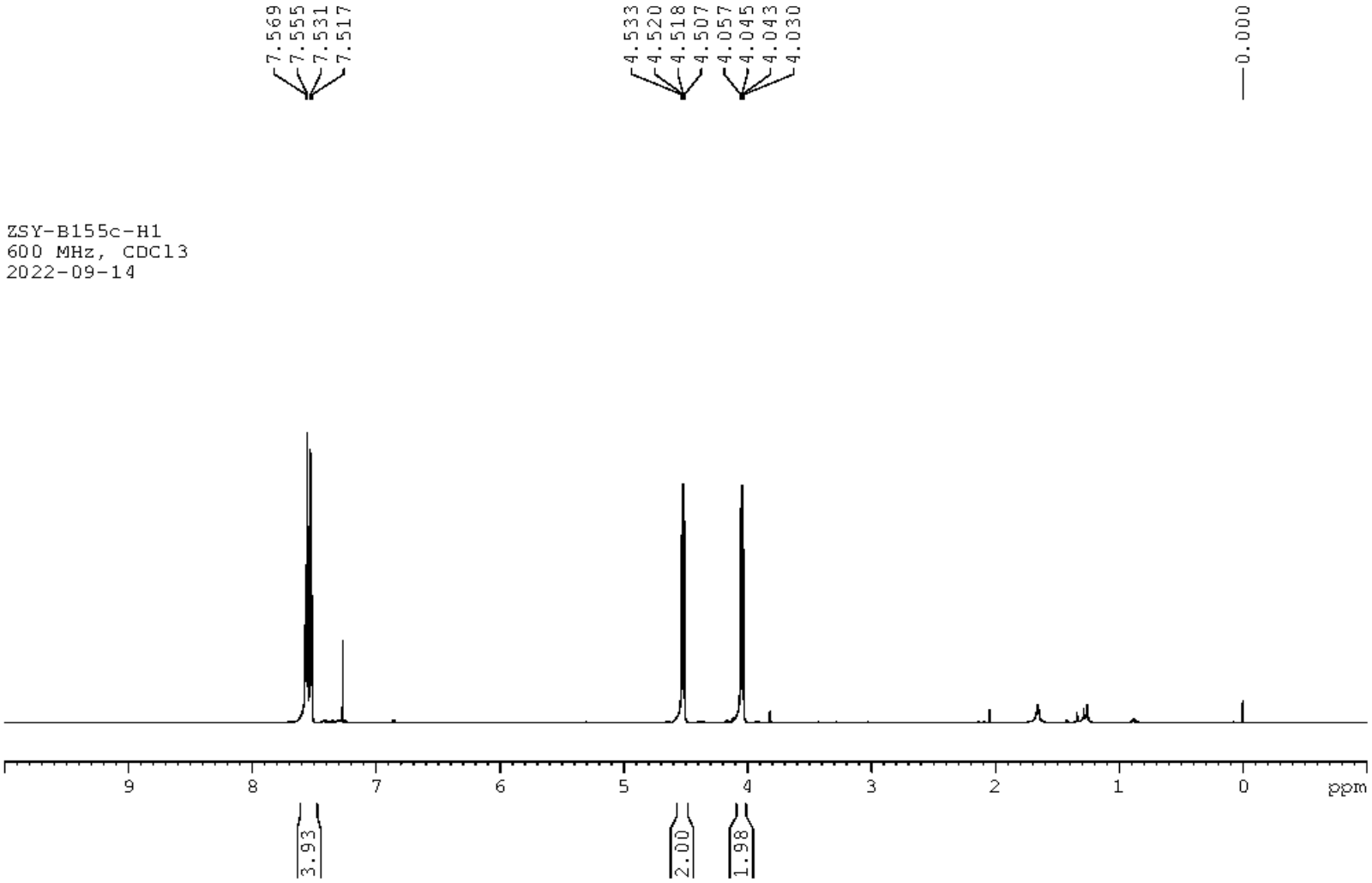
3lb

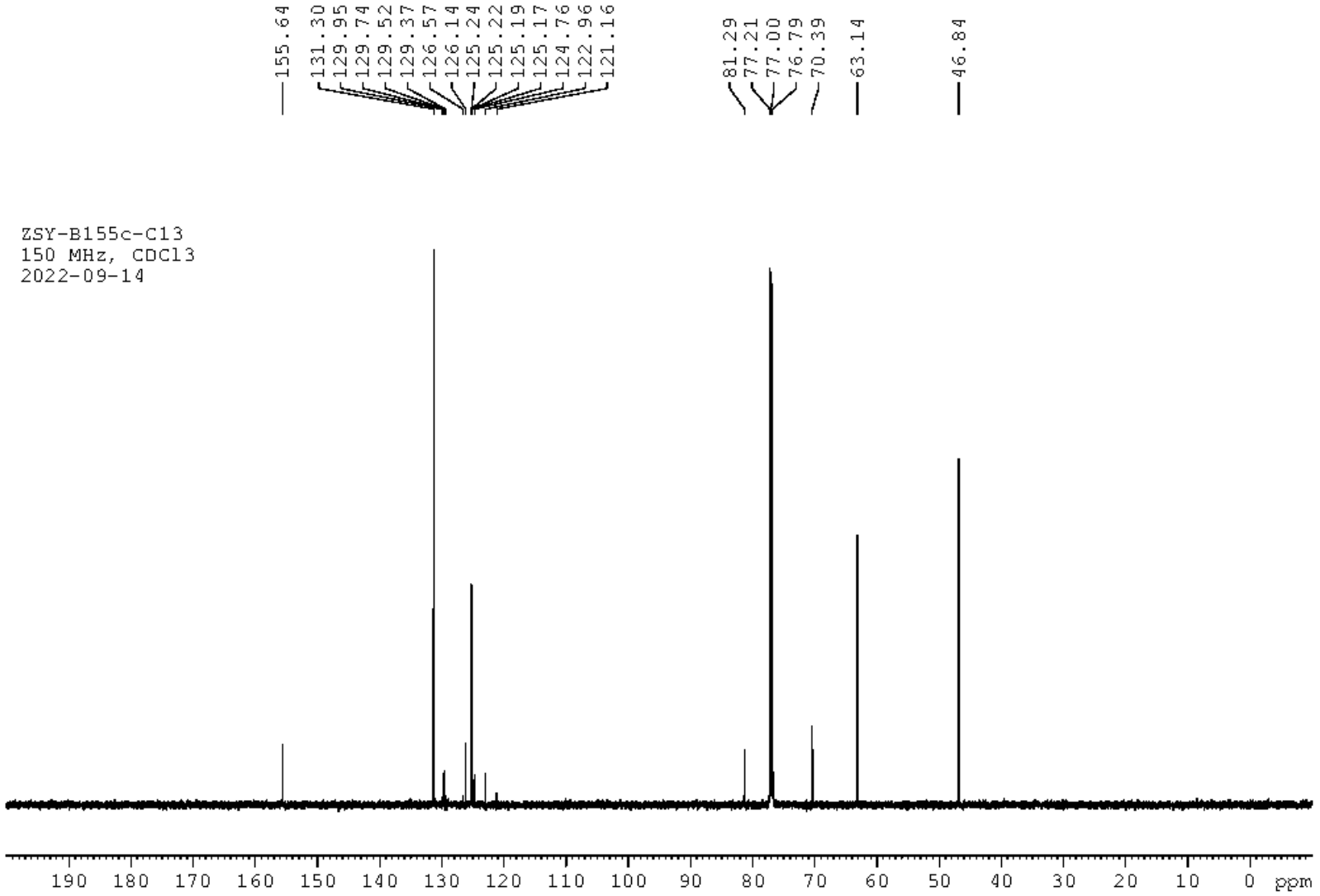

7.390
7.376
6.838
6.823
4.462
4.449
4.435
3.976
3.962
3.949
3.792
0.000
ZSY-B77a-H1
600 MHz, CDCl3
2022-04-26
9
8
7
6
5
4
3
2
1
0
ppm
1.96
2.00
1.99
2.01
3.00

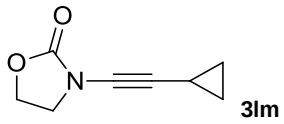

159.55
156.04
133.30
113.80
77.53
77.22
77.00
76.79
70.66
62.98
55.15
46.96
ZSY-B77a-C13
150 MHz, CDCl3
2022-04-26
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
CF3

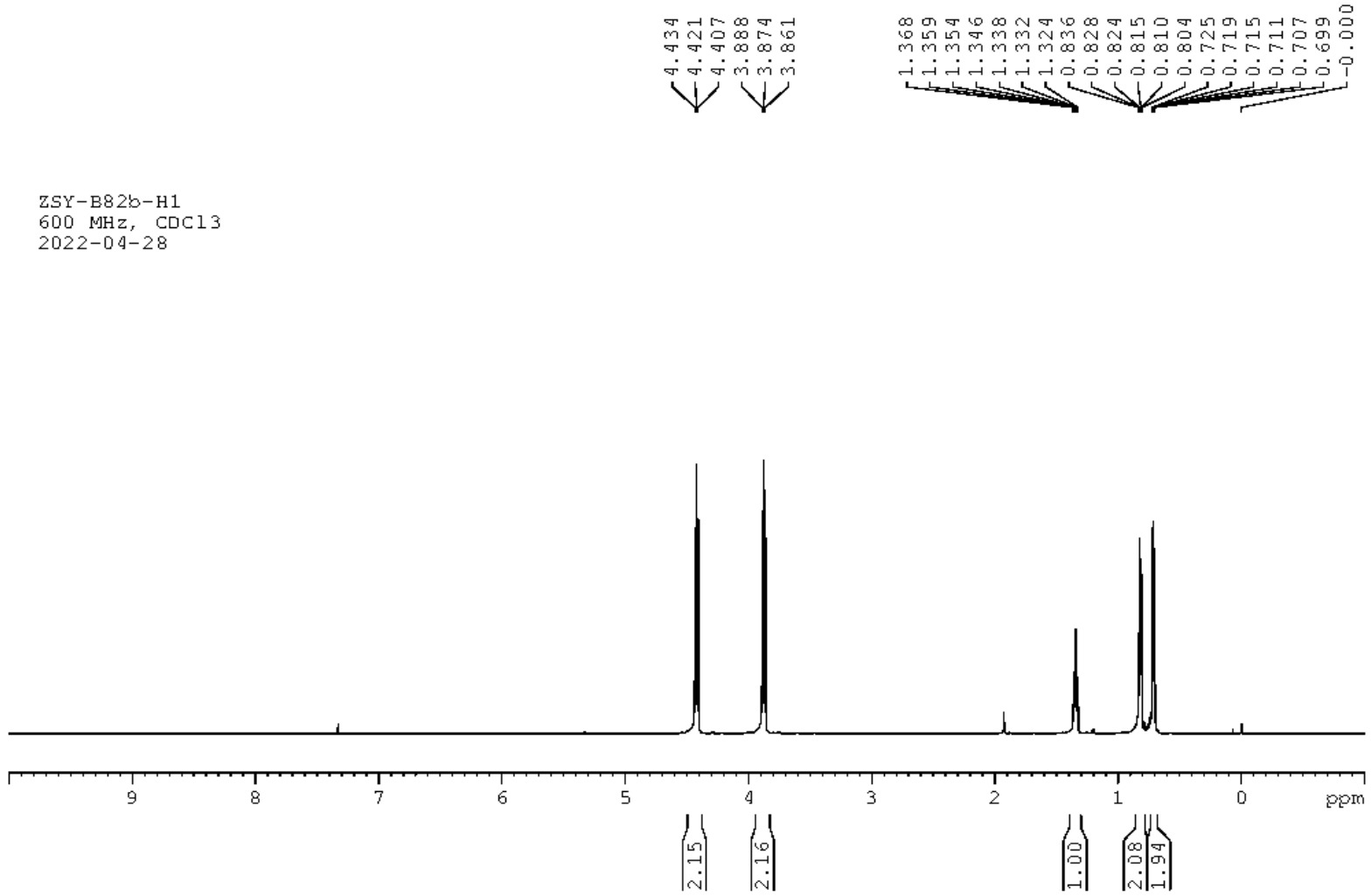
3lc

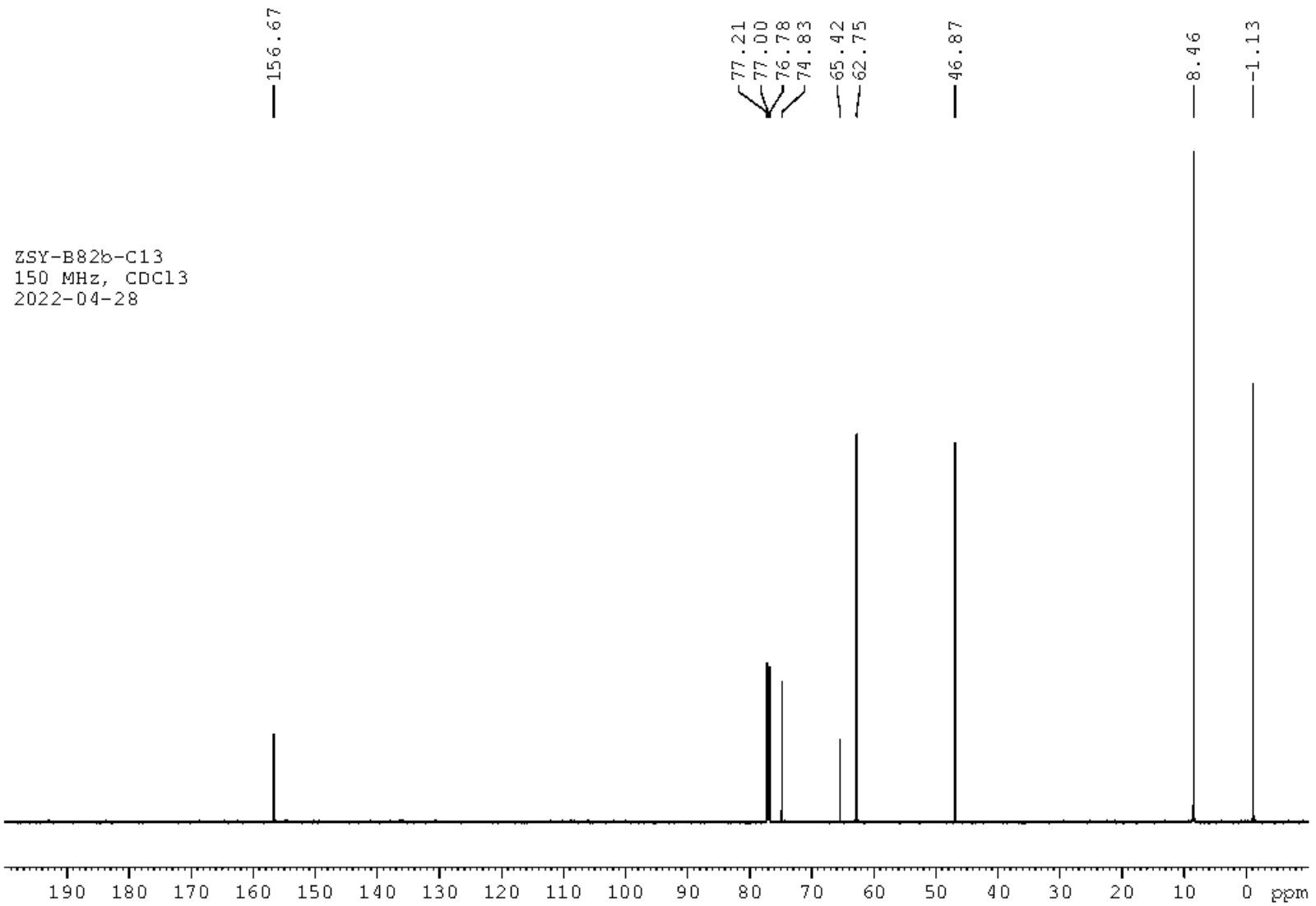

7.569
7.555
7.531
7.517
4.533
4.520
4.518
4.507
4.057
4.045
4.043
4.030
0.000
ZSY-B155c-H1
600 MHz, CDCl3
2022-09-14
9
8
7
6
5
4
3
2
1
0
ppm
3.93
2.00
1.98

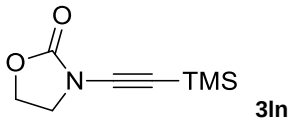

155.64
131.30
129.95
129.74
129.52
129.37
126.57
126.14
125.24
125.22
125.19
125.17
124.76
122.96
121.16
81.29
77.21
77.00
76.79
70.39
63.14
46.84
ZSY-B155c-C13
150 MHz, CDCl3
2022-09-14
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N

