Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

TFA-Promoted Sulfonation/Cascade Cyclization of 2-Propynolphenols with Sodium Sulfinates to 4-Sulfonyl 2*H*-Chromenes under Metal-Free Conditions

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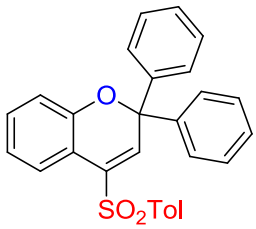
Table of Contents

General Remarks:

Column chromatography was carried out on silica gel. ^{1}H NMR spectra were recorded on 400 MHz in $CDCl_{3,}$ ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$ using TMS as internal standard. IR spectra were recorded on an FT-IR spectrometer and only major peaks are reported in cm^{-1}. Melting points were determined on a microscopic apparatus and were uncorrected. All products were further characterized by HRMS (high resolution mass spectra); copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Solvents were dried under standard method. The petroleum ether was bought from Shanghai Titan Scientific Company in a plastic bucket.

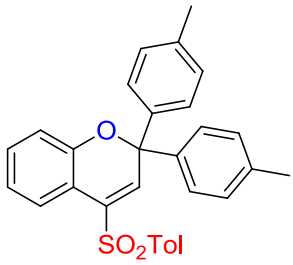
General procedure for the preparation of product 4-sulfonates 2*H*-chromenes 3 and 5: The mixture of 2-propynolphenols (**1** or **4**) (0.1 mmol), sodium sulfinates **2** (0.2 mmol), TFA (0.15 mmol) in CH_3NO_2 (1.0 mL) was stirred at 80°C. After 6.0 h, the completion of the reaction was monitored by TLC. Then, the solvent was concentrated and the residue was purified by flash chromatography on silica gel to afford **3** or **5**.

2,2-diphenyl-4-tosyl-2*H*-chromene (3a):



The resultant residue was purified by flash silica gel column chromatography to afford **3a** as a white solid; mp: 202–204 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 3 H), 6.75 (t, *J* = 7.6 Hz, 1 H), 6.85 (d, *J* = 8.0 Hz, 1 H), 7.06 (t, *J* = 8.0 Hz, 1 H), 7.18 – 7.28 (m, 8 H), 7.31 – 7.35 (m, 5 H), 7.69 – 7.73 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 82.7, 115.4, 117.5, 121.7, 125.1, 126.8, 127.8, 128.2, 128.4, 129.9, 131.1, 135.9, 136.9, 137.1, 142.6, 144.6, 152.5. HRMS (ESI, m/z): calcd for $C_{28}H_{23}O_3S$: $[M+H]^+$ = 439.1362; found: 439.1357.

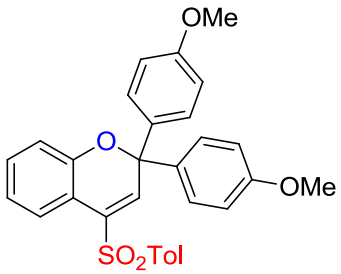
2,2-di-p-tolyl-4-tosyl-2*H*-chromene (3b):



The resultant residue was purified by flash silica gel column chromatography to afford **3b** as a white solid; mp: 192–194 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): 2.24 (s, 6 H), 2.30 (s, 3 H), 6.71 – 6.75 (m, 1 H), 6.82 – 6.84 (m, 1 H), 7.02 – 7.06 (m, 5 H), 7.17 – 7.20 (m, 6 H), 7.32 (s, 1 H), 7.68 – 7.73 (m, 3 H). ^{13}C{H} NMR

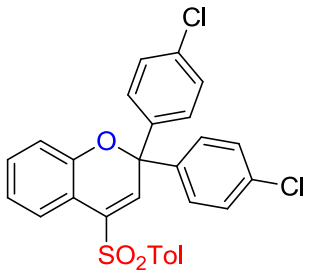
(100 MHz, $CDCl_3$): δ 21.1, 21.6, 82.6, 115.4, 117.5, 121.6, 125.0, 126.8, 127.8, 129.1, 129.9, 131.0, 135.6, 137.0, 137.5, 137.9, 139.9, 144.5, 152.6. HRMS (ESI, m/z): calcd for $C_{30}H_{27}O_3S$: $[M+H]^+$ = 467.1675; found: 467.1673.

2,2-bis(4-methoxyphenyl)-4-tosyl-2*H*-chromene (3c):



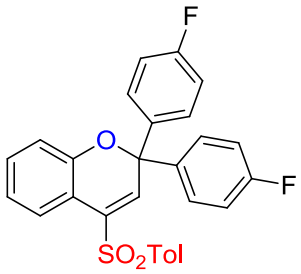
The resultant residue was purified by flash silica gel column chromatography to afford **3c** as a white solid; mp: 198–200 ºC. ^1H NMR (400 MHz, $CDCl_3$): δ 2.29 (s, 3 h), 3.67 (s, 6 H), 6.73 – 6.77 (m, 3 H), 6.85 – 6.89 (m, 5 H), 7.04 – 7.08 (m, 1 H), 7.14 – 7.20 (m, 4 H), 7.32 (s, 1 H), 7.69 – 7.73 (m, 3 H). $^{13}C\{H\}$ NMR (100 MHz, $CDCl_3$): δ 21.6, 55.2, 82.4, 112.9, 113.4, 115.4, 117.5, 119.2, 121.7, 125.1, 127.8, 129.5, 129.9, 131.1, 135.8, 136.9, 144.1, 144.6, 152.5, 159.6. HRMS (ESI, m/z): calcd for $C_{30}H_{27}O_5S$: $[M+H]^+$ = 499.1574; found: 499.1570.

2,2-bis(4-chlorophenyl)-4-tosyl-2*H*-chromene (3d):



The resultant residue was purified by flash silica gel column chromatography to afford **3d** as a white solid; mp: 68–70 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3 H), 6.84 – 6.91 (m, 2 H), 7.13 – 7.17 (m, 1 H), 7.27 – 7.31 (m, 11 H), 7.77 – 7.83 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 81.8, 115.4, 117.5, 122.2, 125.2, 127.8, 128.2, 128.8, 130.0, 131.4, 134.5, 135.7, 136.6, 136.8, 140.8, 144.9, 152.1. HRMS (ESI, m/z): calcd for $C_{28}H_{21}Cl_2O_3S$: $[M+H]^+$ = 507.0583; found: 507.0585.

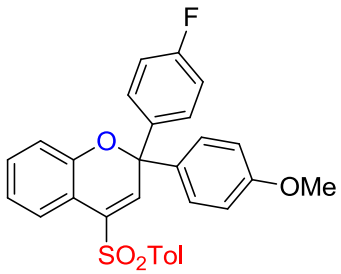
2,2-bis(4-fluorophenyl)-4-tosyl-2*H*-chromene (3e):



The resultant residue was purified by flash silica gel column chromatography to afford **3e** as a white solid; mp: 177–179 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3 H), 6.83 – 6.91 (m, 2 H), 7.03 (t, *J* = 8.4 Hz, 4 H), 7.15 (t, *J* = 8.0 Hz, 1 H), 7.25 – 7.37 (m, 7 H), 7.78 – 7.82 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 81.9, 115.3, 115.4, 115.6, 117.5, 122.0, 125.2, 127.8, 128.7, 128.7,

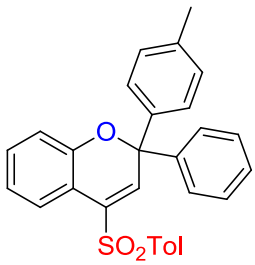
130.0, 131.3, 136.3, 136.4, 136.7, 138.3, 138.3, 144.8, 152.2, 161.2, 163.7. HRMS (ESI, m/z): calcd for $C_{28}H_{21}F_2O_3S$: $[M+H]^+$ = 475.1174; found: 475.1169.

2-(4-fluorophenyl)-2-(4-methoxyphenyl)-4-tosyl-2*H*-chromene (3f):



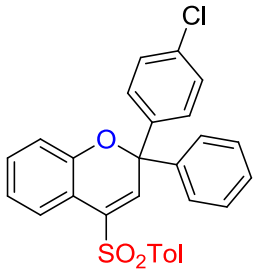
The resultant residue was purified by flash silica gel column chromatography to afford **3f** as a white solid; mp: 157–159 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.29 (s, 3 H), 3.69 (s, 3 H), 6.73 – 6.82 (m, 4 H), 6.93 (t, *J* = 8.4 Hz, 2 H), 7.03 – 7.07 (m, 1 H), 7.17 – 7.20 (m, 4 H), 7.26 – 7.30 (m, 3 H), 7.71 (d, *J* = 8.0 Hz, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.5, 55.2, 82.1, 113.9, 115.2, 115.3, 115.4, 117.5, 121.8, 125.1, 127.8, 128.2, 128.7, 128.7, 129.9, 131.2, 134.4, 135.9, 136.8, 136.9, 128.7, 138.8, 144.7, 152.4, 159.5, 161.1, 163.6. HRMS (ESI, m/z): calcd for $C_{29}H_{24}FO_4S$: $[M+H]^+$ = 487.1374; found: 487.1368.

2-phenyl-2-(p-tolyl)-4-tosyl-2*H*-chromene (3g):



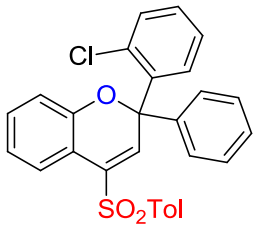
The resultant residue was purified by flash silica gel column chromatography to afford **3g** as a white solid; mp: 196–198 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.24 (s, 3 H), 2.30 (s, 3 H), 6.74 (t, *J* = 7.6 Hz, 1 H), 6.84 (d, *J* = 8.0 Hz, 1 H), 7.03 – 7.07 (m, 3 H), 7.17 – 7.27 (m, 7 H), 7.30 – 7.34 (m, 3 H), 7.69 – 7.73 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.0, 21.5, 82.6, 115.4, 117.5, 121.6, 125.0, 126.7, 126.8, 127.7, 128.0, 128.4, 129.1, 129.9, 131.0, 135.7, 136.9, 137.3, 138.0, 139.7, 142.8, 144.6, 152.6. HRMS (ESI, m/z): calcd for $C_{29}H_{25}O_3S$: $[M+H]^+$ = 453.1519; found: 453.1525.

2-(4-chlorophenyl)-2-phenyl-4-tosyl-2*H*-chromene (3h):



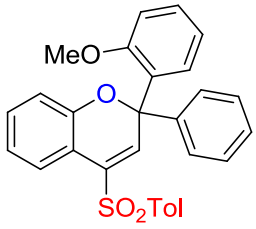
The resultant residue was purified by flash silica gel column chromatography to afford **3h** as a white solid; mp: 154–156 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (s, 3 H), 6.82 – 6.86 (m, 1 H), 6.91 (d, *J* = 8.4 Hz, 1 H), 7.12 – 7.16 (m, 1 H), 7.25 – 7.39 (m, 12 H), 7.78 – 7.81 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 82.2, 115.4, 117.5, 121.9, 125.2, 126.7, 127.8, 128.3, 128.4, 128.6, 128.7, 129.9, 131.3, 134.2, 136.4, 136.8, 141.2, 142.2, 144.7, 152.3. HRMS (ESI, m/z): calcd for $C_{28}H_{22}ClO_3S$: $[M+H]^+$ = 473.0973; found: 473.0971.

2-(2-chlorophenyl)-2-phenyl-4-tosyl-2*H*-chromene (3i):



The resultant residue was purified by flash silica gel column chromatography to afford **3i** as a white solid; mp: 60–62 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): 2.31 (s, 3 H), 6.78 (t, *J* = 8.0 Hz, 1 H), 6.87 (d, *J* = 8.0 Hz, 1 H), 7.06 – 7.10 (m, 1 H), 7.14 – 7.32 (m, 10 H), 7.38 – 7.41 (m, 1 H), 7.52 (s, 1 H), 7.74 – 7.77 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 82.6, 115.3, 117.4, 121.8, 125.1, 126.5, 127.1, 128.0, 128.4, 128.5, 129.5, 129.9, 131.1, 131.8, 132.8, 135.5, `136.2, 136.7, 138.8, 140.9, 144.7, 152.3. HRMS (ESI, m/z): calcd for $C_{28}H_{22}ClO_3S$: $[M+H]^+$ = 473.0973; found: 473.0973.

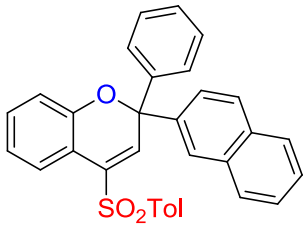
2-(2-methoxyphenyl)-2-phenyl-4-tosyl-2*H*-chromene (3j):



The resultant residue was purified by flash silica gel column chromatography to afford **3j** as a white solid; mp: 174–176 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (s, 3 H), 3.65 (s, 3 H), 6.81 (t, *J* = 7.6 Hz, 1 H), 6.89 – 6.96 (m, 3 H), 7.10 – 7.14 (m, 1 H), 7.24 – 7.36 (m, 8 H), 7.51 (dd, *J* = 1.6, 7.6 Hz, 1 H), 7.72 – 7.76 (m, 2 H), 7.80 (d, *J* = 7.6 Hz, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.5,

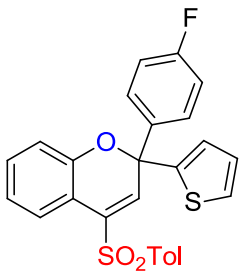
55.7, 82.0, 112.3, 115.4, 117.4, 120.6, 121.6, 124.9, 126.9, 127.7, 127.8, 128.0, 128.1, 129.7, 129.8, 130.7, 134.3, 137.7, 142.2, 144.4, 152.4, 156.1. HRMS (ESI, m/z): calcd for $C_{29}H_{25}O_4S$: $[M+H]^+$ = 469.1468; found: 469.1467.

2-(naphthalen-2-yl)-2-phenyl-4-tosyl-2*H*-chromene (3k):



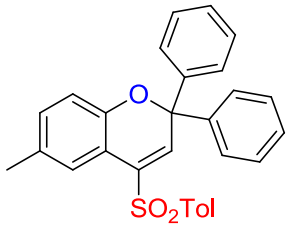
The resultant residue was purified by flash silica gel column chromatography to afford **3k** as a white solid; mp: 203–205 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.27 (s, 3 H), 6.72 – 6.76 (m, 1 H), 6.87 – 6.89 (m, 1 H), 7.02 – 7.06 (m, 1 H), 7.15 – 7.28 (m, 5 H), 7.34 – 7.42 (m, 6 H), 7.70 – 7.80 (m, 6 H), 7.81 (s, 1 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.5, 82.8, 115.5, 117.6, 121.8, 124.6, 125.1, 126.1, 126.4, 126.6, 126.9, 127.6, 127.8, 128.2, 128.4, 128.5, 129.9, 131.2, 132.7, 132.9, 136.2, 136.9, 137.0, 139.7, 142.6, 144.6, 152.5. HRMS (ESI, m/z): calcd for $C_{32}H_{25}O_3S$: $[M+H]^+$ = 489.1519; found: 489.1514.

2-(4-fluorophenyl)-2-(thiophen-2-yl)-4-tosyl-2*H*-chromene (3l):



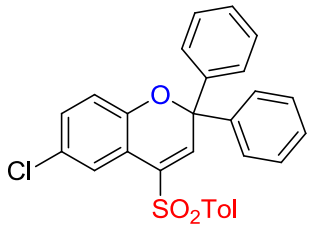
The resultant residue was purified by flash silica gel column chromatography to afford **3l** as a white solid; mp: 164–166 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3 H), 6.84 – 6.94 (m, 4 H), 7.05 (t, *J* = 8.8 Hz, 2 H), 7.13 – 7.18 (m, 1 H), 7.28 – 7.34 (m, 4 H), 7.46 – 7.50 (m, 2 H), 7.81 (d, *J* = 8.4 Hz, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 80.2, 115.2, 115.3, 115.5, 117.6, 122.1, 125.1, 126.7, 126.8, 127.1, 127.8, 128.3, 128.4, 129.9, 131.3, 135.6, 136.2, 136.7, 137.9, 139.9, 144.8, 146.4, 152.0, 161.4, 163.8. HRMS (ESI, m/z): calcd for $C_{26}H_{20}FO_3S_2$: $[M+H]^+$ = 463.0832; found: 463.0834.

6-methyl-2,2-diphenyl-4-tosyl-2*H*-chromene (3m):



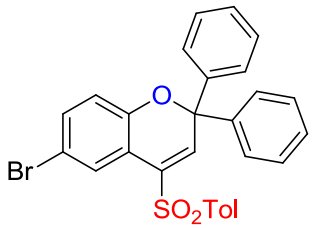
The resultant residue was purified by flash silica gel column chromatography to afford **3m** as a white solid; mp: 219–221 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.17 (s, 3 H), 2.37 (s, 3 H), 6.82 (d, *J* = 8.4 Hz, 1 H), 6.92 (dd, *J* = 1.2, 8.0 Hz, 1 H), 7.24 – 7.34 (m, 8 H), 7.38 – 7.41 (m, 5 H), 7.59 (s, 1 H), 7.79 (d, *J* = 8.4 Hz, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 20.8, 21.6, 82.5, 115.1, 117.2, 125.4, 126.8, 127.8, 128.1, 128.4, 129.9, 130.9, 131.7, 136.0, 136.9, 137.1, 142.7, 144.6, 150.3. HRMS (ESI, m/z): calcd for $C_{29}H_{25}O_3S$: $[M+H]^+$ = 453.1519; found: 453.1519.

6-chloro-2,2-diphenyl-4-tosyl-2*H*-chromene (3n):



The resultant residue was purified by flash silica gel column chromatography to afford **3n** as a yellow solid; mp: 204–206 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.33 (s, 3 H), 6.79 (d, *J* = 8.4 Hz, 1 H), 7.01 (dd, *J* = 2.4, 8.8 Hz, 1 H), 7.23 – 7.30 (m, 12 H), 7.38 (s, 1 H), 7.70 – 7.74 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 83.1, 116.7, 118.8, 124.9, 126.8, 126.8, 127.8, 128.4, 128.5, 130.1, 130.9, 135.3, 136.5, 138.1, 142.1, 144.9, 151.1. HRMS (ESI, m/z): calcd for $C_{28}H_{22}ClO_3S$: $[M+H]^+$ = 473.0973; found: 473.0968.

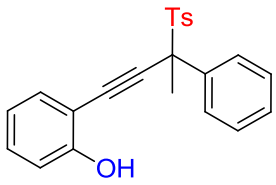
6-bromo-2,2-diphenyl-4-tosyl-2*H*-chromene (3o):



The resultant residue was purified by flash silica gel column chromatography to afford **3o** as a yellow solid; mp: 207–209 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.25 (s, 3 H), 6.66 (d, *J* = 8.8 Hz, 1 H), 7.06 – 7.09 (m, 1 H), 7.10 – 7.22 (m, 12 H), 7.30 (s, 1 H), 7.64 (d, *J* = 8.4 Hz, 2 H), 7.81 (d, *J* = 2.0 Hz, 1 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 83.0, 114.0, 117.2, 119.3, 126.8, 127.8, 127.9,

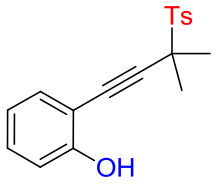
128.4, 128.5, 130.0, 133.8, 135.2, 136.5, 138.0, 142.1, 144.9, 151.6. HRMS (ESI, m/z): calcd for $C_{21}H_{16}N_5O_2$: M+H = 370.1299; found: 370.1301. HRMS (ESI, m/z): calcd for $C_{28}H_{22}BrO_3S$: $[M+H]^+$ = 517.0468; found: 517.0471.

2-(3-phenyl-3-tosylbut-1-yn-1-yl)phenol (3p'):



The resultant residue was purified by flash silica gel column chromatography to afford **3p'** as a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.23 (s, 3 H), 2.35 (s, 3 H), 6.88 (t, *J* = 7.6 Hz, 1 H), 6.90 – 7.03 (m, 1 H), 7.10 (d, *J* = 8.0 Hz, 2 H), 7.27 – 7.37 (m, 8 H), 7.53 (d, *J* = 7.6 Hz, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 22.2, 68.5, 85.0, 93.3, 108.1, 115.4, 120.1, 128.2, 128.7, 128.9, 129.2, 130.6, 131.1, 131.4, 133.9, 145.1, 158.4. HRMS (ESI, m/z): calcd for $C_{23}H_{21}O_3S$: $[M+H]^+$ = 377.1206; found: 377.1208.

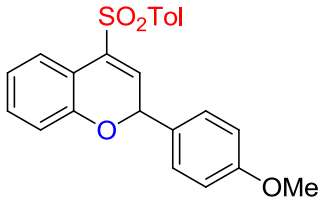
2-(3-methyl-3-tosylbut-1-yn-1-yl)phenol (3q'):



The resultant residue was purified by flash silica gel column chromatography to afford **3q'** as a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.62 (s, 6 H),

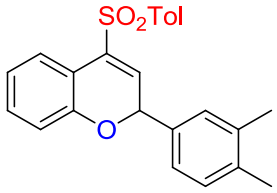
2.38 (s, 3 H), 6.04 (s, 1 H), 6.78 (t, *J* = 7.6 Hz, 1 H), 6.89 (d, *J* = 8.4 Hz, 1 H), 7.14 – 7.16 (m, 1 H), 7.18 – 7.22 (m, 1 H), 7.27 (d, *J* = 8.0 Hz, 2 H), 7.78 (d, *J* = 8.0 Hz, 2 H). $^{13}C\{H\}$ NMR (100 MHz, $CDCl_3$): δ 21.7, 23.5, 59.9, 81.5, 94.5, 108.1, 115.2, 120.2, 129.5, 130.7, 130.9, 131.3, 131.7, 145.4, 157.7. HRMS (ESI, m/z): calcd for $C_{18}H_{18}O_3S$: $[M+H]^+$ = 315.1049; found: 315.1047.