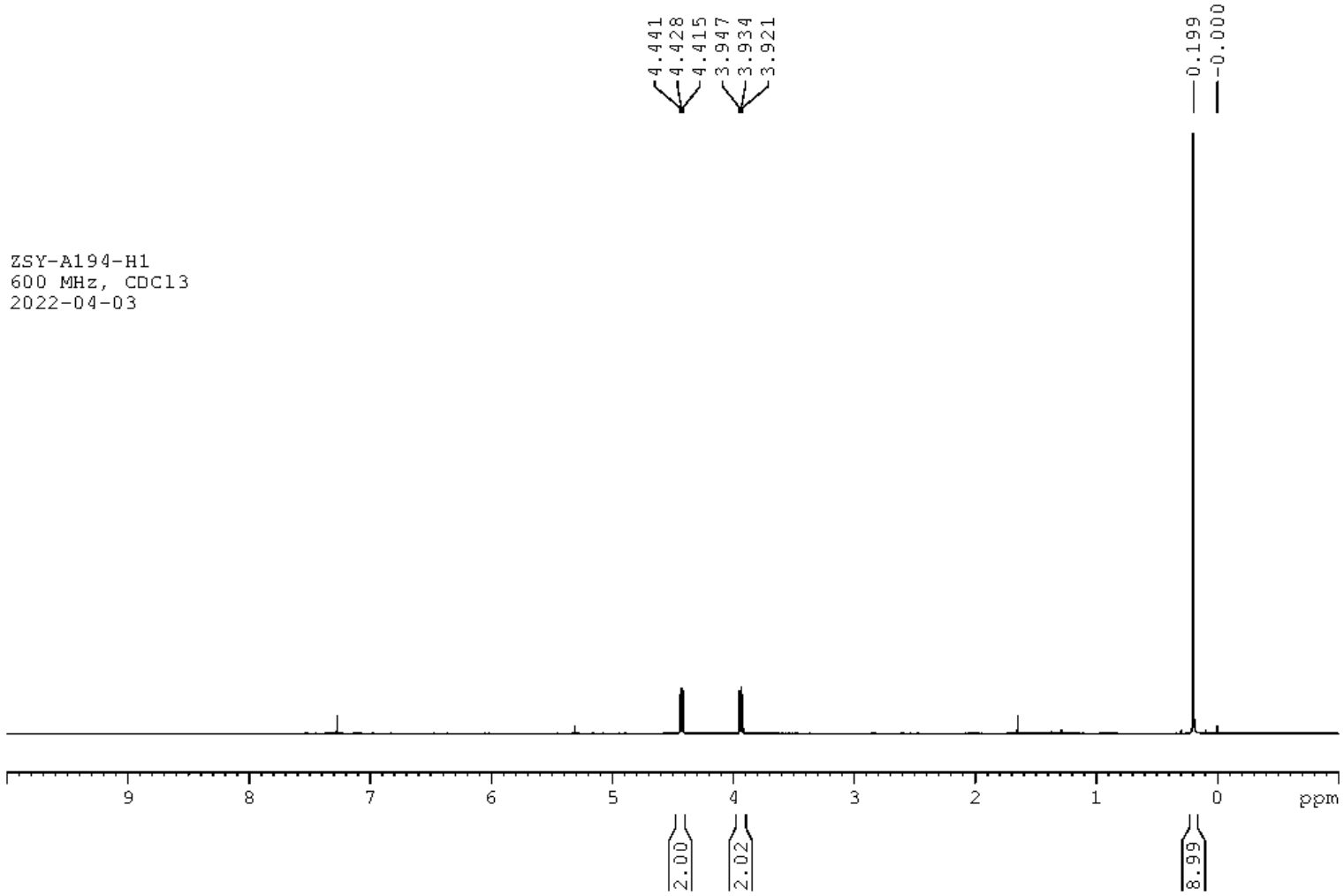
3lm

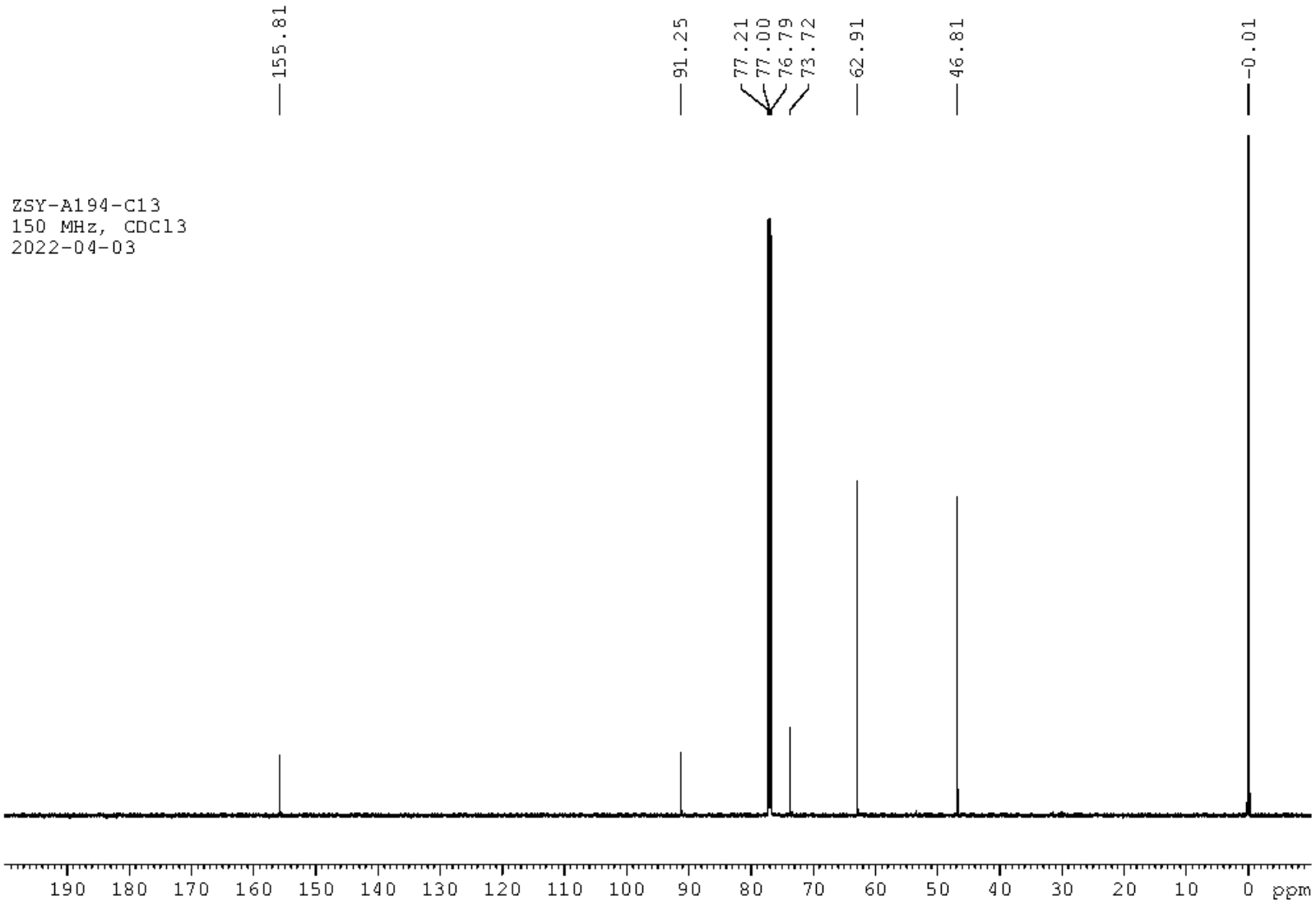

4.434
4.421
4.407
3.888
3.874
3.861
1.368
1.359
1.354
1.346
1.338
1.332
1.324
0.836
0.828
0.824
0.815
0.810
0.804
0.725
0.719
0.715
0.711
0.707
0.699
-0.000
ZSY-B82b-H1
600 MHz, CDCl3
2022-04-28
9
8
7
6
5
4
3
2
1
0
ppm
2.15
2.16
1.00
2.08
1.94

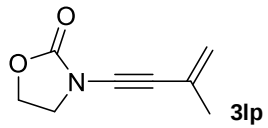

156.67
77.21
77.00
76.78
74.83
65.42
62.75
46.87
8.46
-1.13
ZSY-B82b-C13
150 MHz, CDCl3
2022-04-28
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
TMS

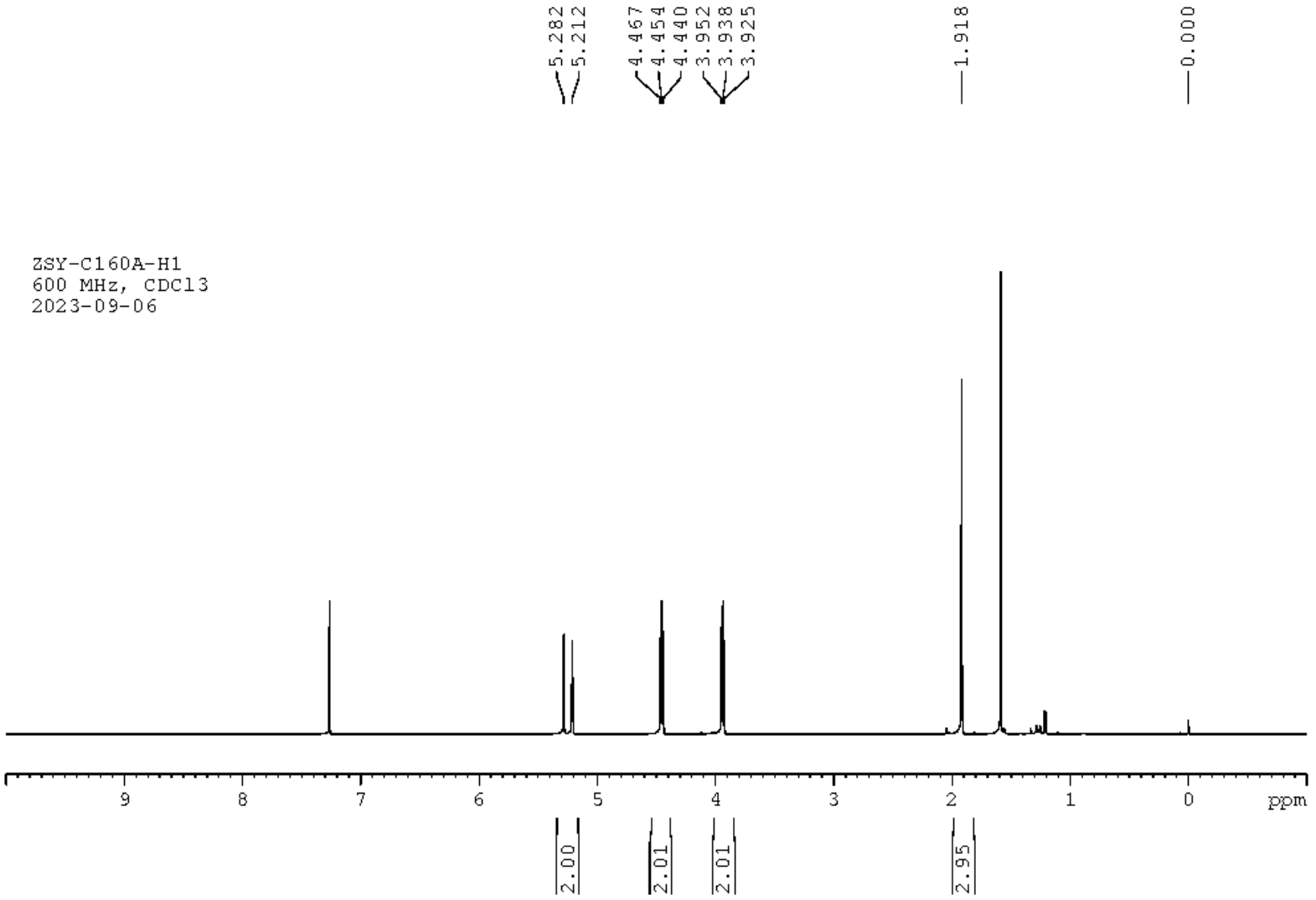
3ln

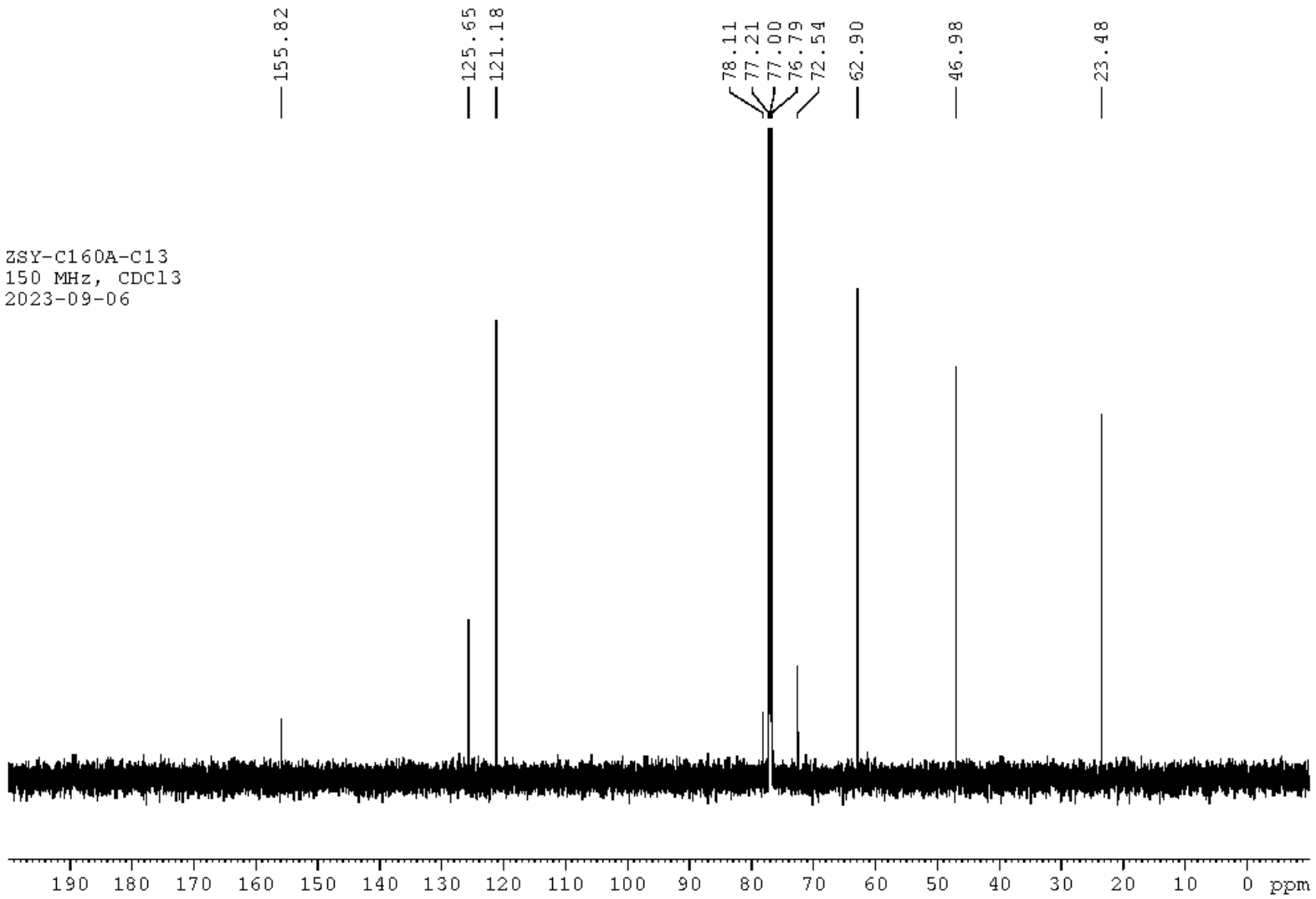

4.441
4.428
4.415
3.947
3.934
3.921
0.199
-0.000
ZSY-A194-H1
600 MHz, CDCl3
2022-04-03
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02
8.99

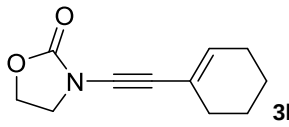

155.81
91.25
77.21
77.00
76.79
73.72
62.91
46.81
-0.01
ZSY-A194-C13
150 MHz, CDCl3
2022-04-03
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N

3lp


5.282
5.212
4.467
4.454
4.440
3.952
3.938
3.925
1.918
0.000
ZSY-C160A-H1
600 MHz, CDCl3
2023-09-06
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
2.01
2.95

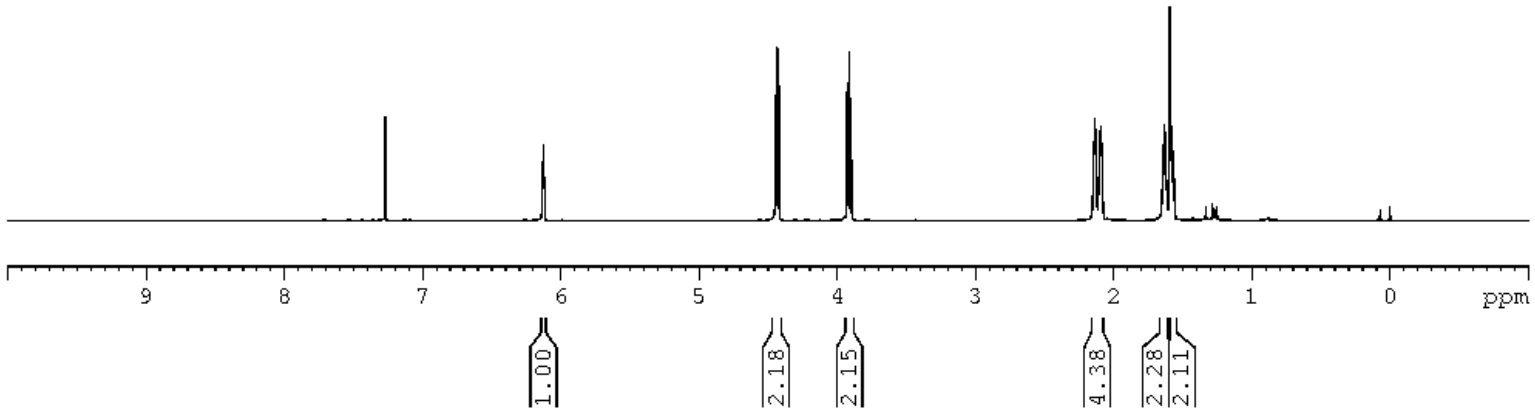

155.82
125.65
121.18
78.11
77.21
77.00
76.79
72.54
62.90
46.98
23.48
ZSY-C160A-C13
150 MHz, CDCl3
2023-09-06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