2-(4-methoxyphenyl)-4-tosyl-2*H*-chromene (5a):



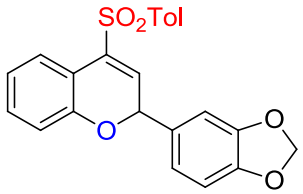
The resultant residue was purified by flash silica gel column chromatography to afford **5a** as a yellow solid; mp: 54–56 ºC. ^1H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3 H), 3.81 (s, 3 H), 5.47 (s, 1 H), 6.86 (d, *J* = 8.8 Hz, 2 H), 6.97 (s, 1 H), 7.17 – 7.29 (m, 4 H), 7.40 – 7.45 (m, 3 H), 7.50 – 7.56 (m, 3 H). $^{13}C\{H\}$ NMR (100 MHz, $CDCl_3$): δ 21.6, 55.3, 70.6, 108.3, 111.3, 114.0, 121.3, 122.3, 123.0, 124.7, 127.9, 129.3, 129.3, 131.7, 134.6, 144.8, 149.1, 154.9, 160.3. HRMS (ESI, m/z): calcd for $C_{23}H_{21}O_4S$: $[M+H]^+$ = 393.1155; found: 393.1162.

2-(3,4-dimethylphenyl)-4-tosyl-2*H*-chromene (5b):



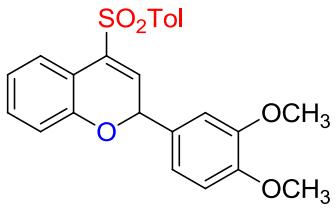
The resultant residue was purified by flash silica gel column chromatography to afford **5b** as a yellow solid; mp: 141–143 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.15 (s, 3 H), 2.16 (s, 3 H), 2.30 (s, 3 H), 5.38 (s, 1 H), 6.89 (s, 1 H), 7.02 (d, *J* = 8.0 Hz, 1 H), 7.09 – 7.20 (m, 6 H), 7.31 (d, *J* = 7.6 Hz, 1 H), 7.46 (d, *J* = 8.0 Hz, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 19.5, 19.7, 21.6, 71.0, 108.2, 111.3, 121.2, 123.0, 124.7, 127.6, 127.8, 127.9, 129.3, 129.3, 129.8, 131.5, 134.7, 136.9, 137.9, 144.7, 149.3, 154.9. HRMS (ESI, m/z): calcd for $C_{24}H_{23}O_3S$: $[M+H]^+$ = 391.1362; found: 391.1357.

2-(benzo[*d*][1,3]dioxol-5-yl)-4-tosyl-2*H*-chromene (5c):



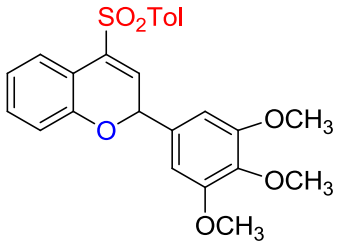
The resultant residue was purified by flash silica gel column chromatography to afford **5c** as a white solid; mp: 165–167 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3 H), 5.43 (s, 1 H), 5.98 (d, *J* = 8.0 Hz, 2 H), 6.74 (d, *J* = 8.4 Hz, 1 H), 6.88 (dd, *J* = 1.6, 8.0 Hz, 1 H), 6.96 (s, 1 H), 7.17 – 7.30 (m, 5 H), 7.41 (d, *J* = 8.4 Hz, 1 H), 7.55 (d, *J* = 8.4 Hz, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 70.8, 101.4, 108.2, 108.3, 110.5, 111.3, 121.3, 123.1, 123.8, 124.7, 124.8, 127.8, 129.2, 129.4, 134.6, 144.9, 147.8, 148.5, 148.9, 154.9. HRMS (ESI, m/z): calcd for $C_{23}H_{19}O_5S$: $[M+H]^+$ = 407.0948; found: 407.0951.

2-(3,4-dimethoxyphenyl)-4-tosyl-2*H*-chromene (5d):



The resultant residue was purified by flash silica gel column chromatography to afford **5d** as a yellow solid; mp: 56–58 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3 H), 3.82 (s, 3 H), 3.86 (s, 3 H), 5.47 (s, 1 H), 6.80 (d, *J* = 8.4 Hz, 1 H), 6.98 (s, 1 H), 7.03 – 7.06 (m, 2 H), 7.17 – 7.30 (m, 4 H), 7.41 (d, *J* = 8.0 Hz, 1 H), 7.51 – 7.56 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.5, 55.8, 70.8, 108.3, 110.9, 111.2, 113.3, 121.3, 122.6, 123.0, 123.2, 124.8, 127.8, 129.2, 129.3, 134.5, 144.8, 148.7, 148.9, 149.7, 154.9. HRMS (ESI, m/z): calcd for $C_{24}H_{23}O_5S$: $[M+H]^+$ = 423.1261; found: 423.1263.

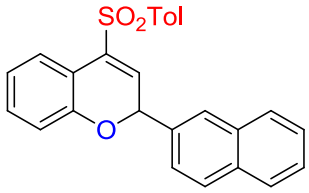
4-tosyl-2-(3,4,5-trimethoxyphenyl)-2*H*-chromene (5e):



The resultant residue was purified by flash silica gel column chromatography to afford **5e** as a yellow solid; mp: 167–169 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3 H), 3.79 (s, 6 H), 3.84 (s, 3 H), 5.44 (s, 1 H), 6.71 (s, 2 H), 7.00 (s, 1 H), 7.19 – 7.31 (m, 4 H), 7.41 (d, *J* = 8.4 Hz, 1 H), 7.53 – 7.57 (m, 3 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.5, 56.1, 60.8, 71.2, 107.7, 108.4, 111.2, 121.3, 123.1, 124.9, 125.7, 127.7, 129.3, 134.5, 138.8, 144.9, 148.7, 153.1, 154.9.

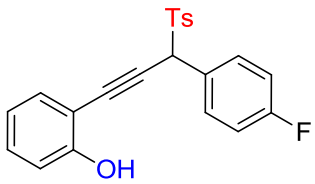
HRMS (ESI, m/z): calcd for $C_{25}H_{25}O_6S$: $[M+H]^+$ = 453.1366; found: 453.1361.

2-(naphthalen-2-yl)-4-tosyl-2*H*-chromene (5f):



The resultant residue was purified by flash silica gel column chromatography to afford **5f** as a yellow solid; mp: 163–165 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.26 (s, 3 H), 5.62 (s, 1 H), 6.98 (s, 1 H), 7.05 (d, *J* = 8.4 Hz, 2 H), 7.12 – 7.22 (m, 2 H), 7.34 – 7.49 (m, 6 H), 7.56 – 7.59 (m, 1 H), 7.69 – 7.74 (m, 3 H), 7.88 (s, 1 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 21.6, 71.4, 108.5, 111.3, 121.3, 123.1, 124.8, 126.4, 126.8, 127.2, 127.6, 127.8, 127.9, 128.2, 128.3, 129.3, 129.4, 130.4, 132.9, 133.3, 134.6, 144.9, 148.9, 155.0. HRMS (ESI, m/z): calcd for $C_{26}H_{21}O_3S$: $[M+H]^+$ = 413.1206; found: 413.1208.

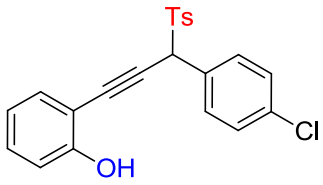
2-(3-(4-fluorophenyl)-3-tosylprop-1-yn-1-yl)phenol (5g'):



The resultant residue was purified by flash silica gel column chromatography to afford **5g'** as a yellow solid; mp: 131–133 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.41 (s, 3 H), 5.34 (s, 1 H), 6.87 (t, *J* = 7.6 Hz, 1 H), 6.97 – 7.04 (m, 3 H), 7.23

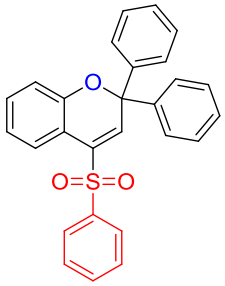
– 7.29 (m, 4 H), 7.31 – 7.37 (m, 2 H), 7.53 (d, *J* = 8.0 Hz, 2 H). $^{13}C\{H\}$ NMR (100 MHz, $CDCl_3$): δ 21.6, 65.3, 84.9, 87.6, 107.8, 115.4, 115.5, 115.7, 120.2, 125.6, 125.6, 129.5, 129.8, 131.3, 131.4, 131.7, 131.7, 132.3, 145.7, 158.1, 162.2, 164.7. HRMS (ESI, m/z): calcd for $C_{22}H_{18}FO_3S$: $[M+H]^+$ = 381.0955; found: 381.0952.

2-(3-(4-chlorophenyl)-3-tosylprop-1-yn-1-yl)phenol (5h'):



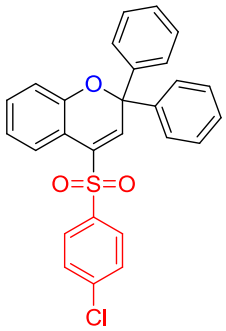
The resultant residue was purified by flash silica gel column chromatography to afford **5h'** as a white solid; mp: 126–128 ºC. ^1H NMR (400 MHz, $CDCl_3$): δ 2.35 (s, 3 H), 5.25 (s, 1 H), 6.21 (s, 1H), 6.79 (t, *J* = 7.6 Hz, 1 H), 6.91 (d, *J* = 8.4 Hz, 1 H), 7.17 – 7.23 (m, 8 H), 7.47 (d, *J* = 8.4 Hz, 2 H). $^{13}C\{H\}$ NMR (100 MHz, $CDCl_3$): δ 21.7, 65.4, 85.0, 87.4, 107.8, 115.4, 120.2, 128.3, 128.8, 129.5, 129.8, 131.2, 131.3, 131.4, 132.3, 135.8, 145.7, 158.1. HRMS (ESI, m/z): calcd for $C_{22}H_{18}ClO_3S$: $[M+H]^+$ = 397.0660; found: 397.0666.

2,2-diphenyl-4-(phenylsulfonyl)-2*H*-chromene (3aa):



The resultant residue was purified by flash silica gel column chromatography to afford **3aa** as a yellow solid; mp: 171–173 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.80 – 6.84 (m, 1 H), 6.93 (d, *J* = 8.0 Hz, 1 H), 7.11 – 7.16 (m, 1 H), 7.27 – 7.50 (m, 13 H), 7.54 – 7.58 (m, 1 H), 7.77 (dd, *J* = 1.2, 9.2 Hz, 1 H), 7.90 – 7.93 (m, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 82.7, 115.3, 117.5, 121.7, 125.0, 126.8, 127.6, 128.2, 128.5, 129.3, 131.2, 133.6, 135.7, 137.5, 139.9, 142.6, 152.5. HRMS (ESI, m/z): calcd for $C_{27}H_{21}O_3S$: $[M+H]^+$ = 425.1206; found: 425.1201.

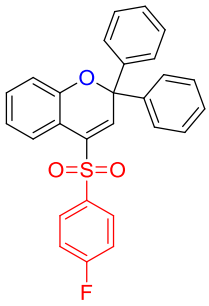
4-((4-chlorophenyl)sulfonyl)-2,2-diphenyl-2*H*-chromene (3ab):



The resultant residue was purified by flash silica gel column chromatography to afford **3ab** as a yellow solid; mp: 195–197 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.82 – 6.86 (m, 1 H), 6.95 (d, *J* = 8.0 Hz, 1 H), 7.14 – 7.18 (m, 1 H), 7.28 – 7.38 (m, 10 H), 7.40 – 7.47 (m, 3 H), 7.75 (dd, *J* = 1.2, 8.0 Hz, 1 H), 7.84 (d, *J* = 8.8 Hz, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 82.7, 115.1, 117.7, 121.8, 124.8,

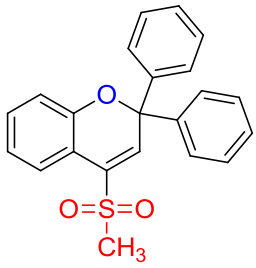
126.8, 128.3, 128.5, 129.2, 129.6, 131.4, 135.5, 137.9, 138.4, 140.4, 142.5, 152.5. HRMS (ESI, m/z): calcd for $C_{27}H_{20}ClO_3S$: $[M+H]^+$ = 459.0816; found: 459.0818.

4-((4-fluorophenyl)sulfonyl)-2,2-diphenyl-2*H*-chromene (3ac):



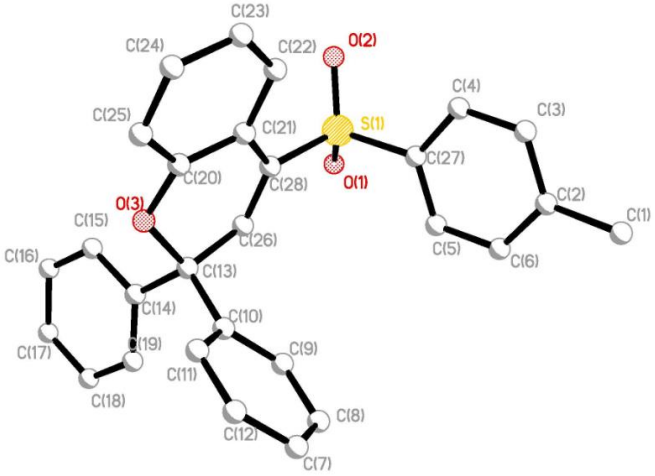
The resultant residue was purified by flash silica gel column chromatography to afford **3ac** as a white solid; mp: 166–168 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.82 – 6.86 (m, 1 H), 6.94 – 6.96 (m, 1 H), 7.15 (t, *J* = 8.0 Hz, 3 H), 7.27 – 7.41 (m, 10 H), 7.44 (s, 1 H), 7.77 (dd, *J* = 0.8, 8.0 Hz, 1 H), 7.91 – 7.94 (m, 2 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 82.7, 115.1, 116.5, 116.8, 117.7, 121.8, 124.9, 126.8, 128.2, 128.5, 130.5, 130.6, 131.4, 135.6, 135.9, 137.7, 142.5, 152.6, 164.4, 166.9. HRMS (ESI, m/z): calcd for $C_{27}H_{20}FO_3S$: $[M+H]^+$ = 443.1112; found: 443.1113.

4-(methylsulfonyl)-2,2-diphenyl-2*H*-chromene (3ad):



The resultant residue was purified by flash silica gel column chromatography to afford **3ad** as a white solid; mp: 188–190 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.05 (s, 3 H), 6.96 (t, *J* = 7.6 Hz, 1 H), 7.05 (d, *J* = 8.4 Hz, 1 H), 7.24 – 7.35 (m, 8 H), 7.39 – 7.41 (m, 4 H), 7.87 (d, *J* = 7.6 Hz, 1 H). ^{13}C{H} NMR (100 MHz, $CDCl_3$): δ 42.5, 82.5, 115.5, 117.9, 122.2, 124.5, 126.7, 128.2, 128.5, 131.5, 135.5, 137.3, 142.4, 152.6. HRMS (ESI, m/z): calcd for $C_{22}H_{19}O_3S$: $[M+H]^+$ = 363.1049; found: 363.1047.

Crystal preparation and X-ray diffraction analysis of compound 3a



X-ray structure of 3a

Datablock: 1

Bond precision: C-C = 0.0029 A Wavelength=0.71073

Cell: a=10.465(2) b=9.797(2) c=22.032(5)
alpha=90 beta=95.834(3) gamma=90
Temperature: 296 K

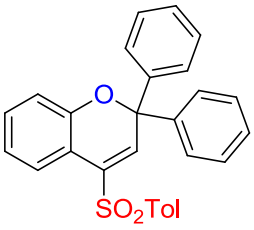
	Calculated	Reported
Volume	2247.1(8)	2247.2(8)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H22 O3 S	?
Sum formula	C28 H22 O3 S	C28 H22 O3 S
Mr	438.52	438.51
Dx,g cm-3	1.296	1.296
Z	4	4
Mu (mm-1)	0.172	0.172
F000	920.0	920.0
F000'	920.89	
h,k,lmax	13,12,28	13,12,28
Nref	5206	4989
Tmin,Tmax	0.950,0.963	
Tmin'	0.950	

Correction method= Not given

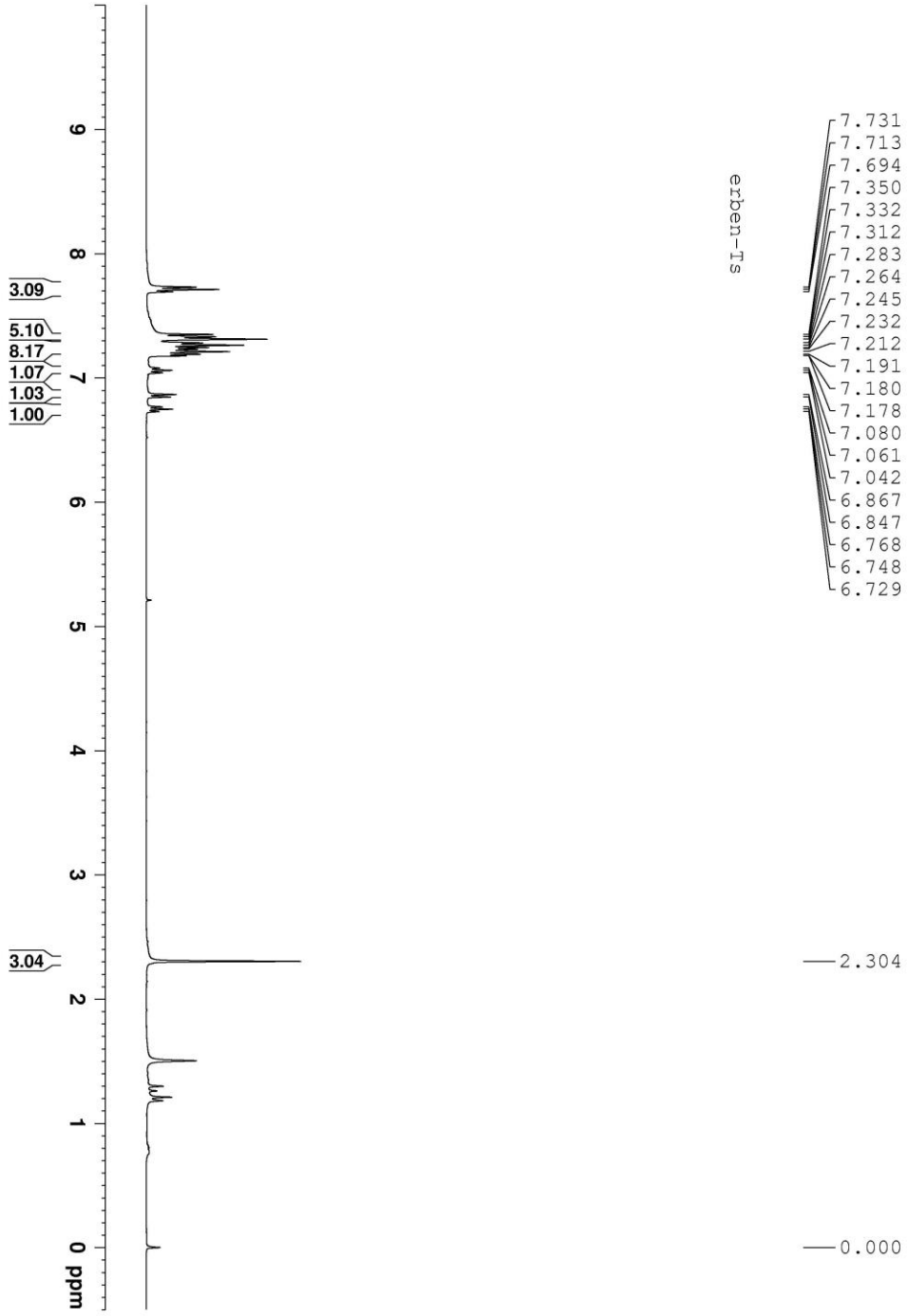
Data completeness= 0.958 Theta(max)= 27.577

R(reflections)= 0.0448(4168) wR2(reflections)= 0.1194(4989)

S = 1.093 Npar= 290


O
SO2Tol

3a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5.10
8.17
1.07
1.03
1.00
3.04
9
8
7
6
5
4
3
2
1
0 ppm
erben-Ts
7.731
7.713
7.694
7.350
7.332
7.312
7.283
7.264
7.245
7.232
7.212
7.191
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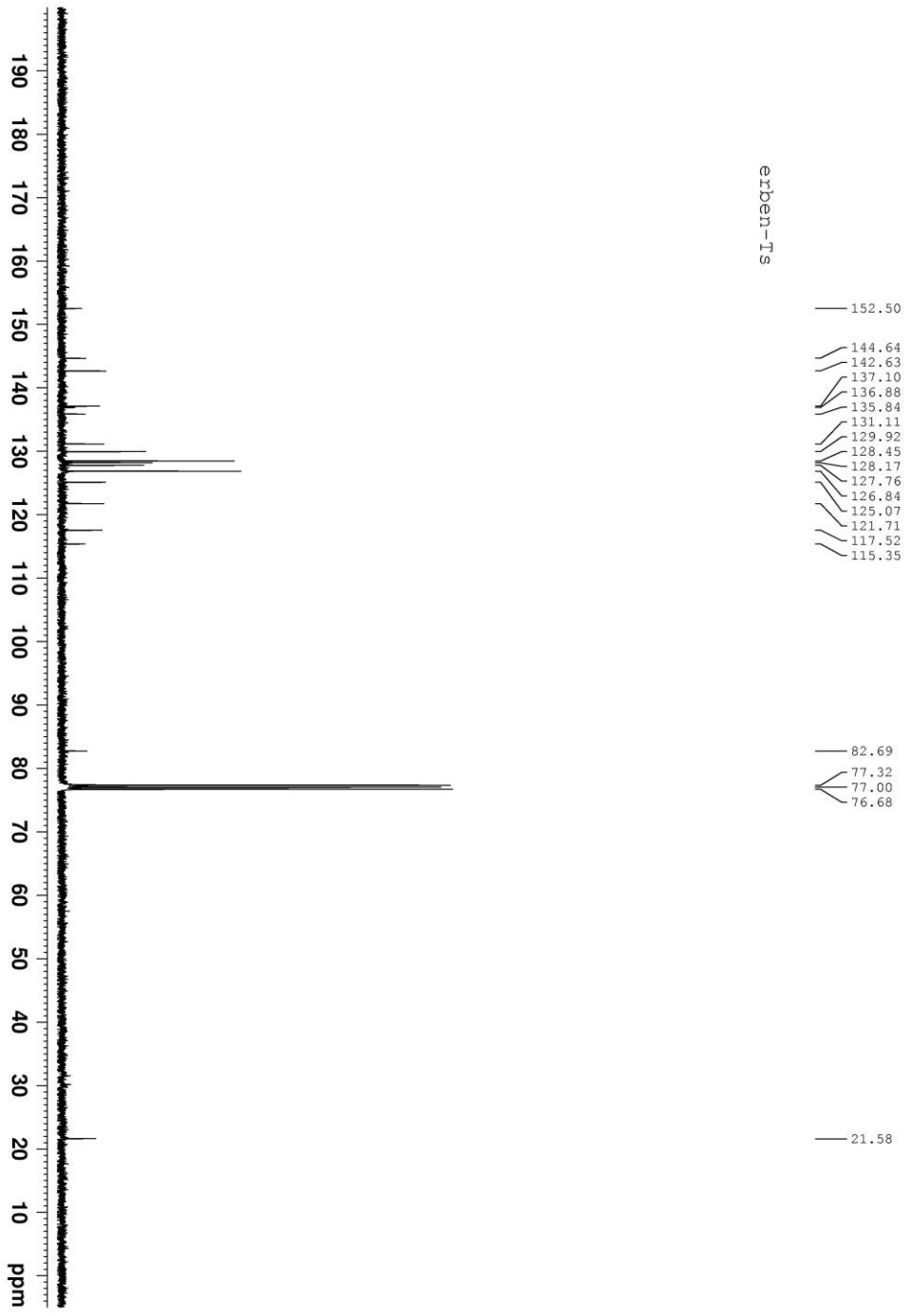
6.768
6.748
6.729
2.304
0.000