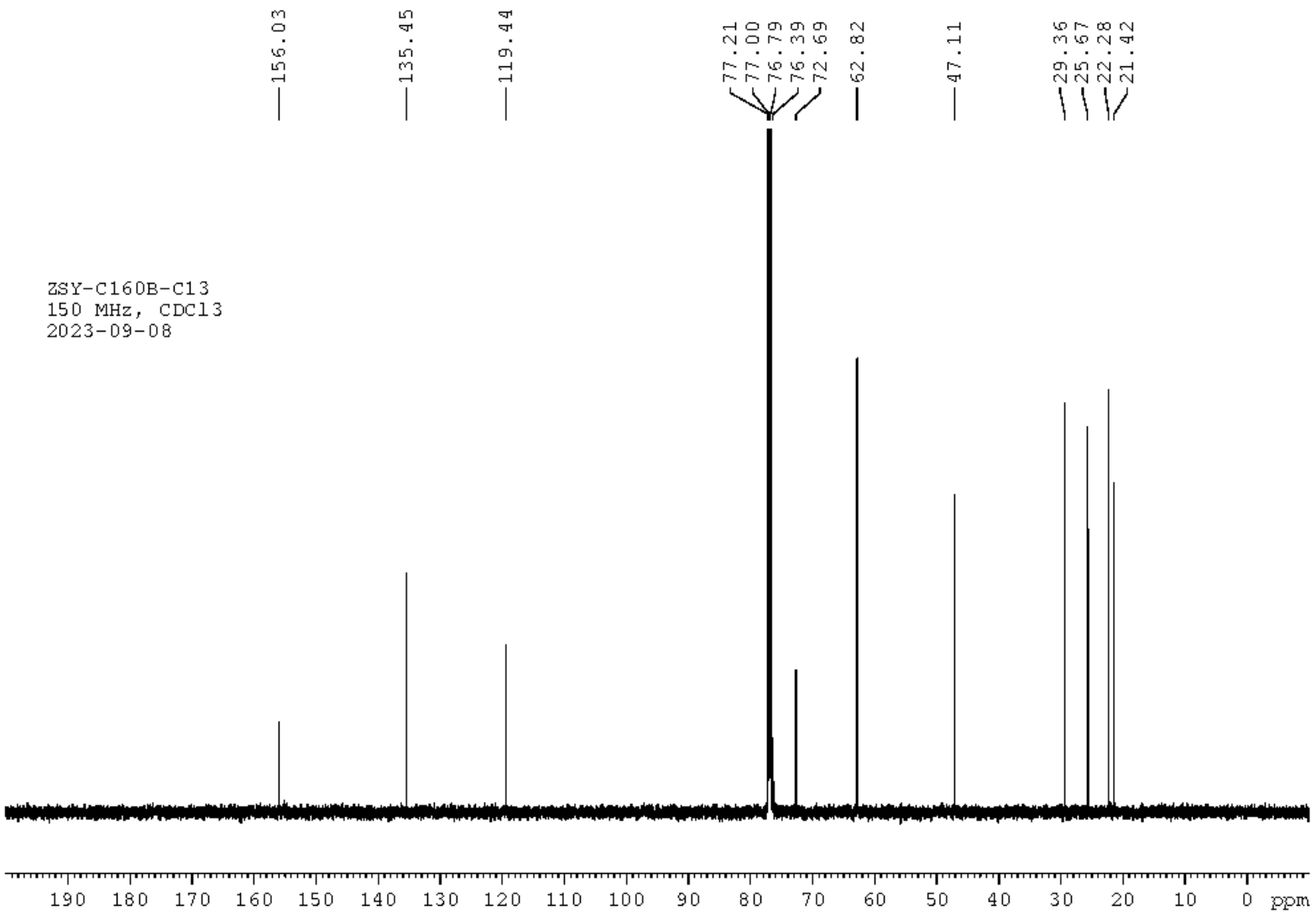


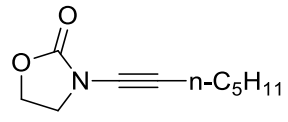
3lq

6.132
6.129
6.126
6.123
6.119
4.448
4.435
4.421
3.927
3.913
3.900
2.148
2.138
2.134
2.124
2.106
2.100
2.096
2.090
2.085
2.080
1.655
1.645
1.639
1.636
1.630
1.627
1.619
1.616
1.586
1.583
1.576
1.573
1.567
1.558
0.000

ZSY-C160B-H1
600 MHz, CDCl3
2023-09-08

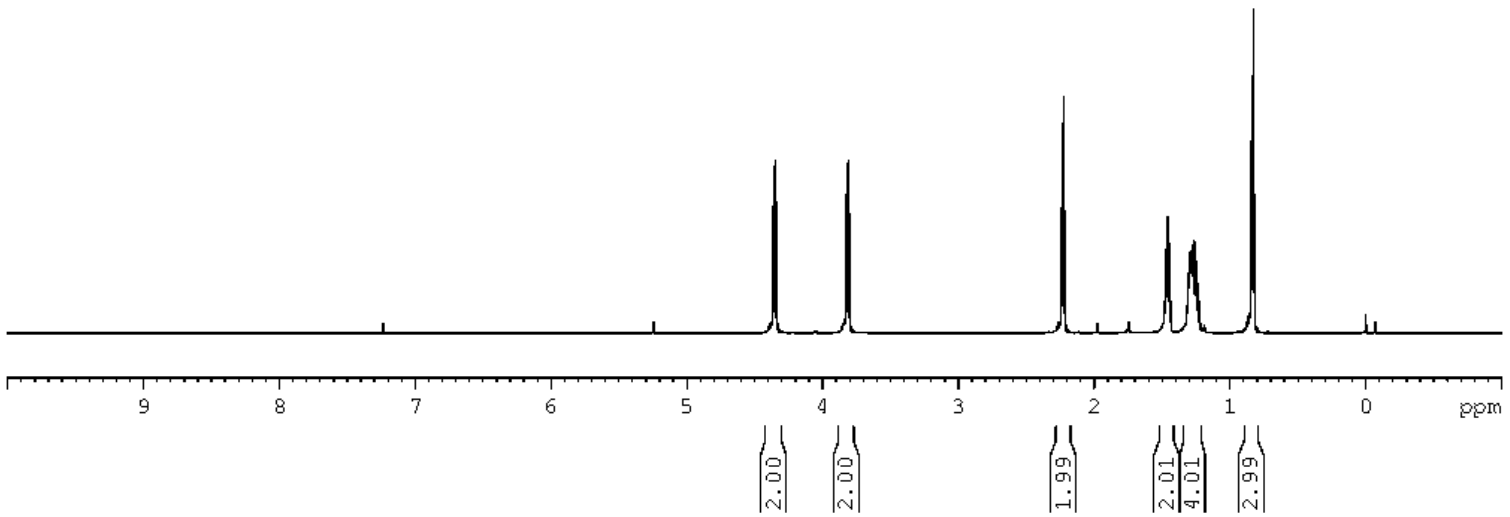


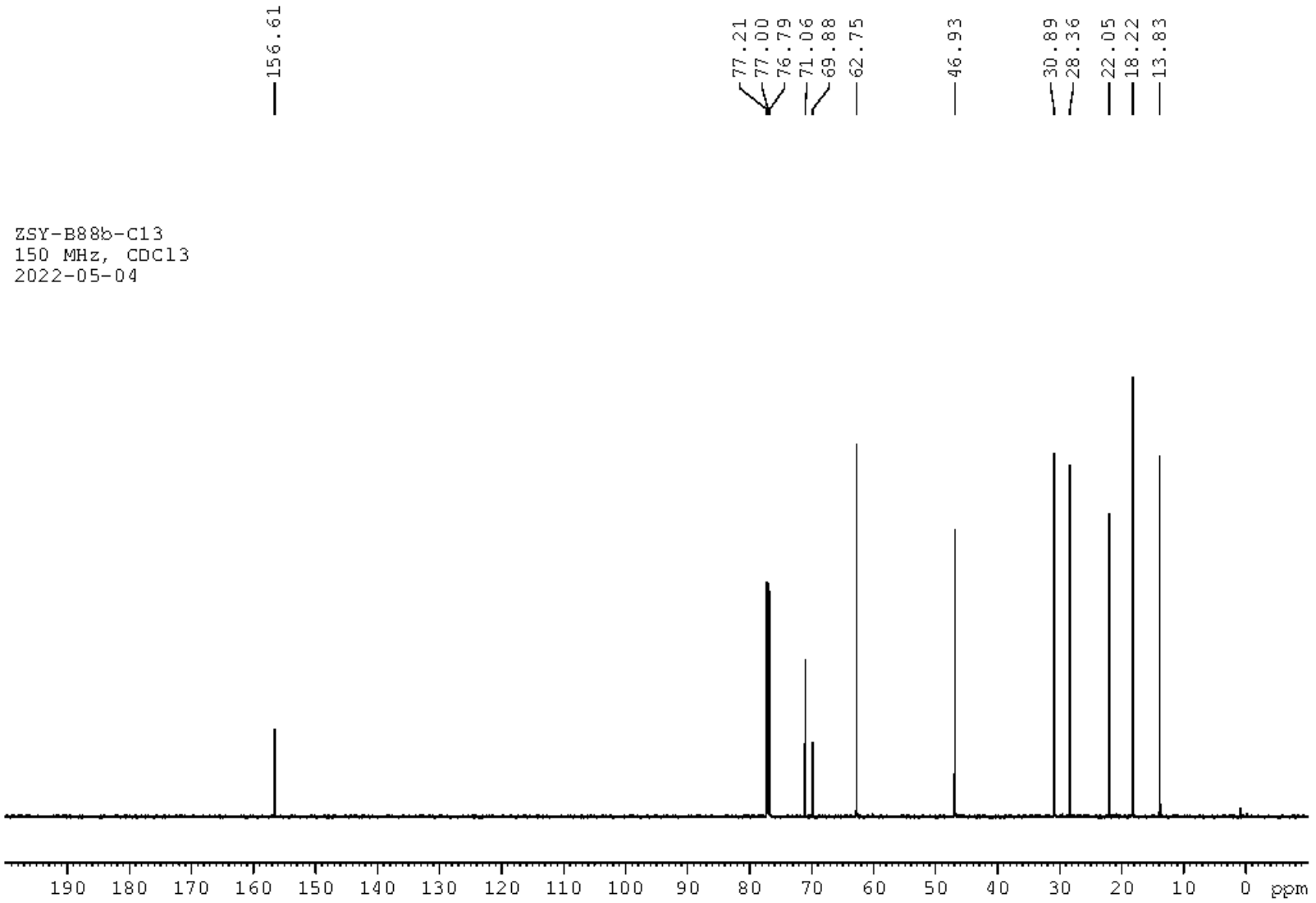

156.03
135.45
119.44
77.21
77.00
76.79
76.39
72.69
62.82
47.11
29.36
25.67
22.28
21.42
ZSY-C160B-C13
150 MHz, CDCl3
2023-09-08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

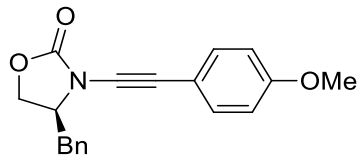


3Ir

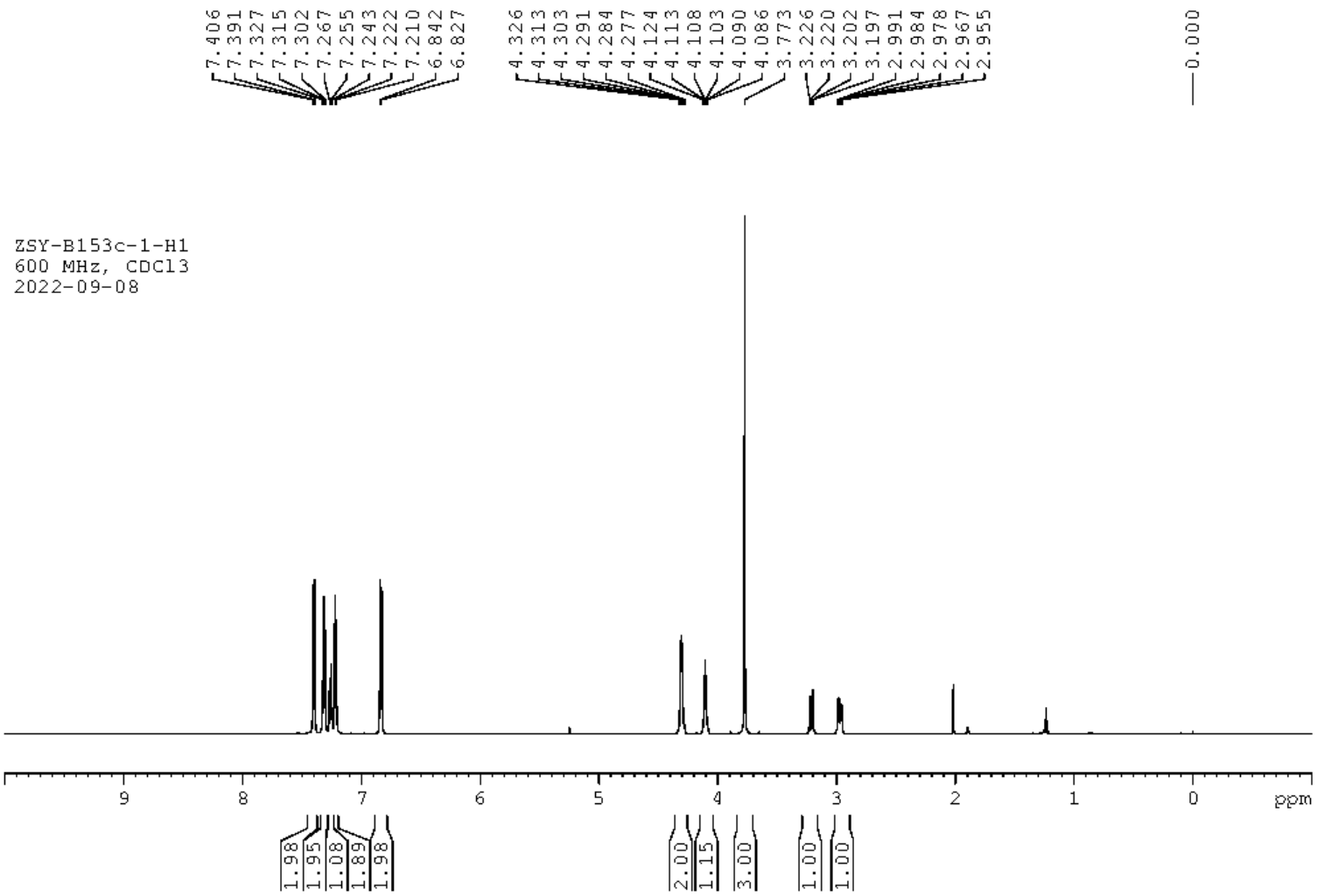
ZSY-B88b-H1
600 MHz, CDCl3
2022-05-04

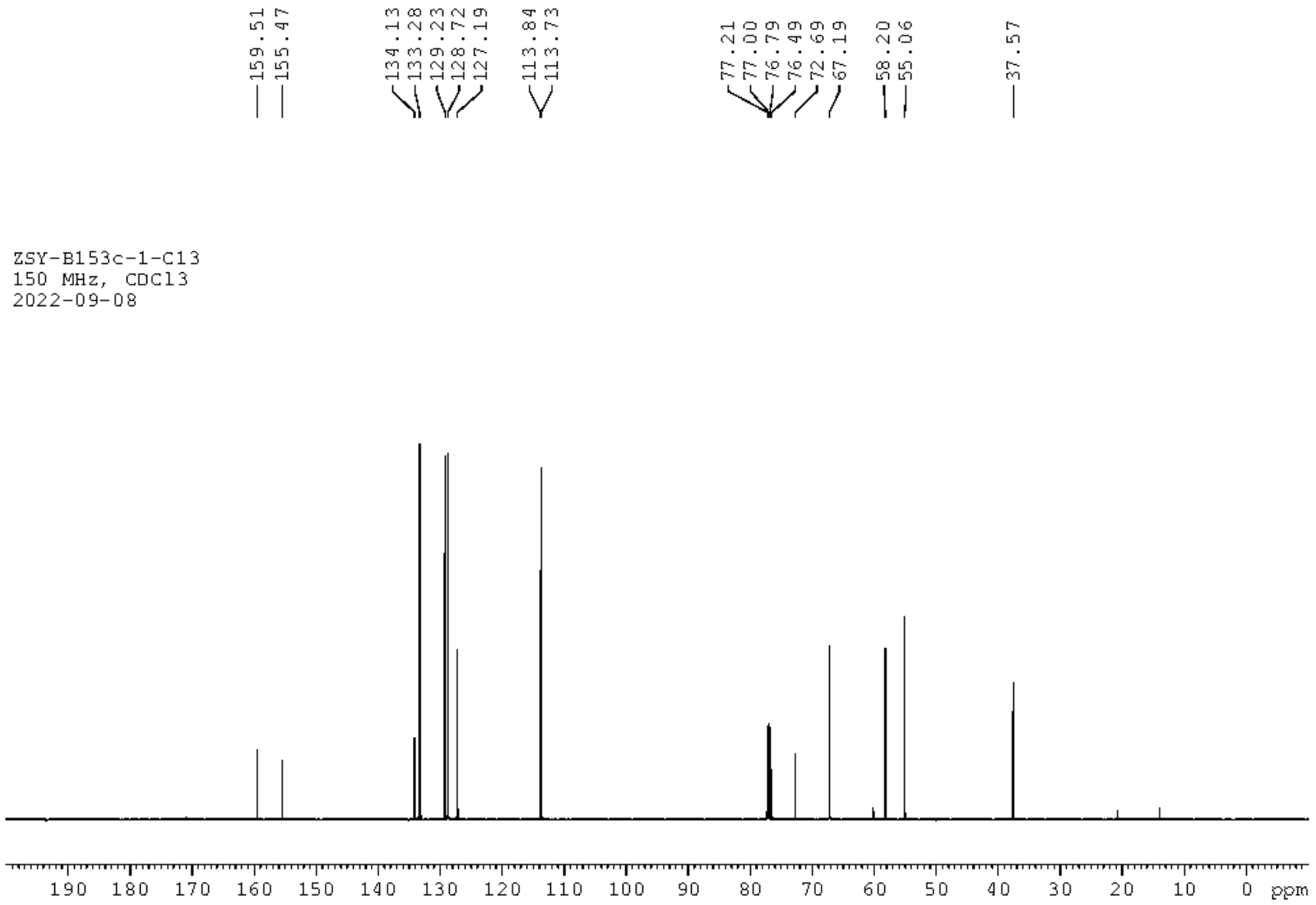


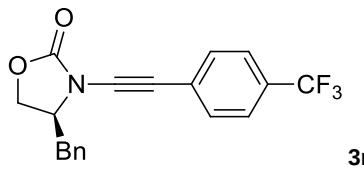

156.61
77.21
77.00
76.79
71.06
69.88
62.75
46.93
30.89
28.36
22.05
18.22
13.83
ZSY-B88b-C13
150 MHz, CDCl3
2022-05-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
OMe
Bn

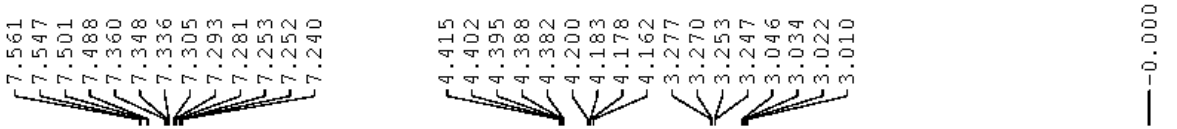
3mb


7.406
7.391
7.327
7.315
7.302
7.267
7.255
7.243
7.222
7.210
6.842
6.827
4.326
4.313
4.303
4.291
4.284
4.277
4.124
4.113
4.108
4.103
4.090
4.086
3.773
3.226
3.220
3.202
3.197
2.991
2.984
2.978
2.967
2.955
0.000
ZSY-B153c-1-H1
600 MHz, CDCl3
2022-09-08
9
8
7
6
5
4
3
2
1
0
ppm
1.98
1.95
1.08
1.89
1.98
2.00
1.15
3.00
1.00
1.00


159.51
155.47
134.13
133.28
129.23
128.72
127.19
113.84
113.73
77.21
77.00
76.79
76.49
72.69
67.19
58.20
55.06
37.57
ZSY-B153c-1-C13
150 MHz, CDCl3
2022-09-08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
CF3
Bn

3mc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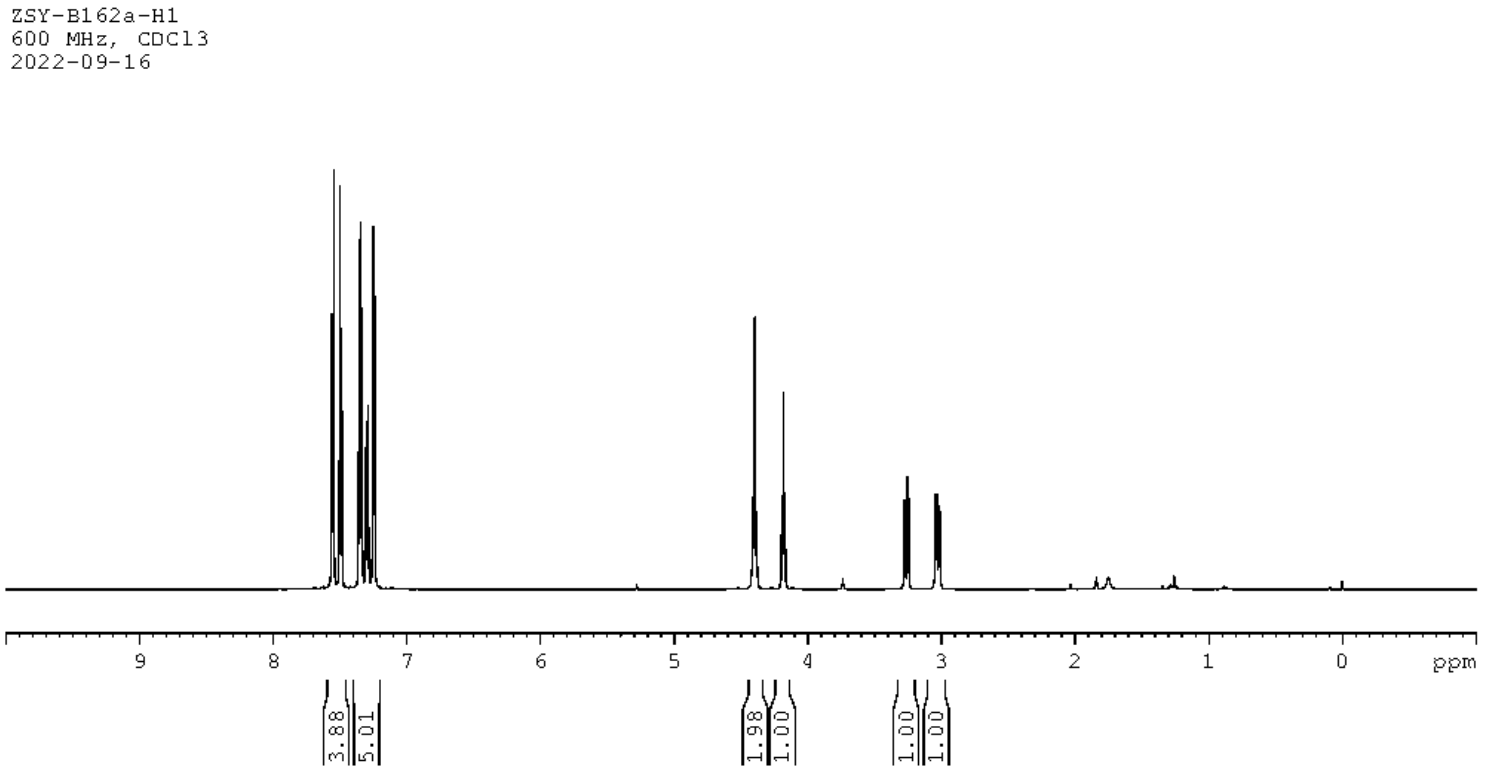
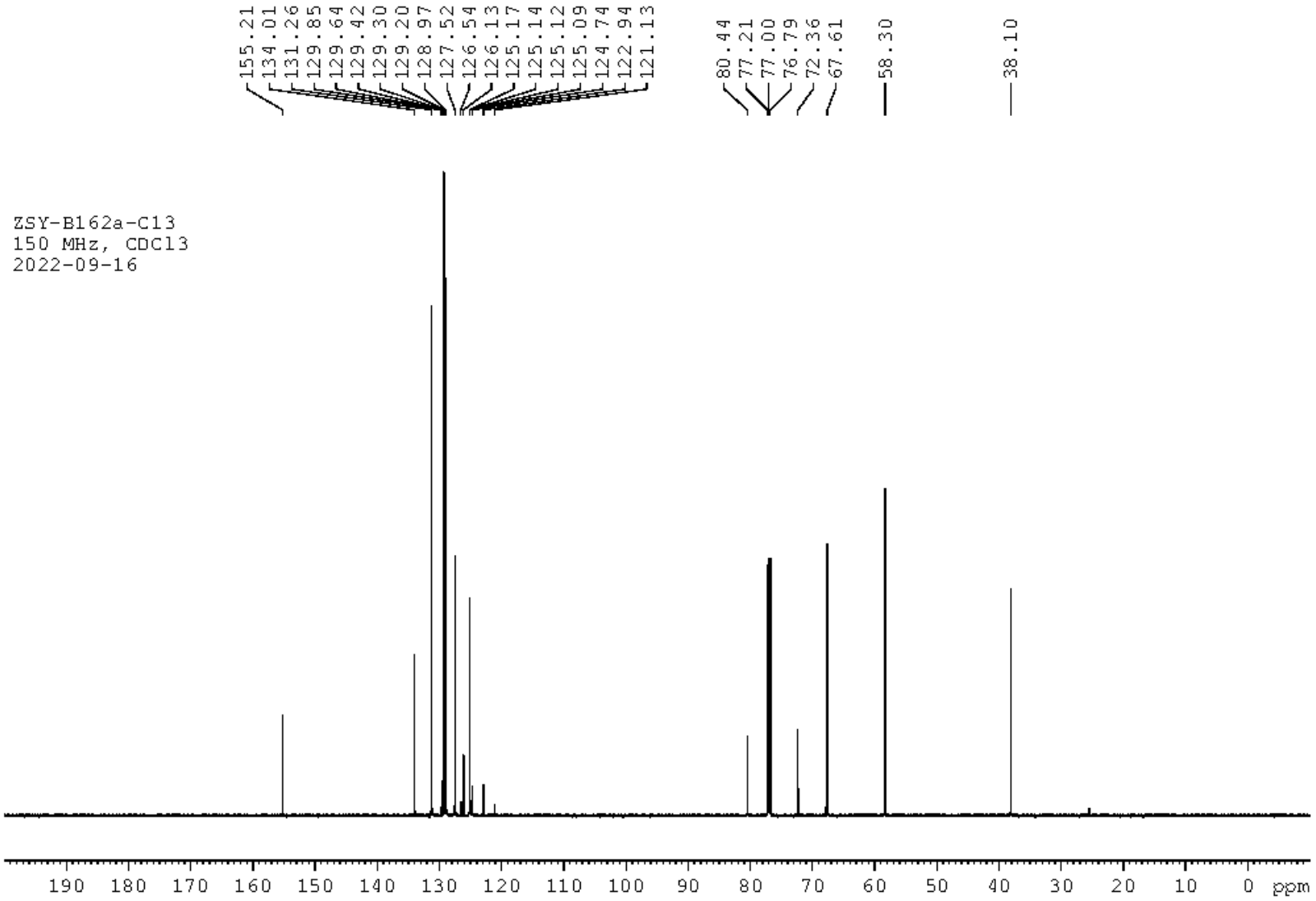
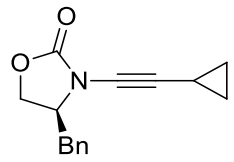
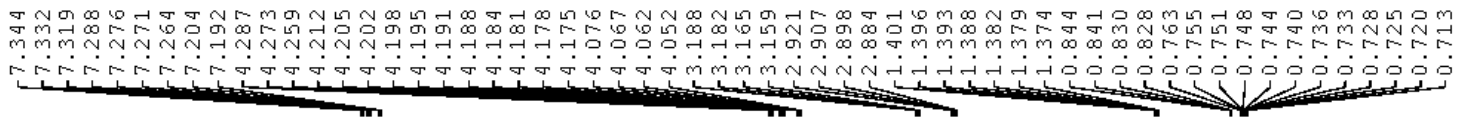
7.547
7.501
7.488
7.360
7.348
7.336
7.305
7.293
7.281
7.253
7.252
7.240
4.415
4.402
4.395
4.388
4.382
4.200
4.183
4.178
4.162
3.277
3.270
3.253
3.247
3.046
3.034
3.022
3.010
0.000


ZSY-B162a-H1
600 MHz, CDCl3
2022-09-16
9
8
7
6
5
4
3
2
1
0
ppm
3.88
5.01
1.98
1.00
1.00
1.00

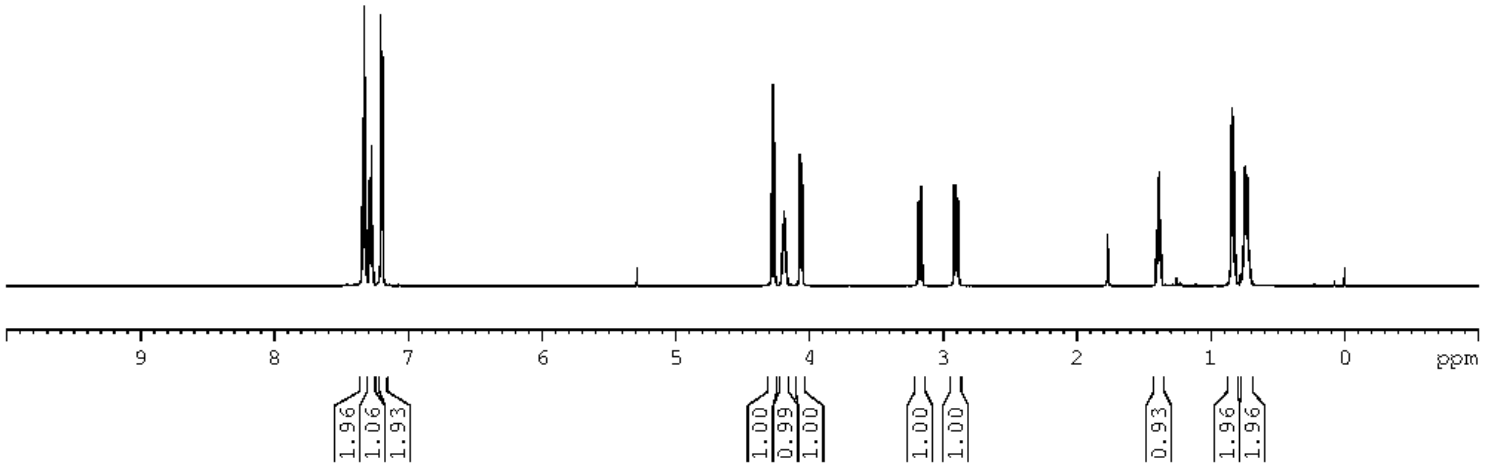

155.21
134.01
131.26
129.85
129.64
129.42
129.30
129.20
128.97
127.52
126.54
126.13
125.17
125.14
125.12
125.09
124.74
122.94
121.13
80.44
77.21
77.00
76.79
72.36
67.61
58.30
38.10
ZSY-B162a-C13
150 MHz, CDCl3
2022-09-16
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