erben-Ts
152.50
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142.63
137.10
136.88
135.84
131.11
129.92
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128.17
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125.07
121.71
117.52
115.35
82.69
77.32
77.00
76.68
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80
70
60
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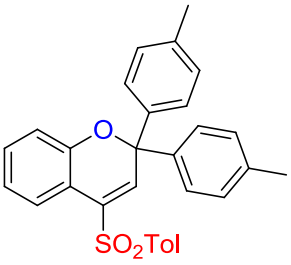
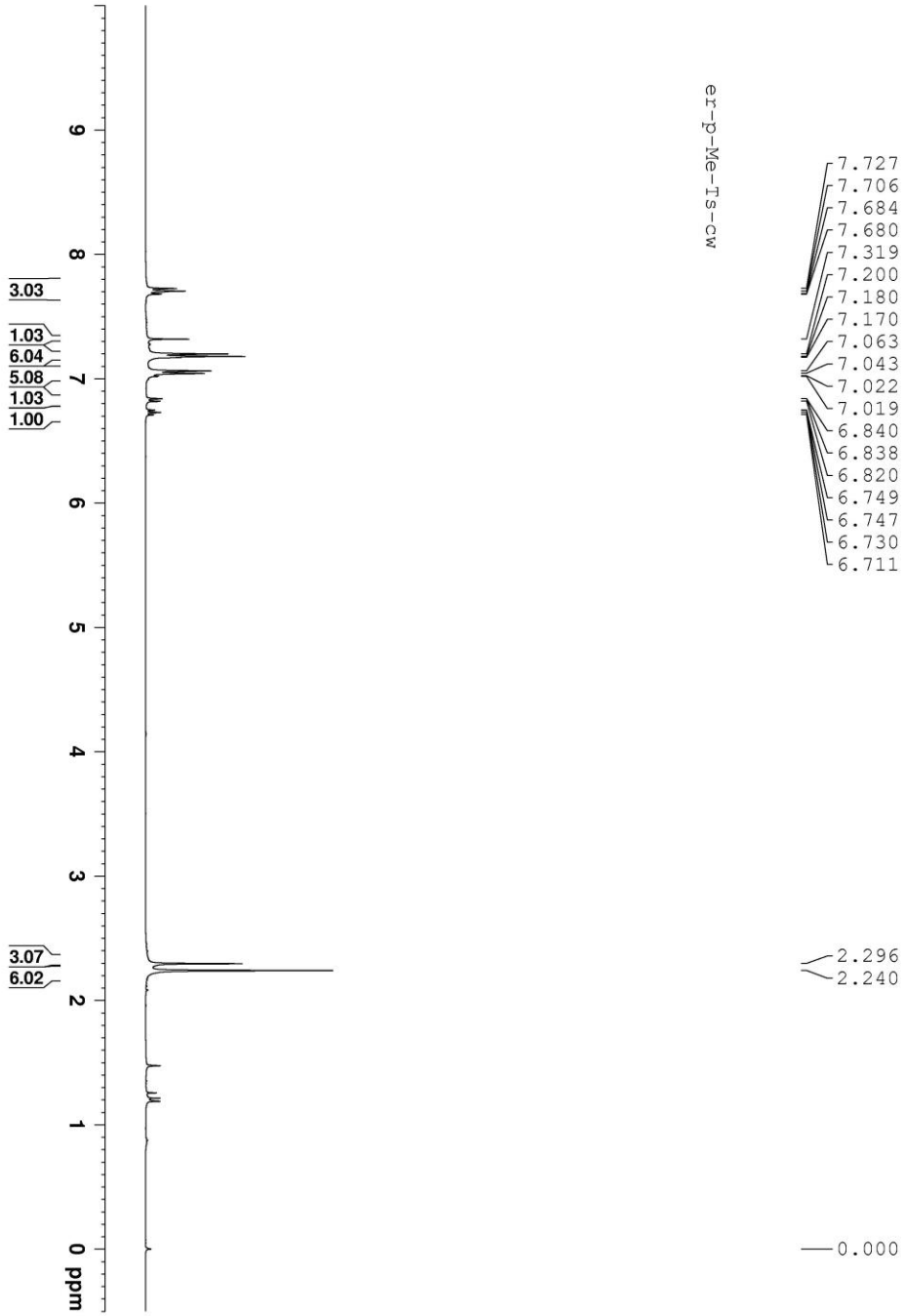
40
30
20
10
ppm