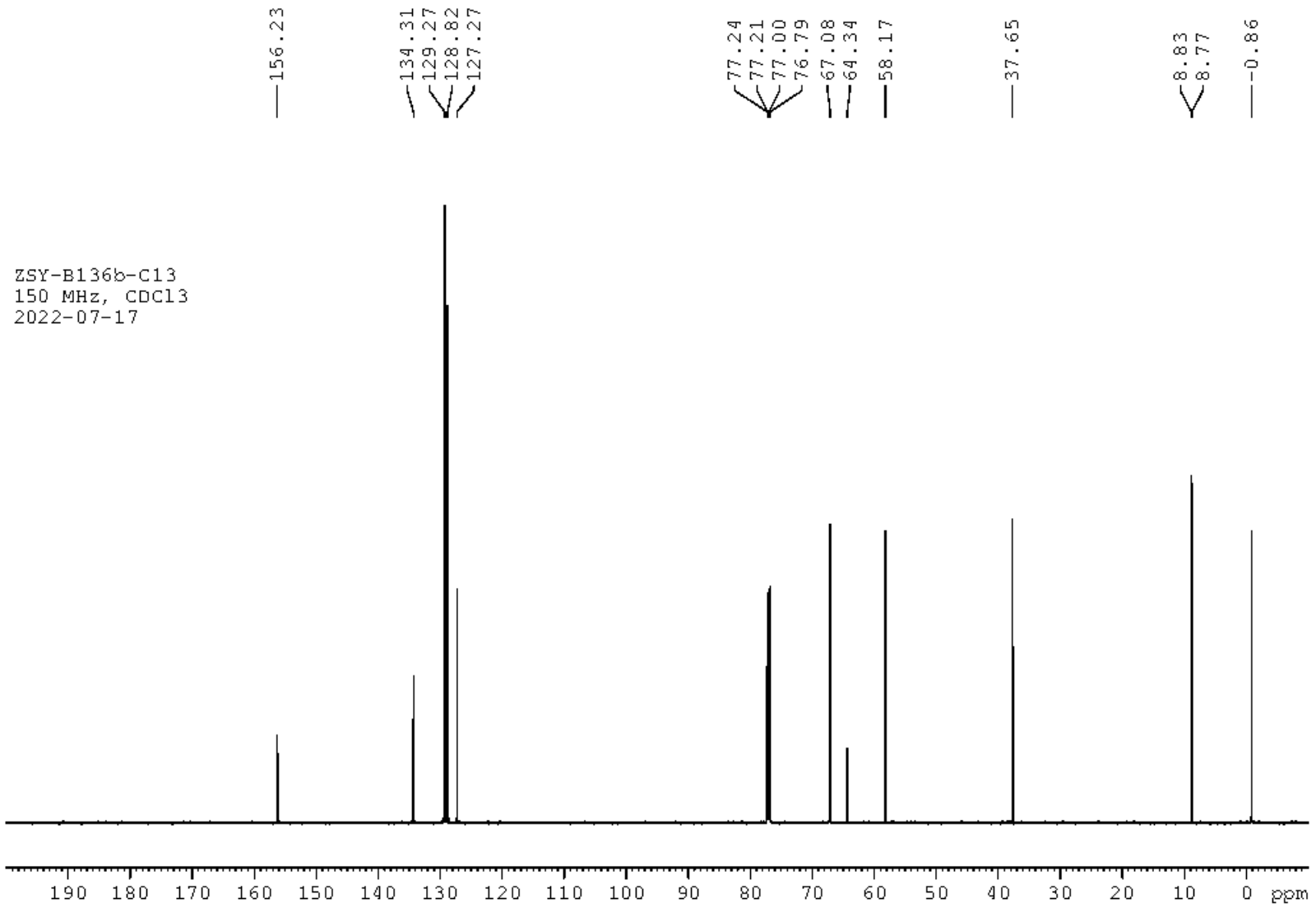


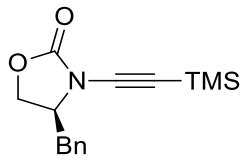
3mm



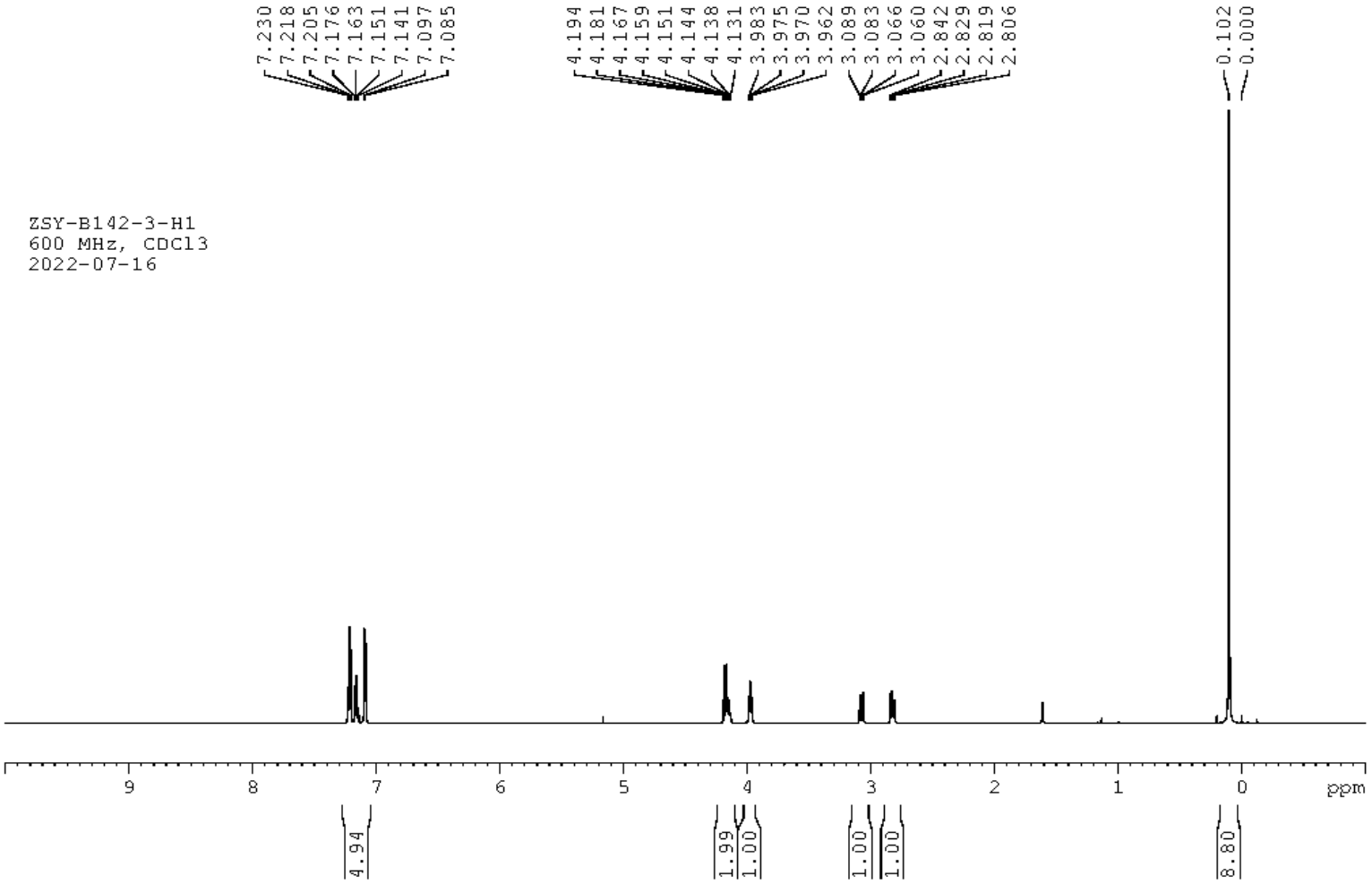
ZSY-B136b-H1
600 MHz, CDCl3
2022-07-17

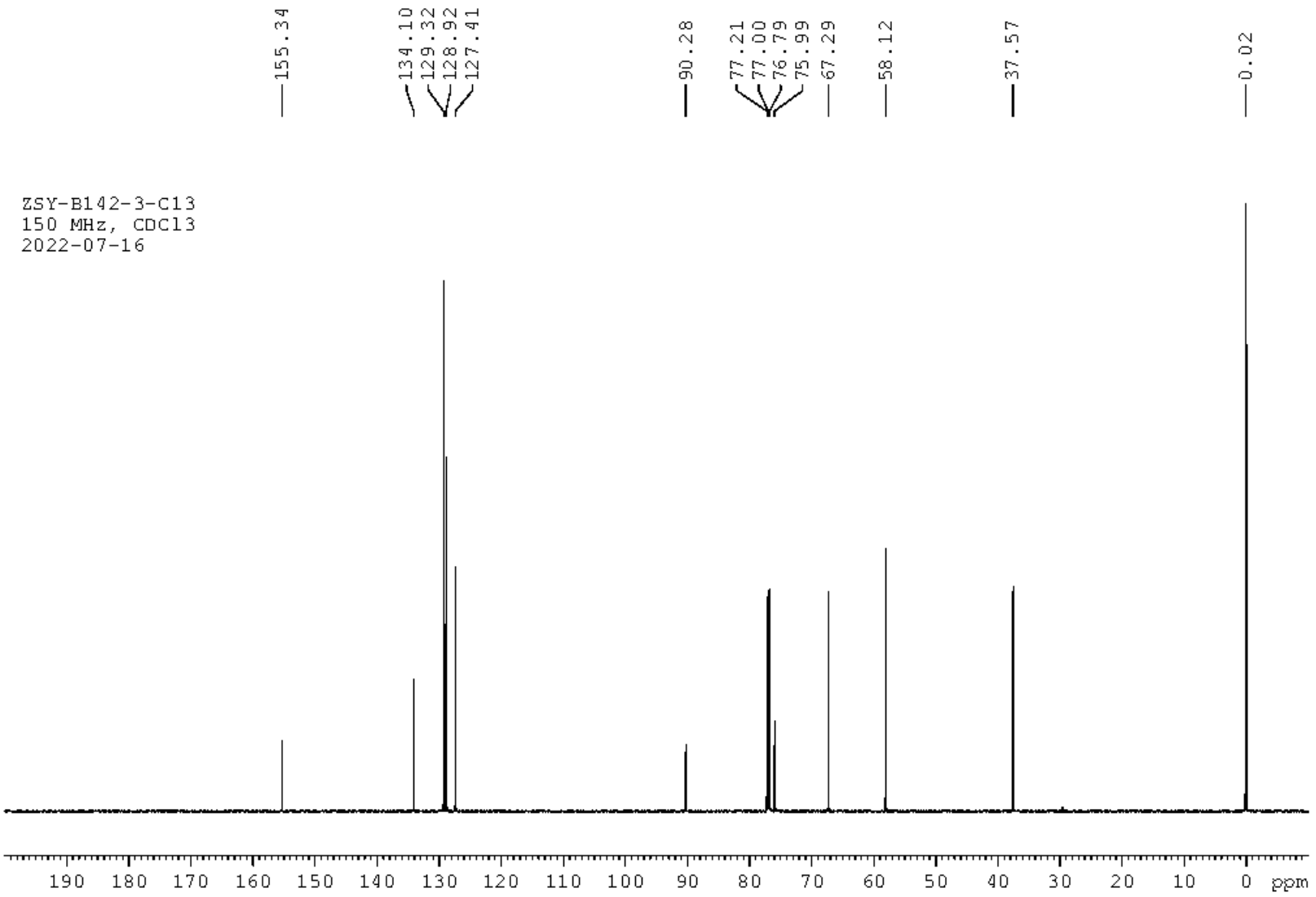


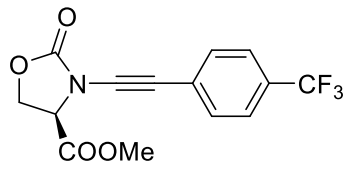

156.23
134.31
129.27
128.82
127.27
77.24
77.21
77.00
76.79
67.08
64.34
58.17
37.65
8.83
8.77
-0.86
ZSY-B136b-C13
150 MHz, CDCl3
2022-07-17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
O
N
TMS
Bn

3mn

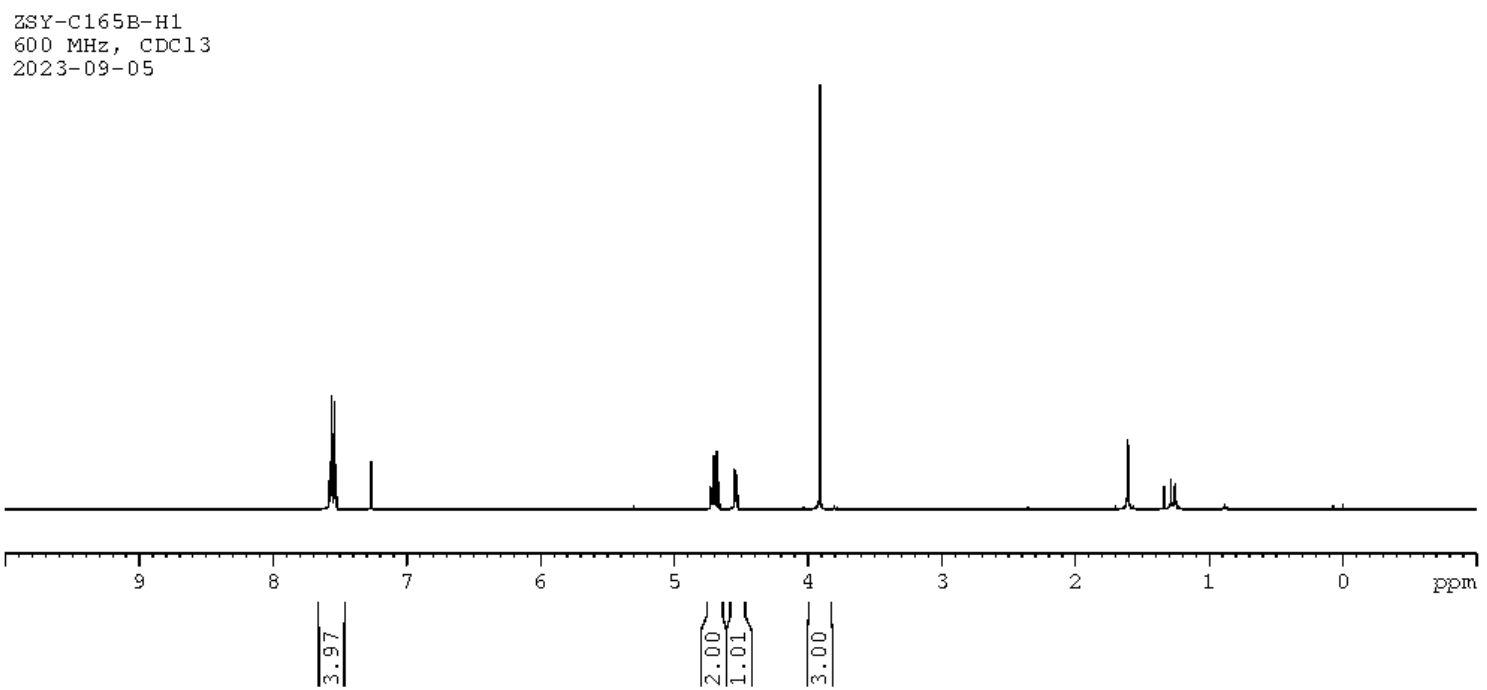

7.230
7.218
7.205
7.176
7.163
7.151
7.141
7.097
7.085
4.194
4.181
4.167
4.159
4.151
4.144
4.138
4.131
3.983
3.975
3.970
3.962
3.089
3.083
3.066
3.060
2.842
2.829
2.819
2.806
0.102
0.000
ZSY-B142-3-H1
600 MHz, CDCl3
2022-07-16
9
8
7
6
5
4
3
2
1
0
ppm
4.94
1.99
1.00
1.00
1.00
8.80

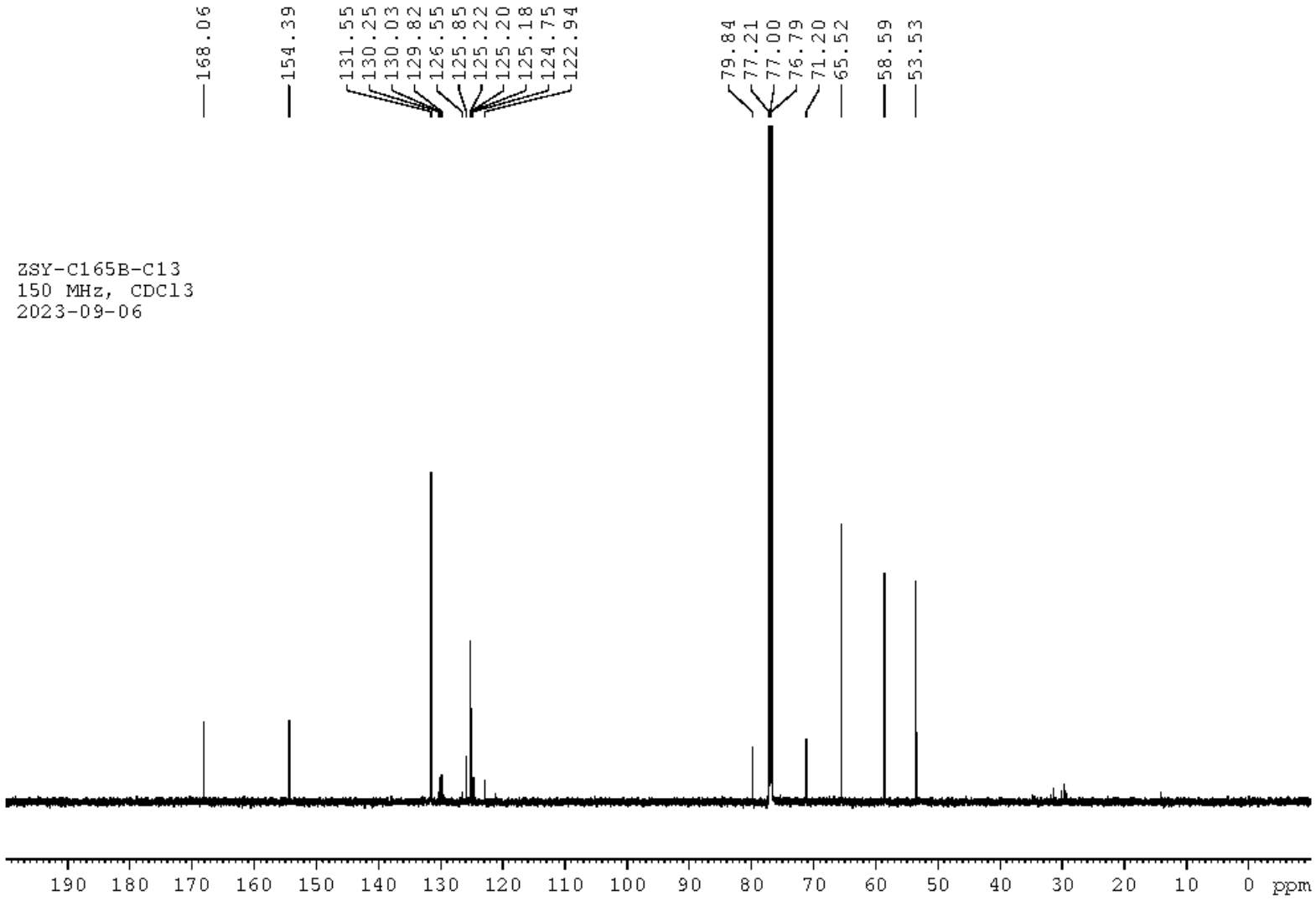

155.34
134.10
129.32
128.92
127.41
90.28
77.21
77.00
76.79
75.99
67.29
58.12
37.57
0.02
ZSY-B142-3-C13
150 MHz, CDCl3
2022-07-16
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