O
SO2Tol

3b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7.706
7.684
7.680
7.319
7.200
7.180
7.170
7.063
7.043
7.022
7.019
6.840
6.838
6.820
6.749
6.747
6.730
6.711
2.296
2.240
0.000
3.03
1.03
6.04
5.08
1.03
1.00
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6.02
9
8
7
6
5
4
3
2
1
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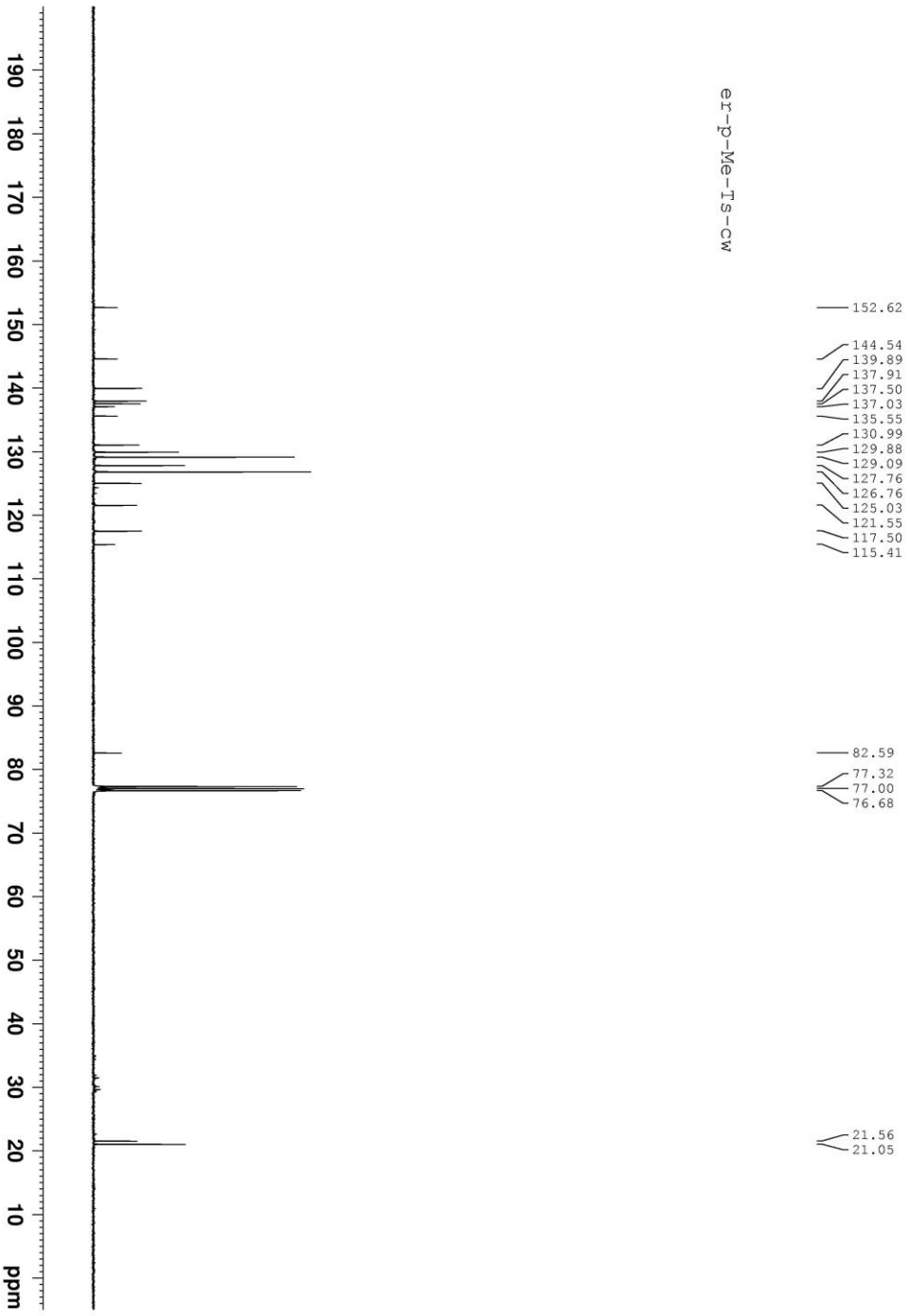
er-p-Me-Is-cw
152.62
144.54
139.89
137.91
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121.55
117.50
115.41
82.59
77.32
77.00
76.68
21.56
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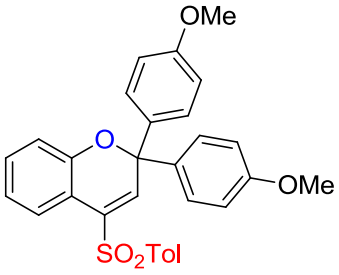
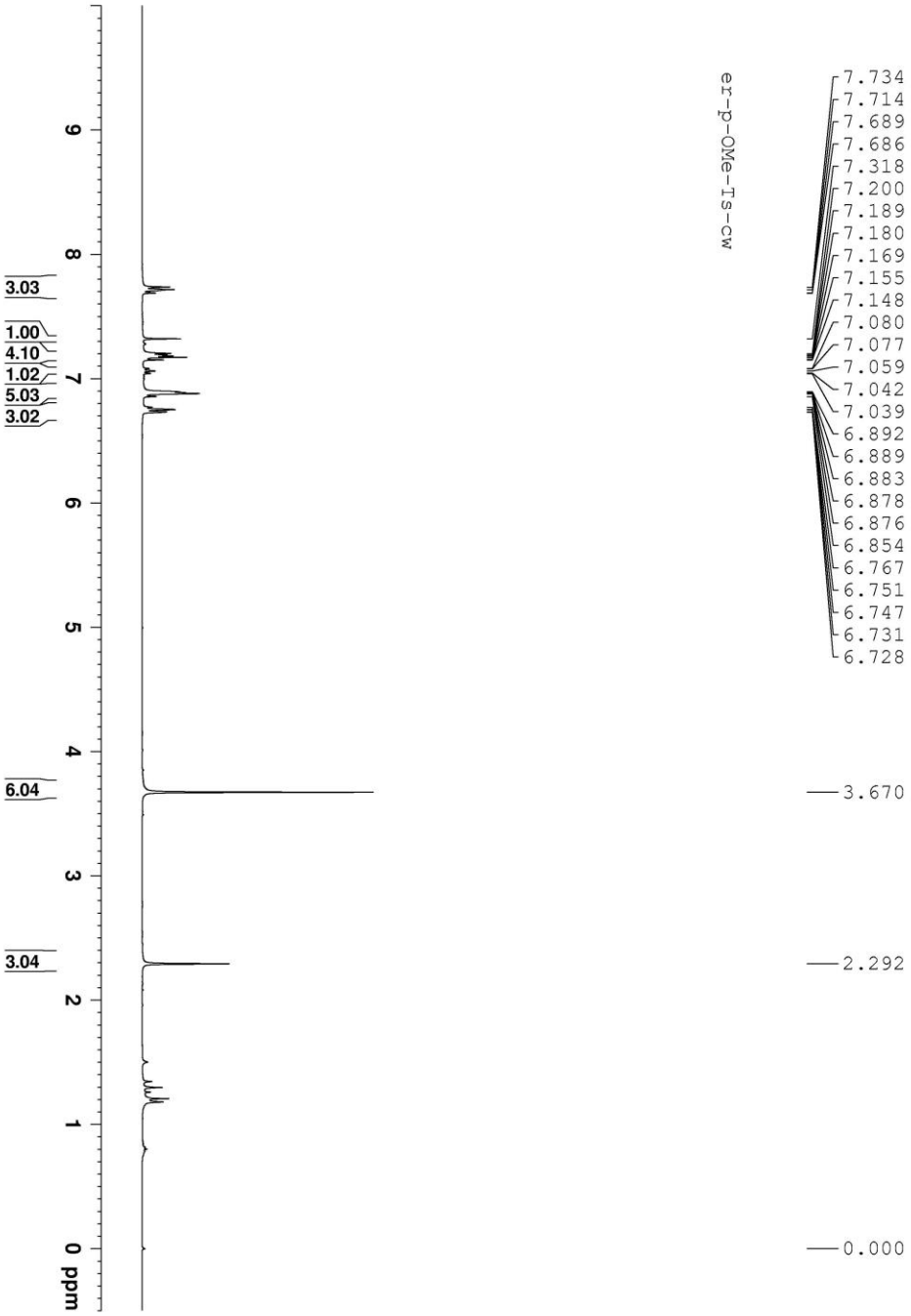
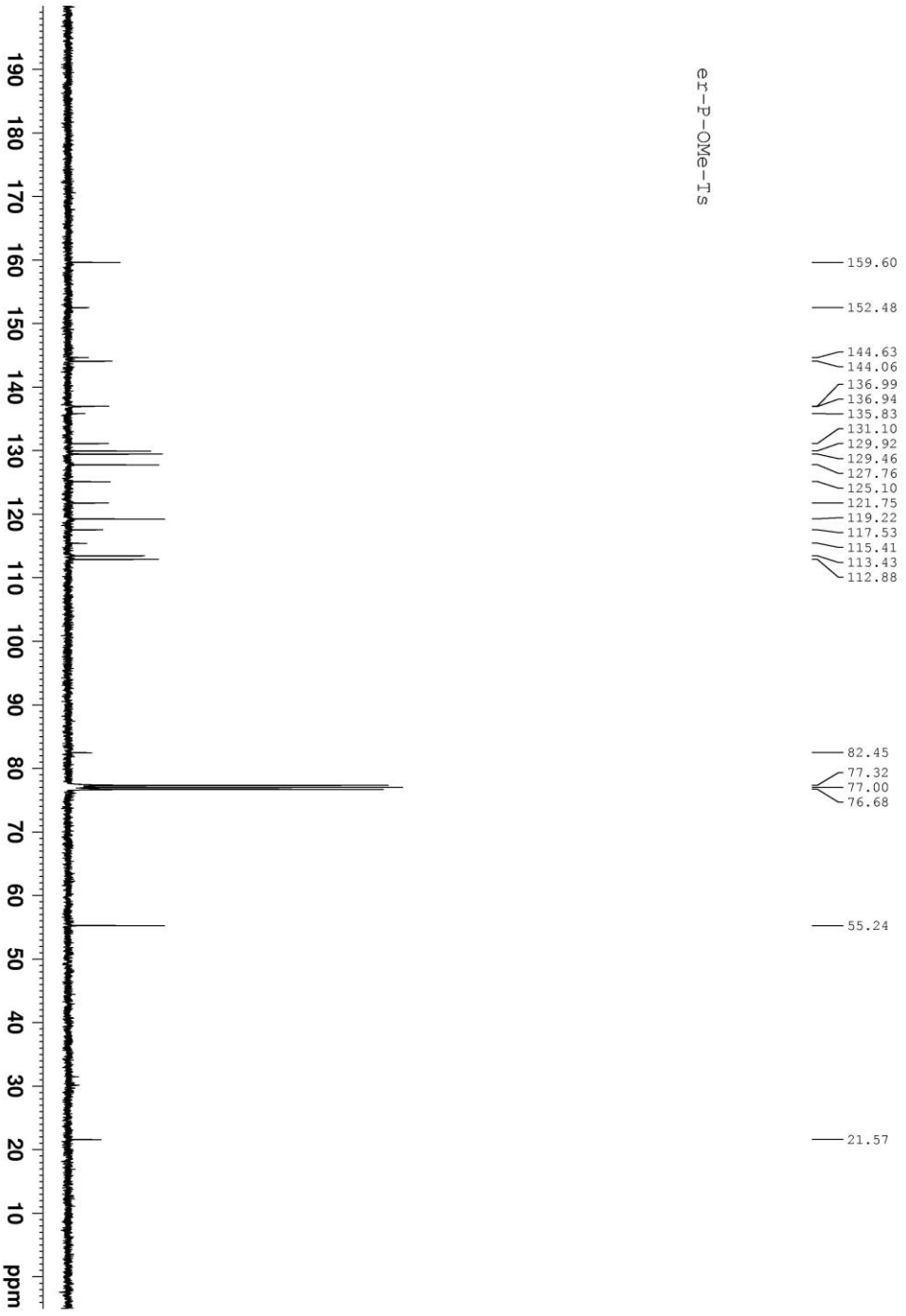
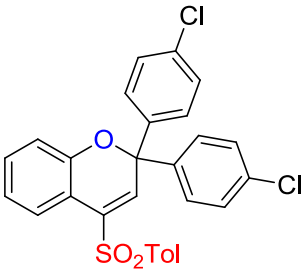
90
80
70
60
50
40
30
20
10
ppm