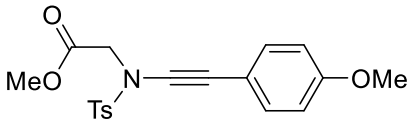

O
O
N
CF3
COOMe

3nc

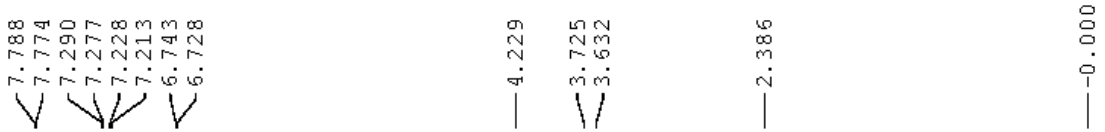

7.574
7.560
7.541
7.527
4.726
4.719
4.710
4.704
4.693
4.678
4.663
4.548
4.542
4.534
4.527
3.908

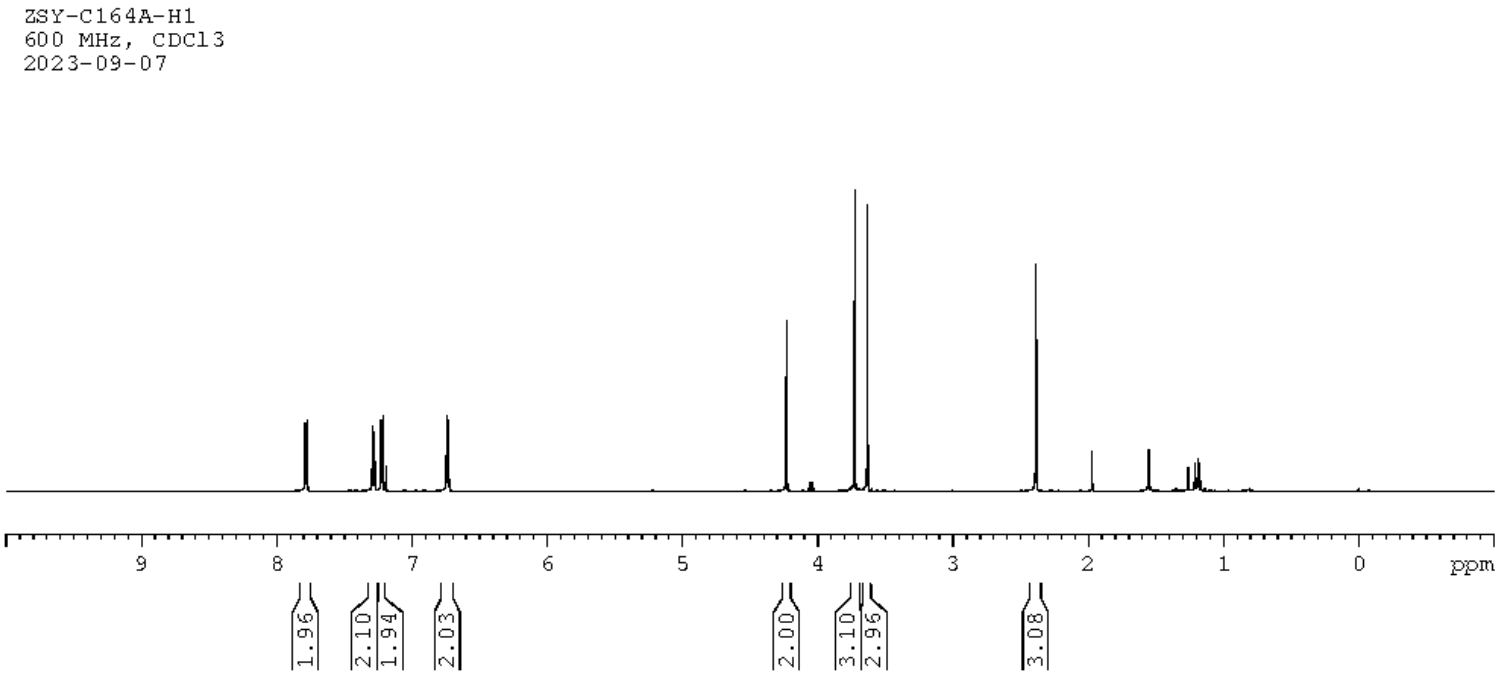

ZSY-C165B-H1
600 MHz, CDCl3
2023-09-05
9
8
7
6
5
4
3
2
1
0
ppm
3.97
2.00
1.01
3.00

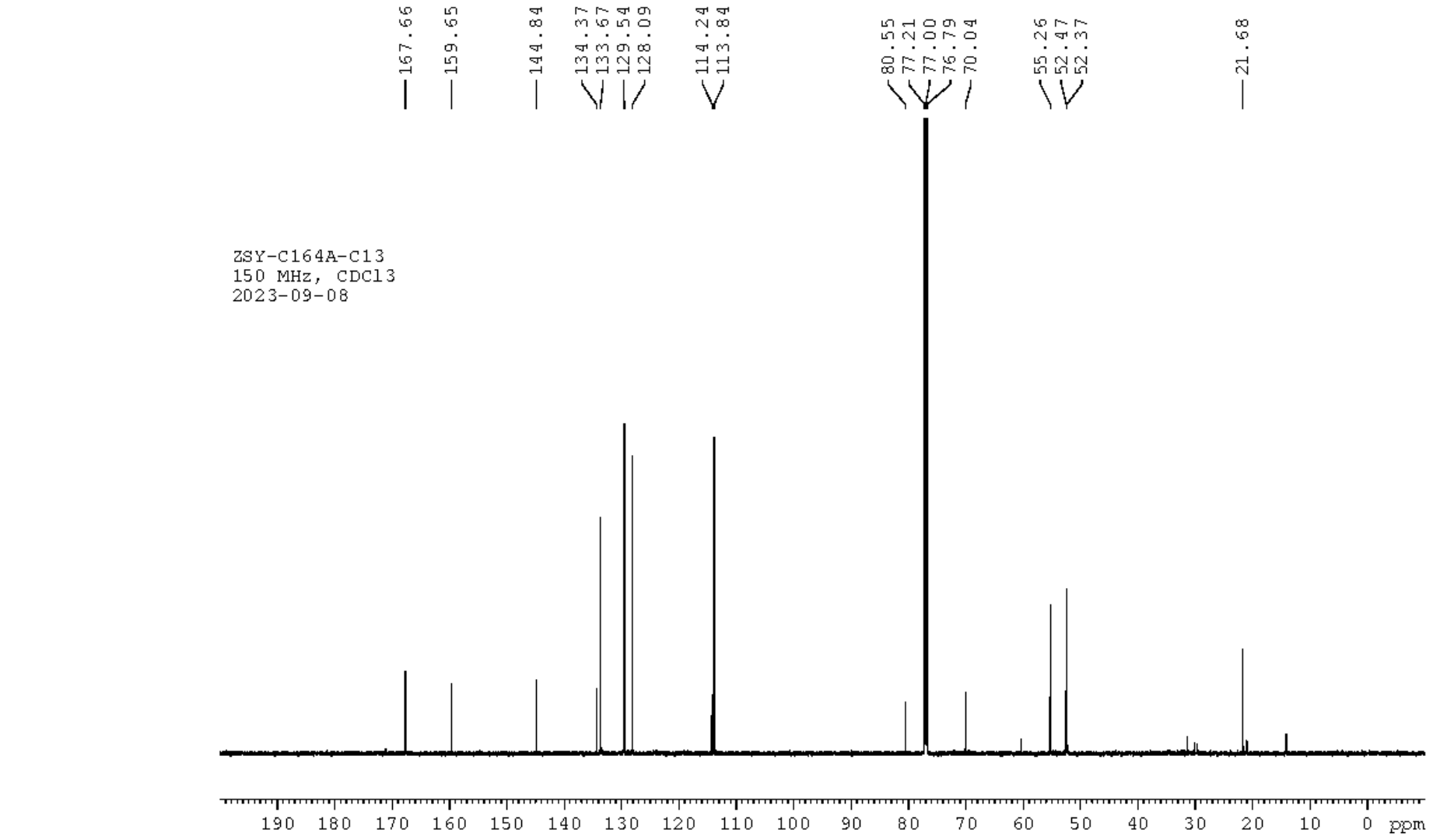

168.06
154.39
131.55
130.25
130.03
129.82
126.55
125.85
125.22
125.20
125.18
124.75
122.94
79.84
77.21
77.00
76.79
71.20
65.52
58.59
53.53
ZSY-C165B-C13
150 MHz, CDCl3
2023-09-06
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

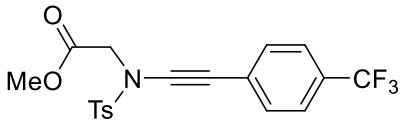

O
MeO
N
Ts
OMe

3sb

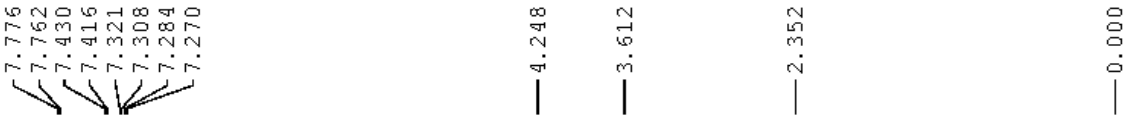

7.788
7.774
7.290
7.277
7.228
7.213
6.743
6.728
4.229
3.725
3.632
2.386
0.000

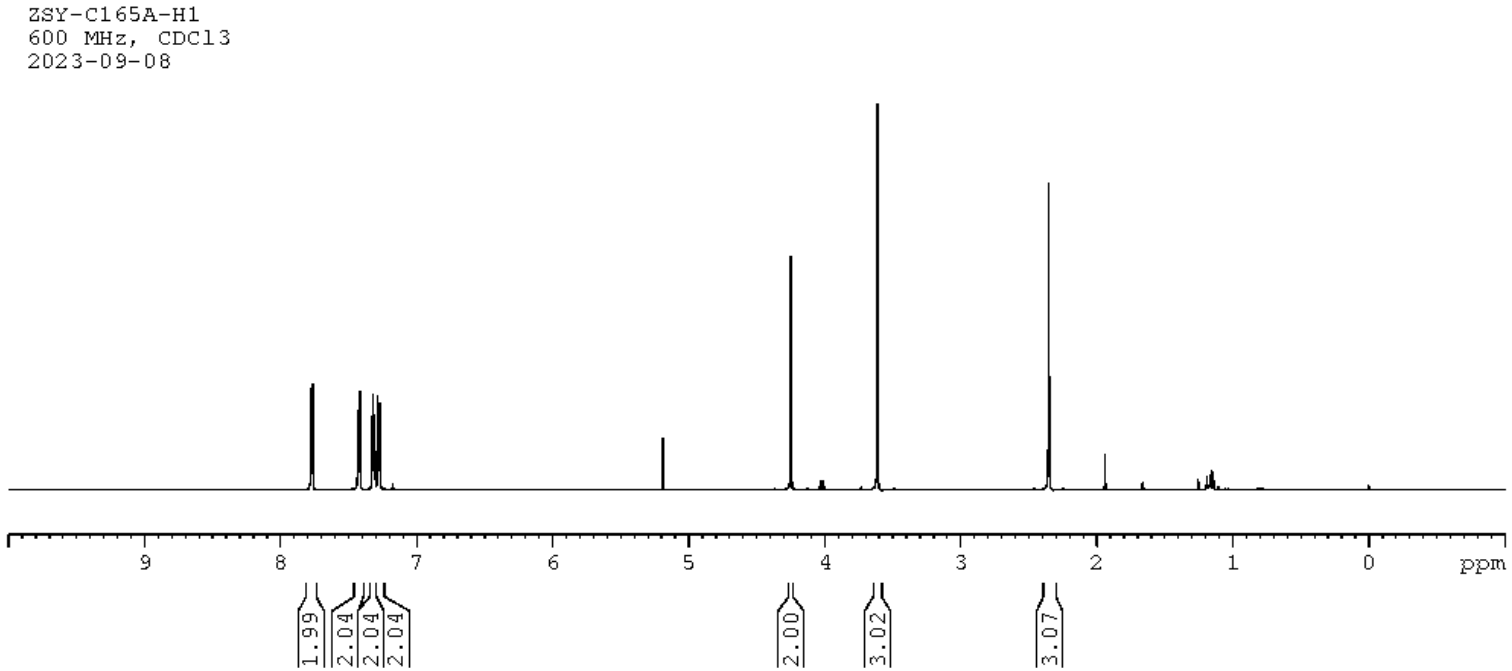

ZSY-C164A-H1
600 MHz, CDCl3
2023-09-07
9
8
7
6
5
4
3
2
1
0
ppm
1.96
2.10
1.94
2.03
2.00
3.10
2.96
3.08

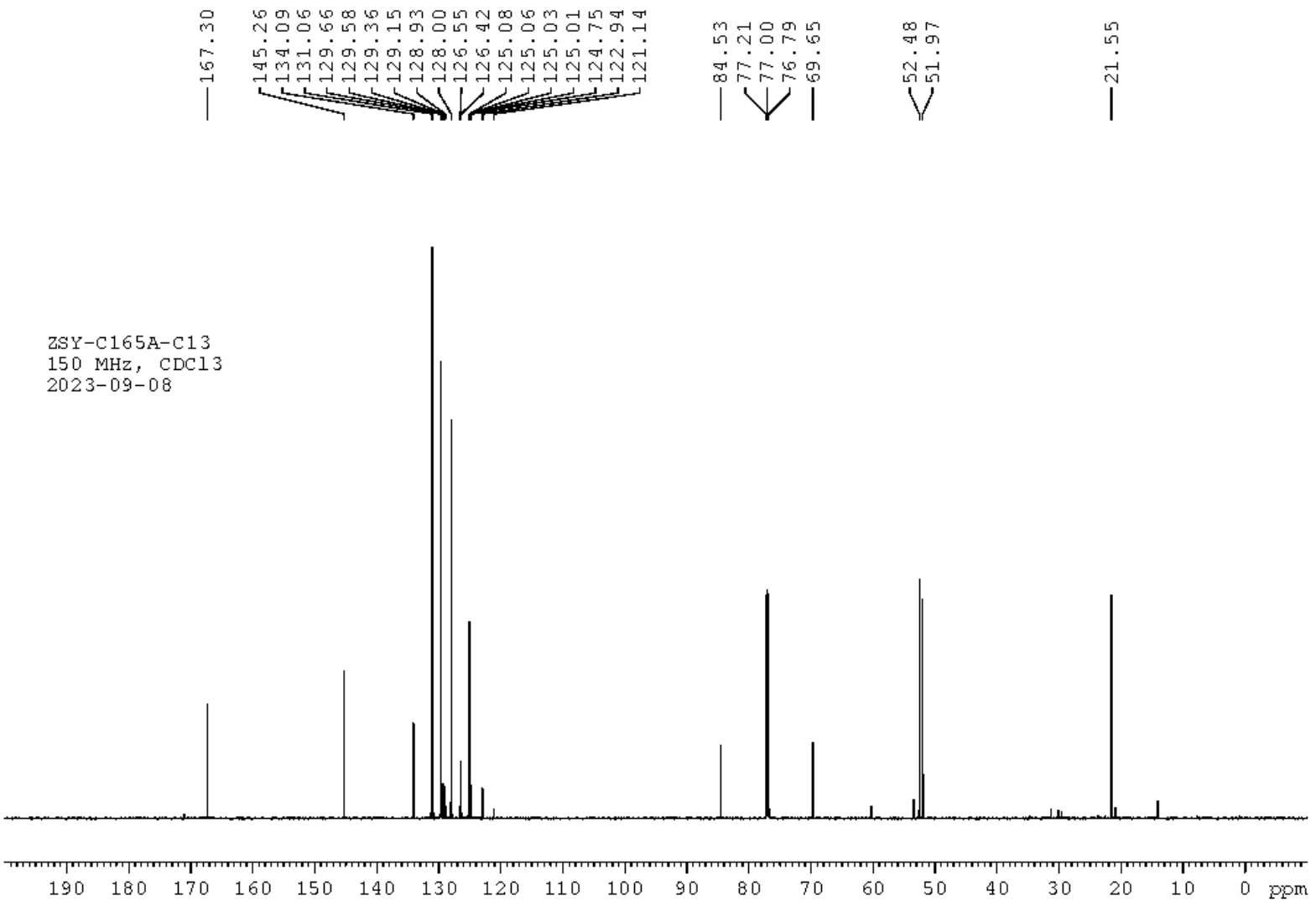

167.66
159.65
144.84
134.37
133.67
129.54
128.09
114.24
113.84
80.55
77.21
77.00
76.79
70.04
55.26
52.47
52.37
21.68
ZSY-C164A-C13
150 MHz, CDCl3
2023-09-08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

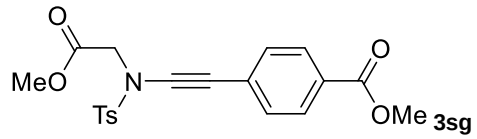

O
MeO
N
Ts
CF3

3sc

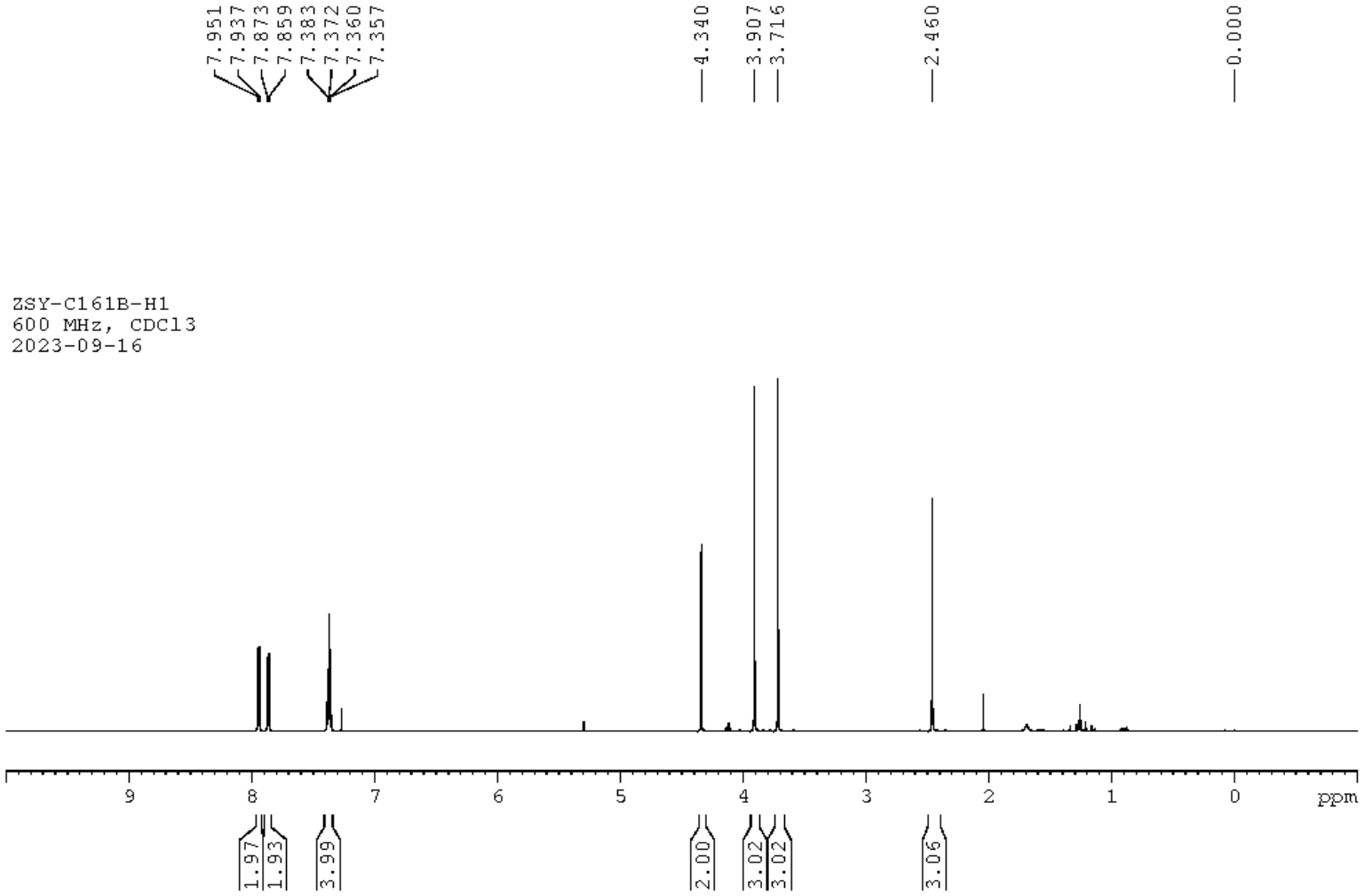

7.776
7.762
7.430
7.416
7.321
7.308
7.284
7.270
4.248
3.612
2.352
0.000

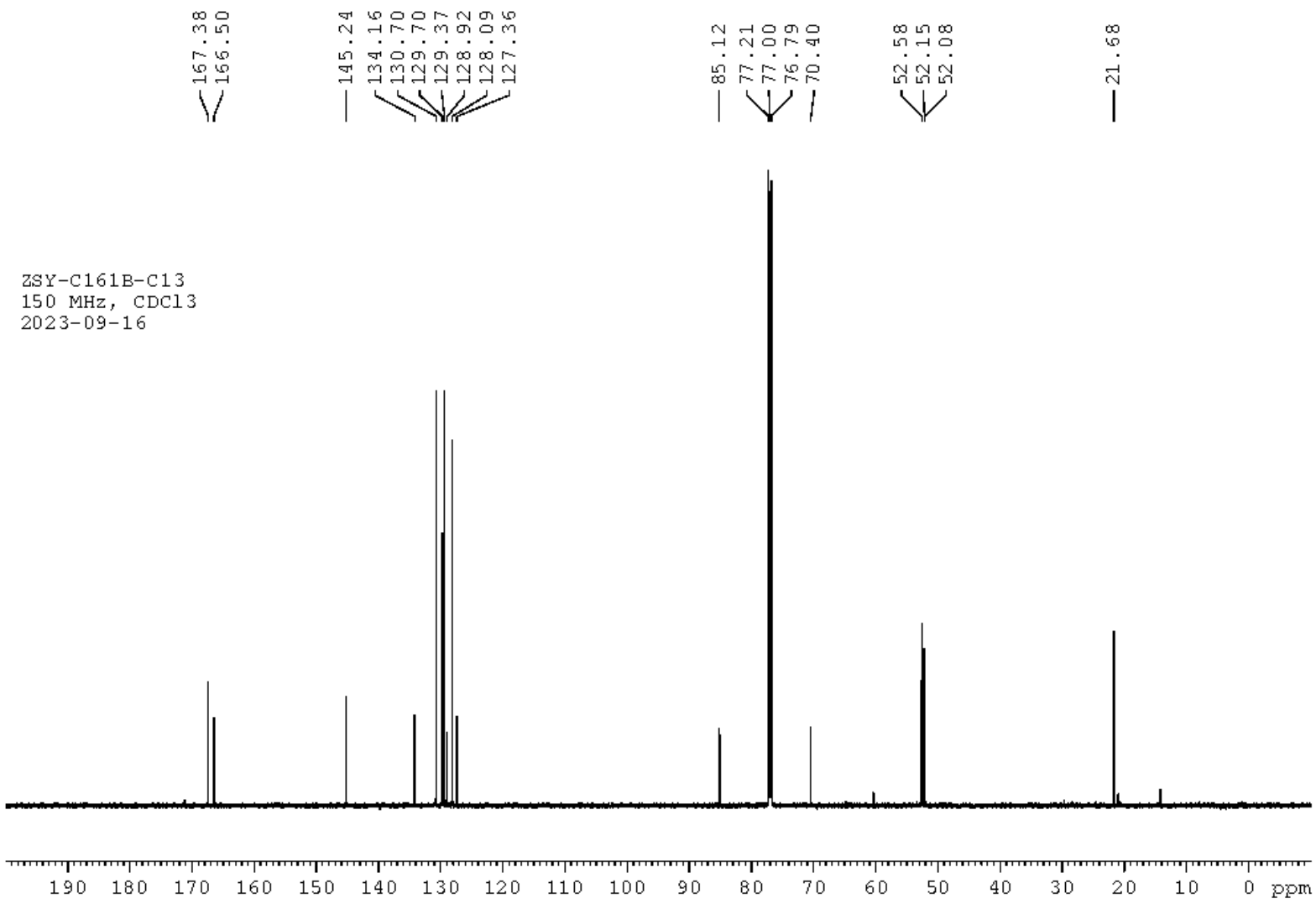

ZSY-C165A-H1
600 MHz, CDCl3
2023-09-08
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.04
2.04
2.04
2.00
3.02
3.07

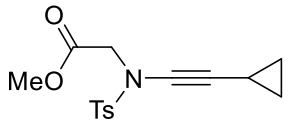

167.30
145.26
134.09
131.06
129.66
129.58
129.36
129.15
128.93
128.00
126.55
126.42
125.08
125.06
125.03
125.01
124.75
122.94
121.14
84.53
77.21
77.00
76.79
69.65
52.48
51.97
21.55
ZSY-C165A-C13
150 MHz, CDCl3
2023-09-08
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
MeO
N
Ts
O
OMe

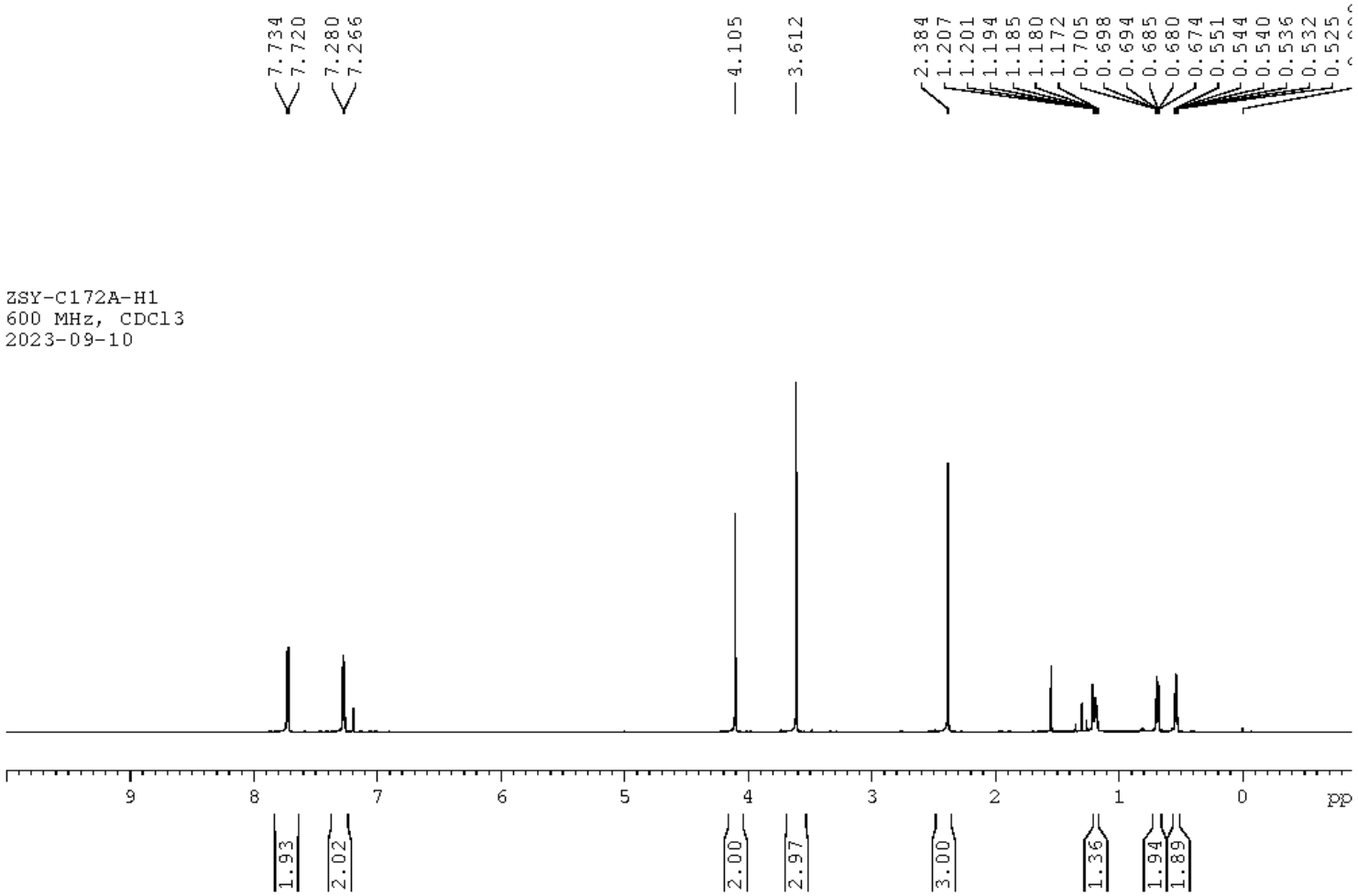
3sg

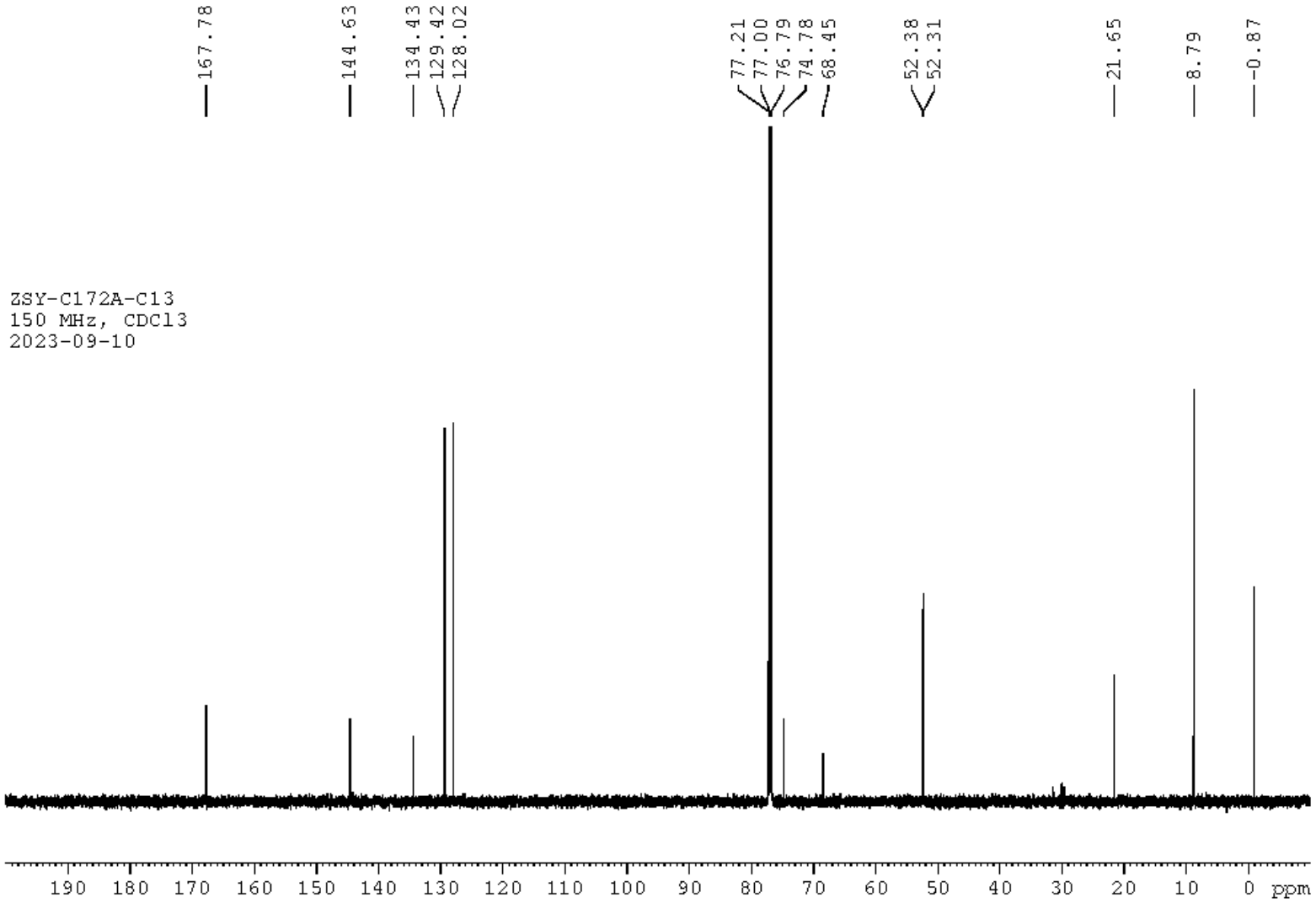

7.951
7.937
7.873
7.859
7.383
7.372
7.360
7.357
4.340
3.907
3.716
2.460
0.000
ZSY-C161B-H1
600 MHz, CDCl3
2023-09-16
9
8
7
6
5
4
3
2
1
0
ppm
1.97
1.93
3.99
2.00
3.02
3.02
3.06

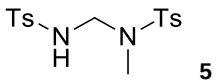

167.38
166.50
145.24
134.16
130.70
129.70
129.37
128.92
128.09
127.36
85.12
77.21
77.00
76.79
70.40
52.58
52.15
52.08
21.68
ZSY-C161B-C13
150 MHz, CDCl3
2023-09-16
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