OMe
O
OMe
SO2Tol

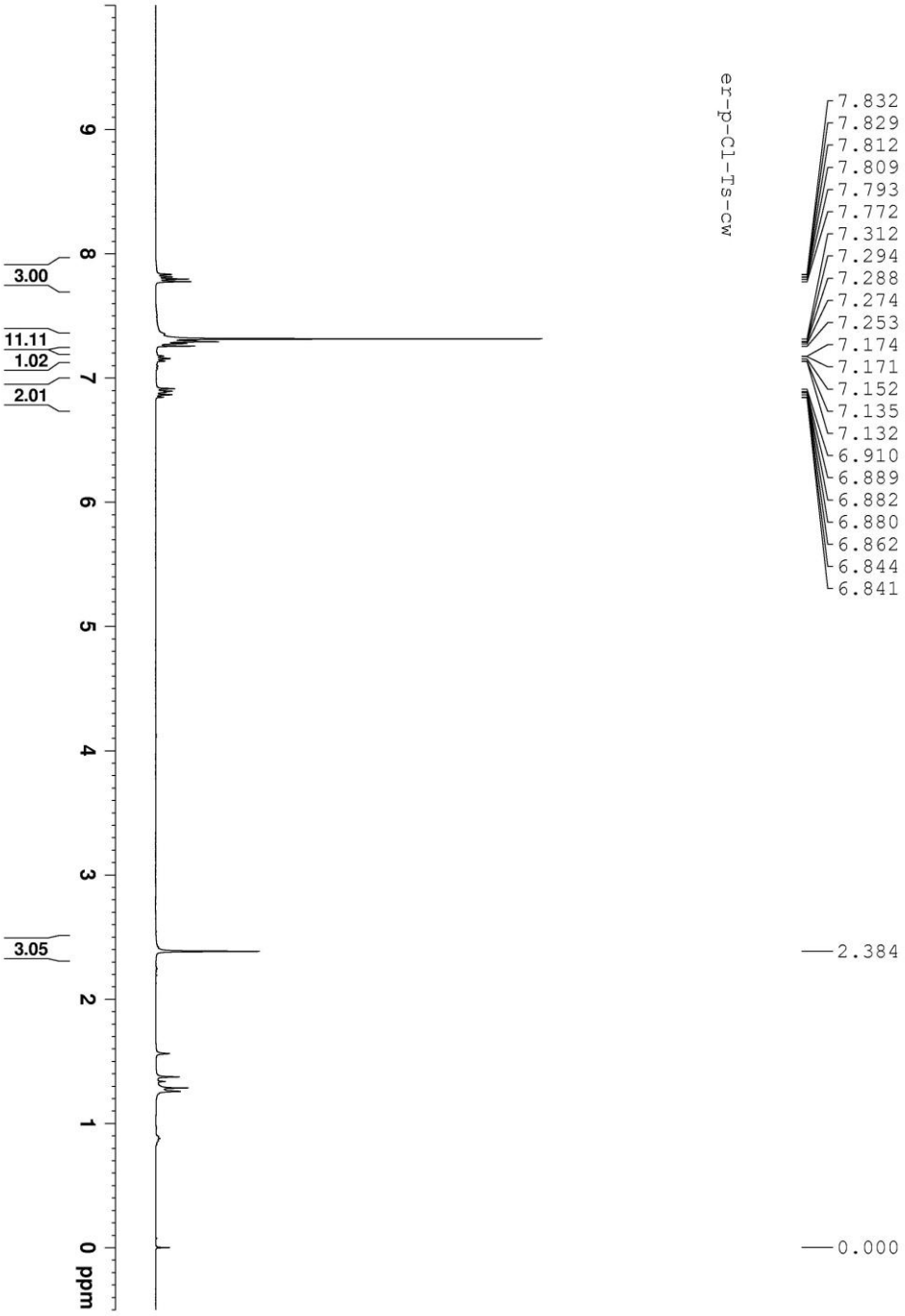
3c

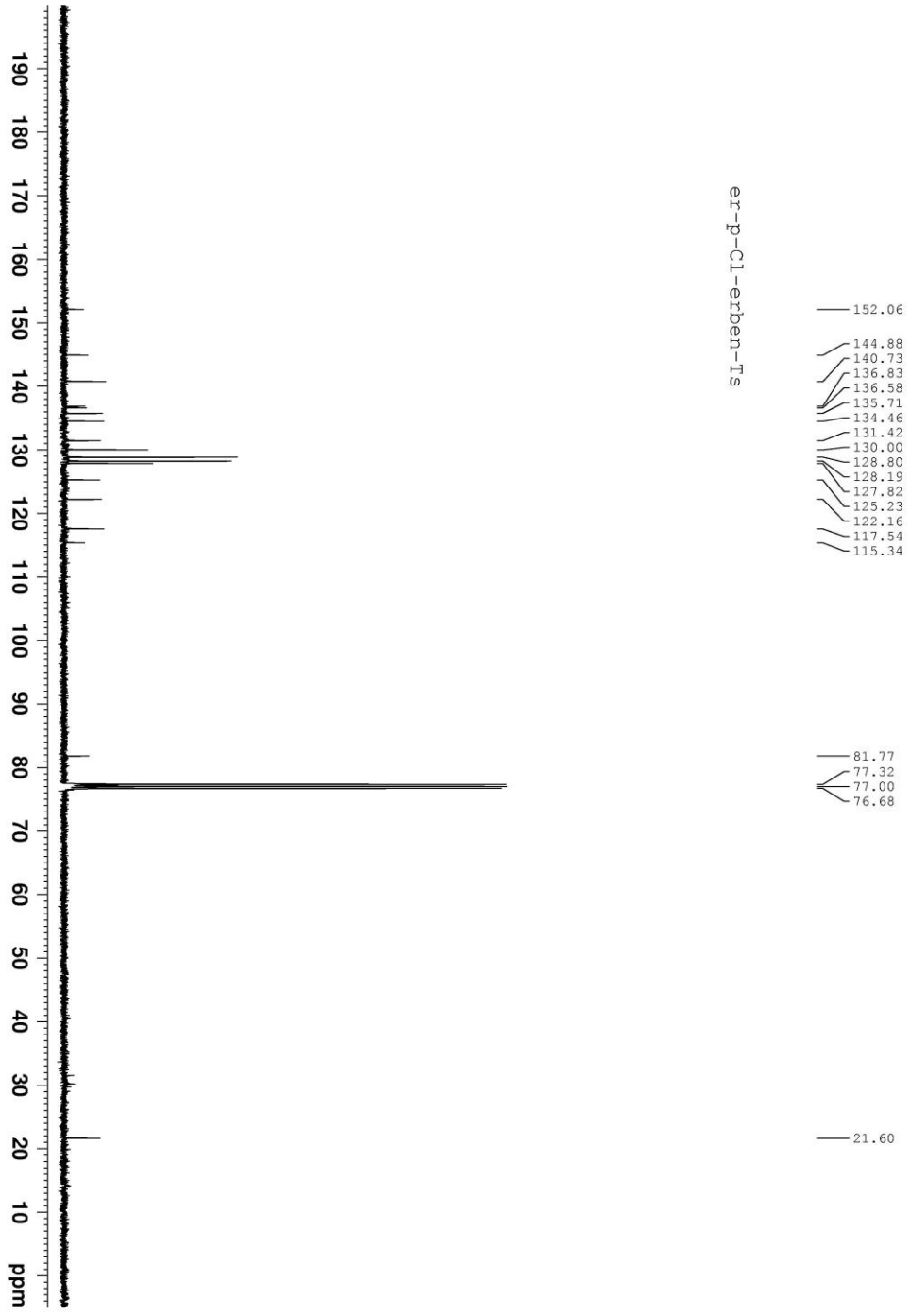

erp-OMe-1s-cw
7.734
7.714
7.689
7.686
7.318
7.200
7.189
7.180
7.169
7.155
7.148
7.080
7.077
7.059
7.042
7.039
6.892
6.889
6.883
6.878
6.876
6.854
6.767
6.751
6.747
6.731
6.728
3.670
2.292
0.000
3.03
1.00
4.10
1.02
5.03
3.02
6.04
3.04
9
8
7
6
5
4
3
2
1
0 ppm

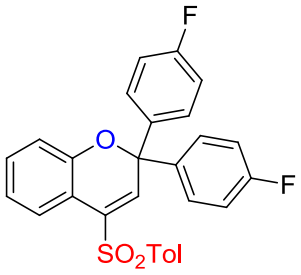

er-p-OMe-1s
159.60
152.48
144.63
144.06
136.99
136.94
135.83
131.10
129.92
129.46
127.76
125.10
121.75
119.22
117.53
115.41
113.43
112.88
82.45
77.32
77.00
76.68
55.24
21.57
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
O
Cl
SO2Tol