O
MeO
N
Ts

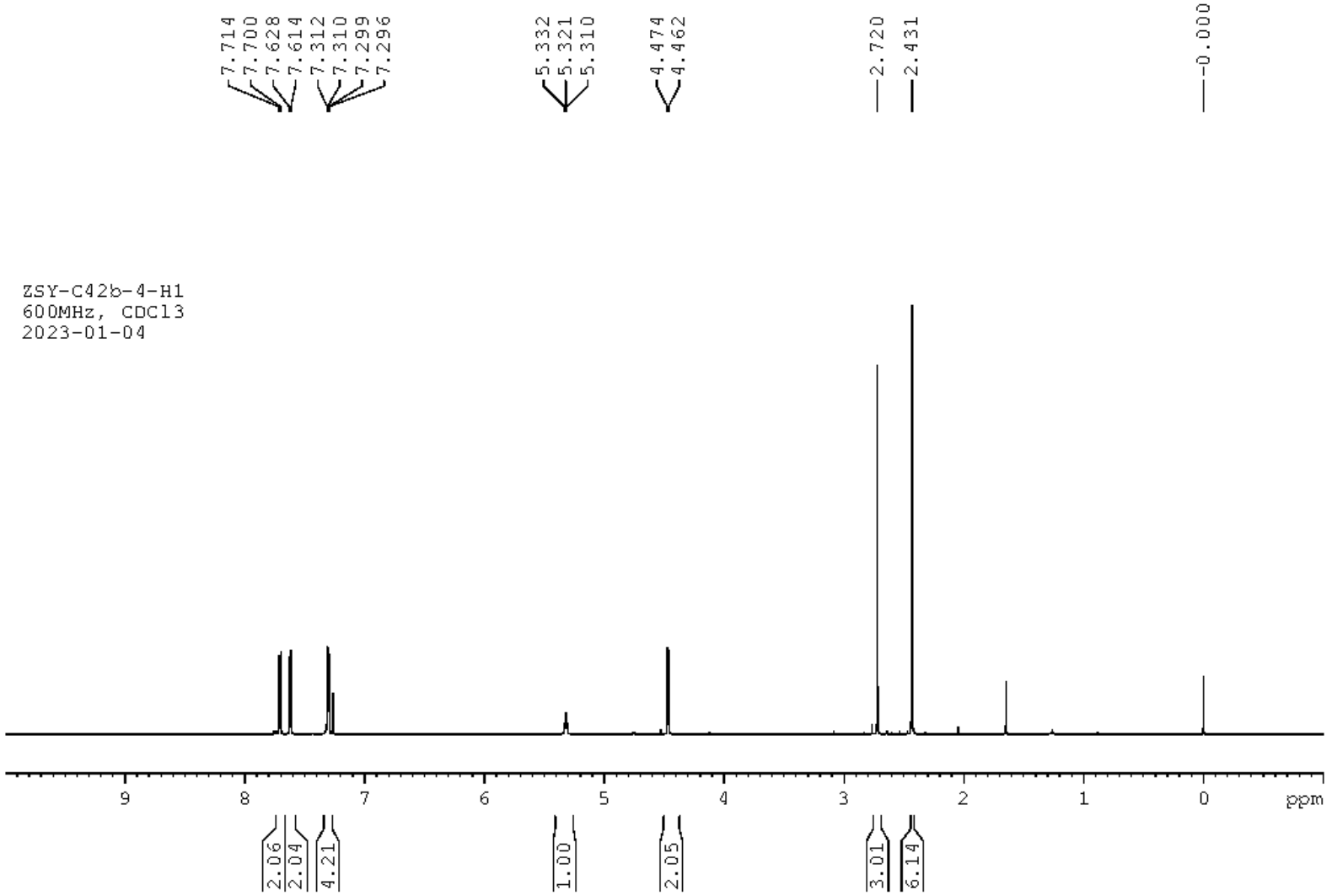
3sm

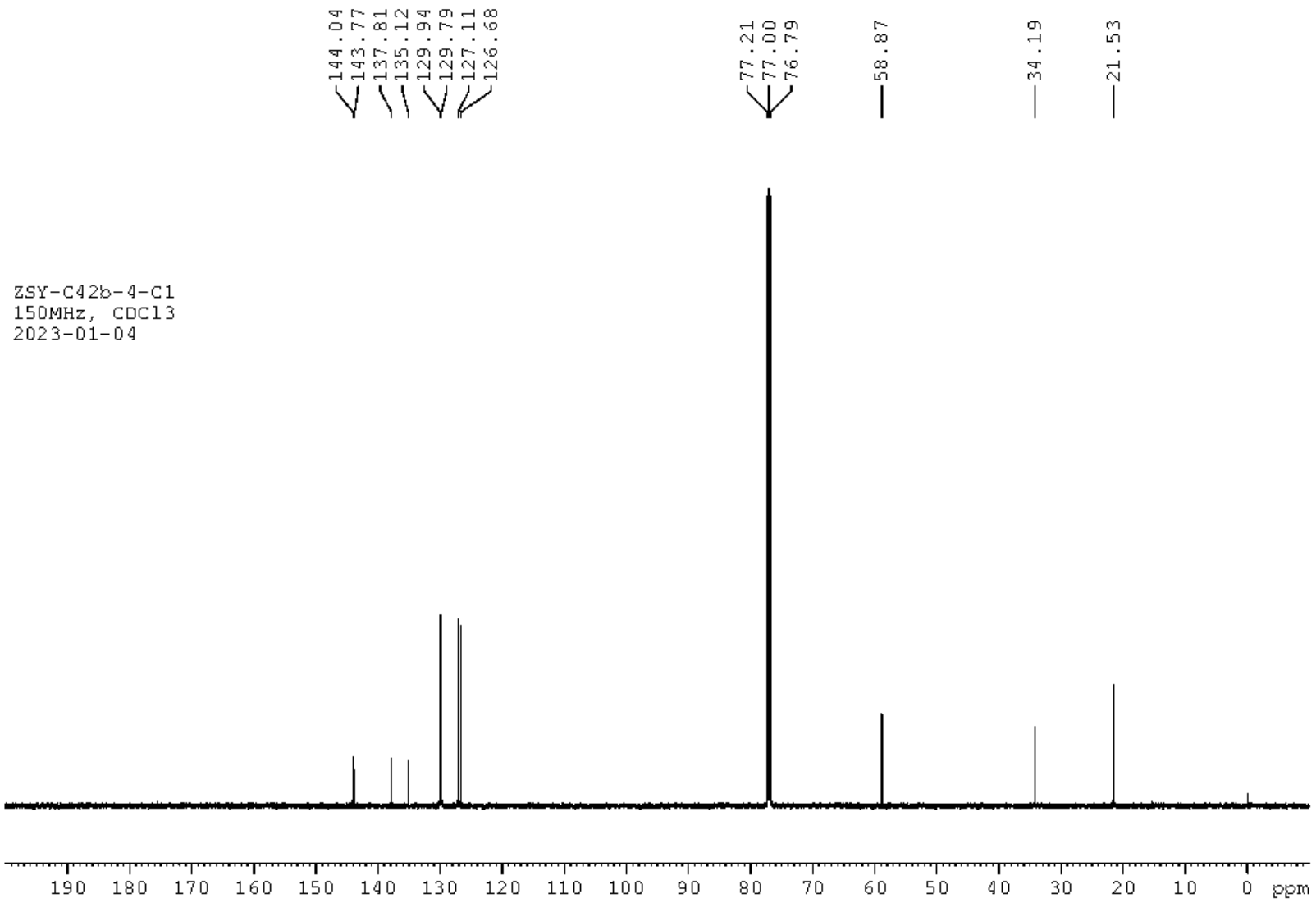

7.734
7.720
7.280
7.266
4.105
3.612
2.384
1.207
1.201
1.194
1.185
1.180
1.172
0.705
0.698
0.694
0.685
0.680
0.674
0.551
0.544
0.540
0.536
0.532
0.525
ZSY-C172A-H1
600 MHz, CDCl3
2023-09-10
9
8
7
6
5
4
3
2
1
0
ppm
1.93
2.02
2.00
2.97
3.00
1.36
1.94
1.89

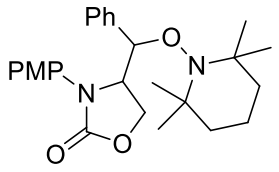

167.78
144.63
134.43
129.42
128.02
77.21
77.00
76.79
74.78
68.45
52.38
52.31
21.65
8.79
-0.87
ZSY-C172A-C13
150 MHz, CDCl3
2023-09-10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ts
N
H
N
Ts

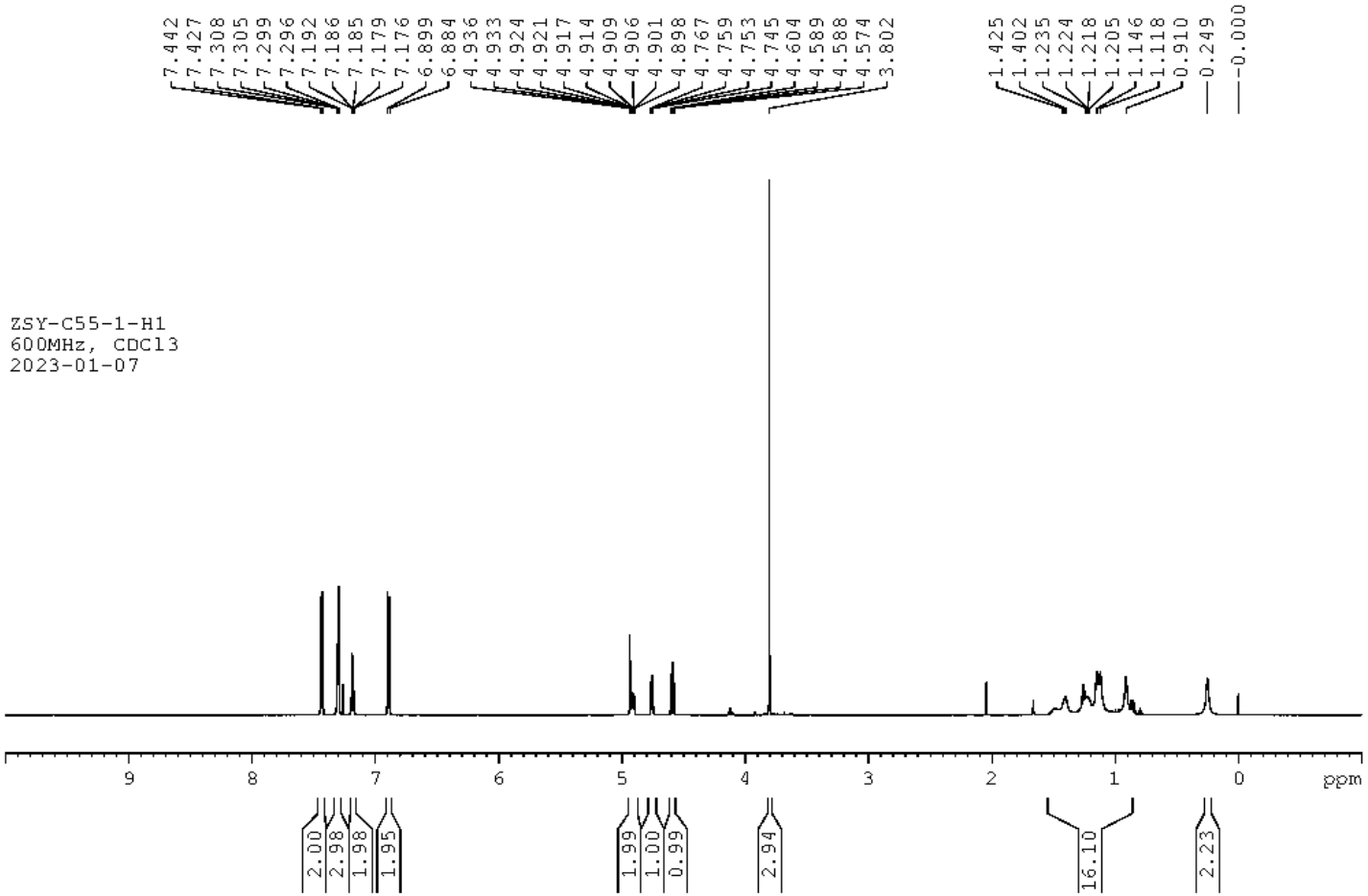
5

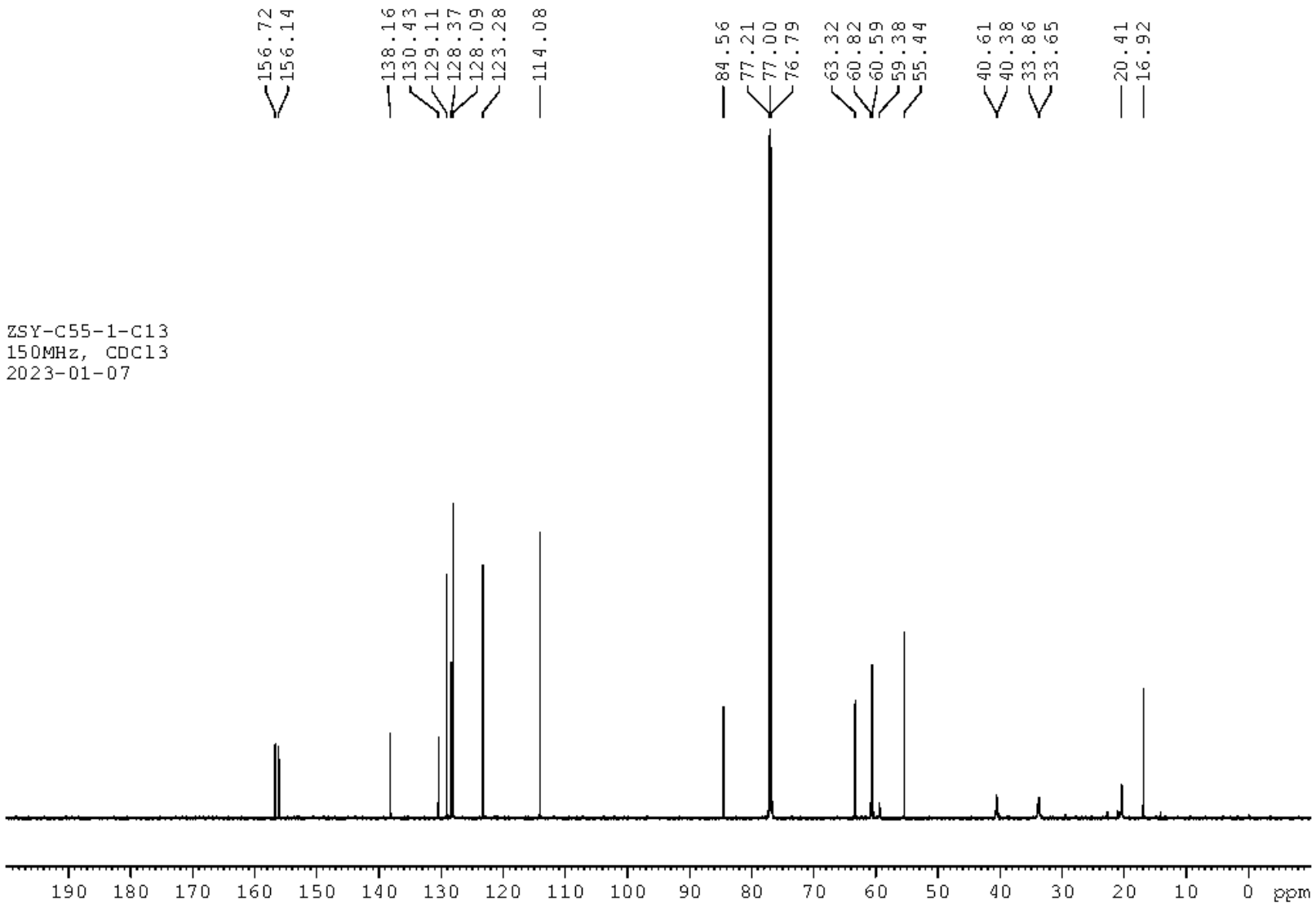

7.714
7.700
7.628
7.614
7.312
7.310
7.299
7.296
5.332
5.321
5.310
4.474
4.462
2.720
2.431
0.000
ZSY-C42b-4-H1
600MHz, CDCl3
2023-01-04
9
8
7
6
5
4
3
2
1
0
ppm
2.06
2.04
4.21
1.00
2.05
3.01
6.14


144.04
143.77
137.81
135.12
129.94
129.79
127.11
126.68
77.21
77.00
76.79
58.87
34.19
21.53
ZSY-C42b-4-C1
150MHz, CDCl3
2023-01-04
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Ph
O
N
PMP
N
O
O

8


7.442
7.427
7.308
7.305
7.299
7.296
7.192
7.186
7.185
7.179
7.176
6.899
6.884
4.936
4.933
4.924
4.921
4.917
4.914
4.909
4.906
4.901
4.898
4.767
4.759
4.753
4.745
4.604
4.589
4.588
4.574
3.802
1.425
1.402
1.235
1.224
1.218
1.205
1.146
1.118
0.910
0.249
0.000
ZSY-C55-1-H1
600MHz, CDCl3
2023-01-07
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.98
1.98
1.95
1.99
1.00
0.99
2.94
16.10
2.23


156.72
156.14
138.16
130.43
129.11
128.37
128.09
123.28
114.08
84.56
77.21
77.00
76.79
63.32
60.82
60.59
59.38
55.44
40.61
40.38
33.86
33.65
20.41
16.92
ZSY-C55-1-C13
150MHz, CDCl3
2023-01-07
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

6. References

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