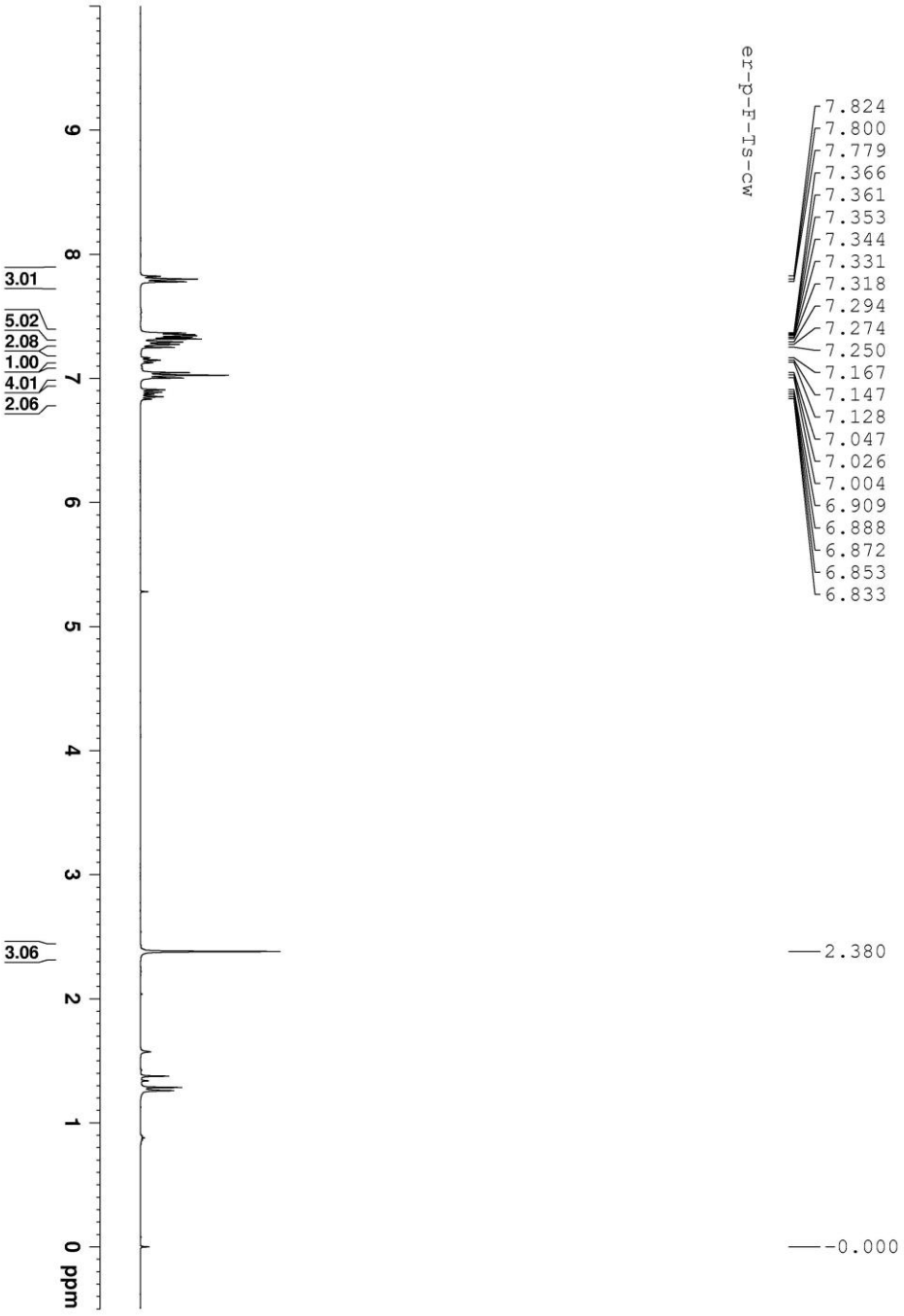
3d

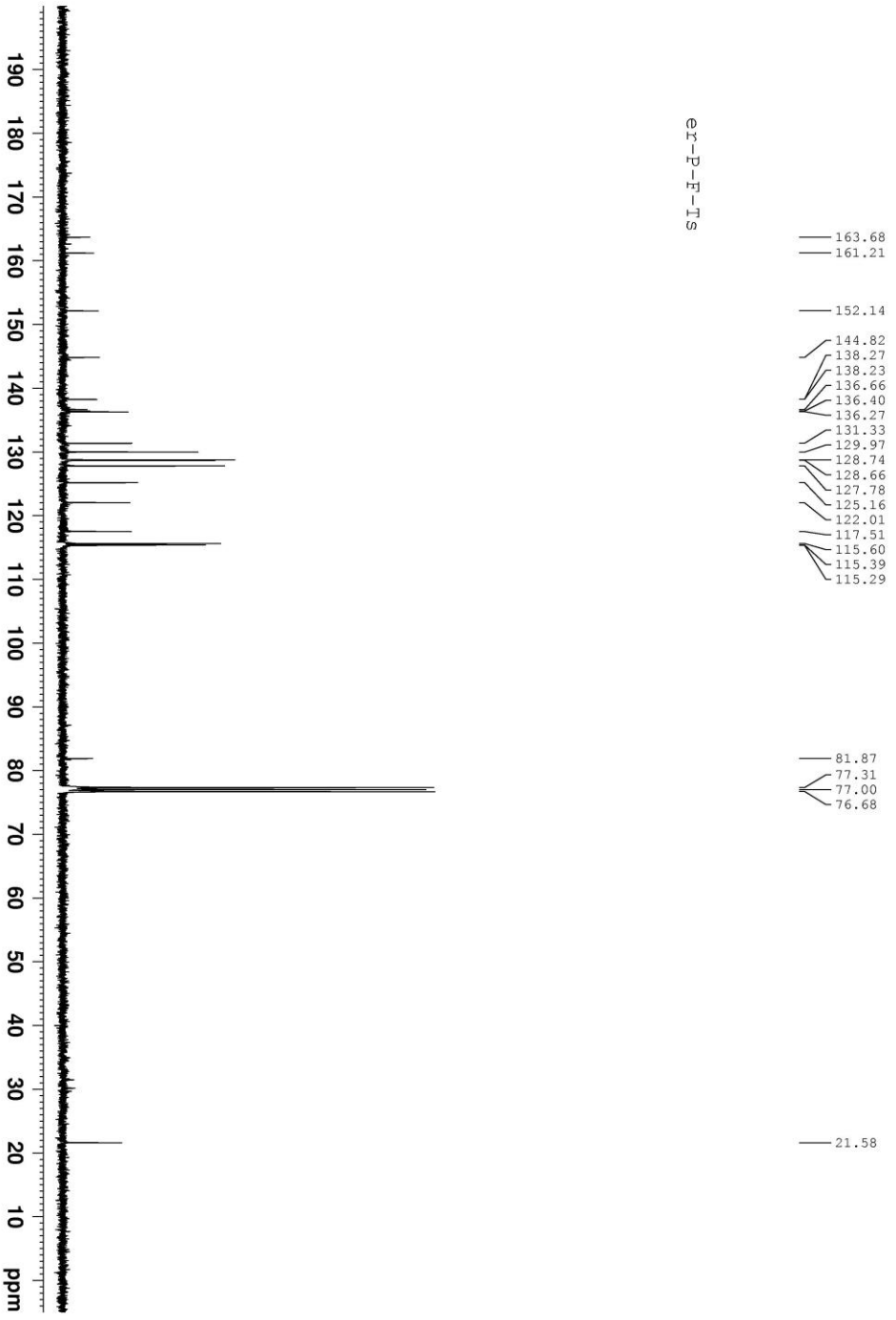

re-p-Cl-1s-cm
7.832
7.829
7.812
7.809
7.793
7.772
7.312
7.294
7.288
7.274
7.253
7.174
7.171
7.152
7.135
7.132
6.910
6.889
6.882
6.880
6.862
6.844
6.841
2.384
0.000
3.00
11.11
1.02
2.01
3.05
9
8
7
6
5
4
3
2
1
0 ppm

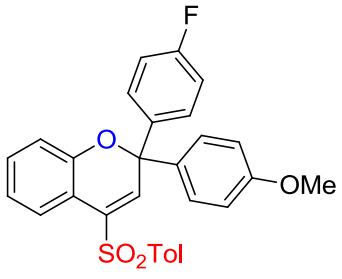

er-p-Cl-erben-Ts
152.06
144.88
140.73
136.83
136.58
135.71
134.46
131.42
130.00
128.80
128.19
127.82
125.23
122.16
117.54
115.34
81.77
77.32
77.00
76.68
21.60
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


F
O
F
SO2Tol

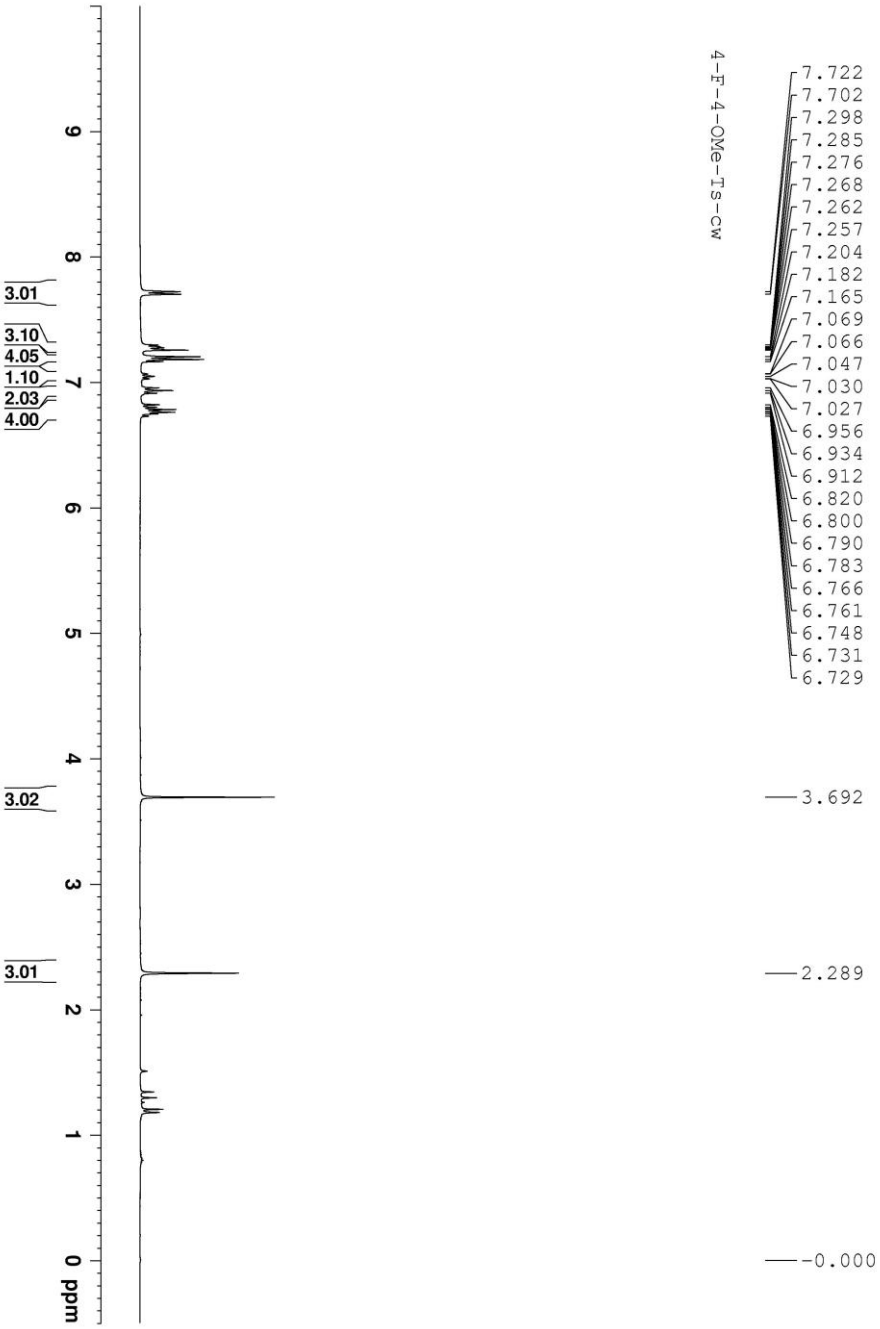
3e

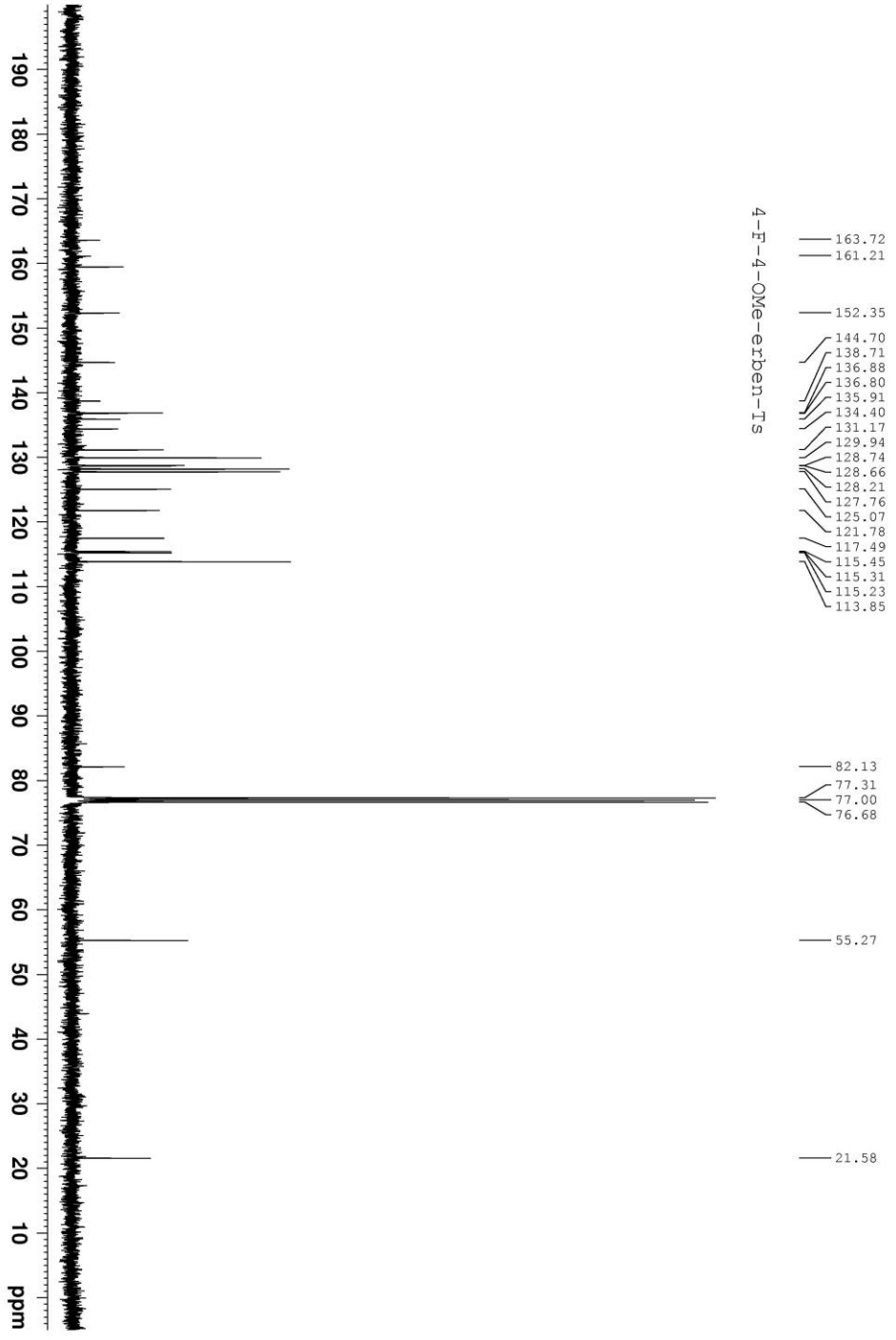

er-p-F-Is-cw
7.824
7.800
7.779
7.366
7.361
7.353
7.344
7.331
7.318
7.294
7.274
7.250
7.167
7.147
7.128
7.047
7.026
7.004
6.909
6.888
6.872
6.853
6.833
3.01
5.02
2.08
1.00
4.01
2.06
3.06
2.380
-0.000
ppm

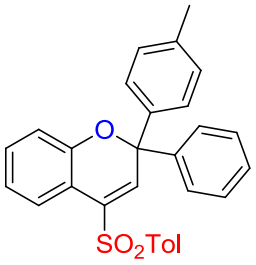

er-P-F-Ts
163.68
161.21
152.14
144.82
138.27
138.23
136.66
136.40
136.27
131.33
129.97
128.74
128.66
127.78
125.16
122.01
117.51
115.60
115.39
115.29
81.87
77.31
77.00
76.68
21.58
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


F
O
OMe
SO2Tol

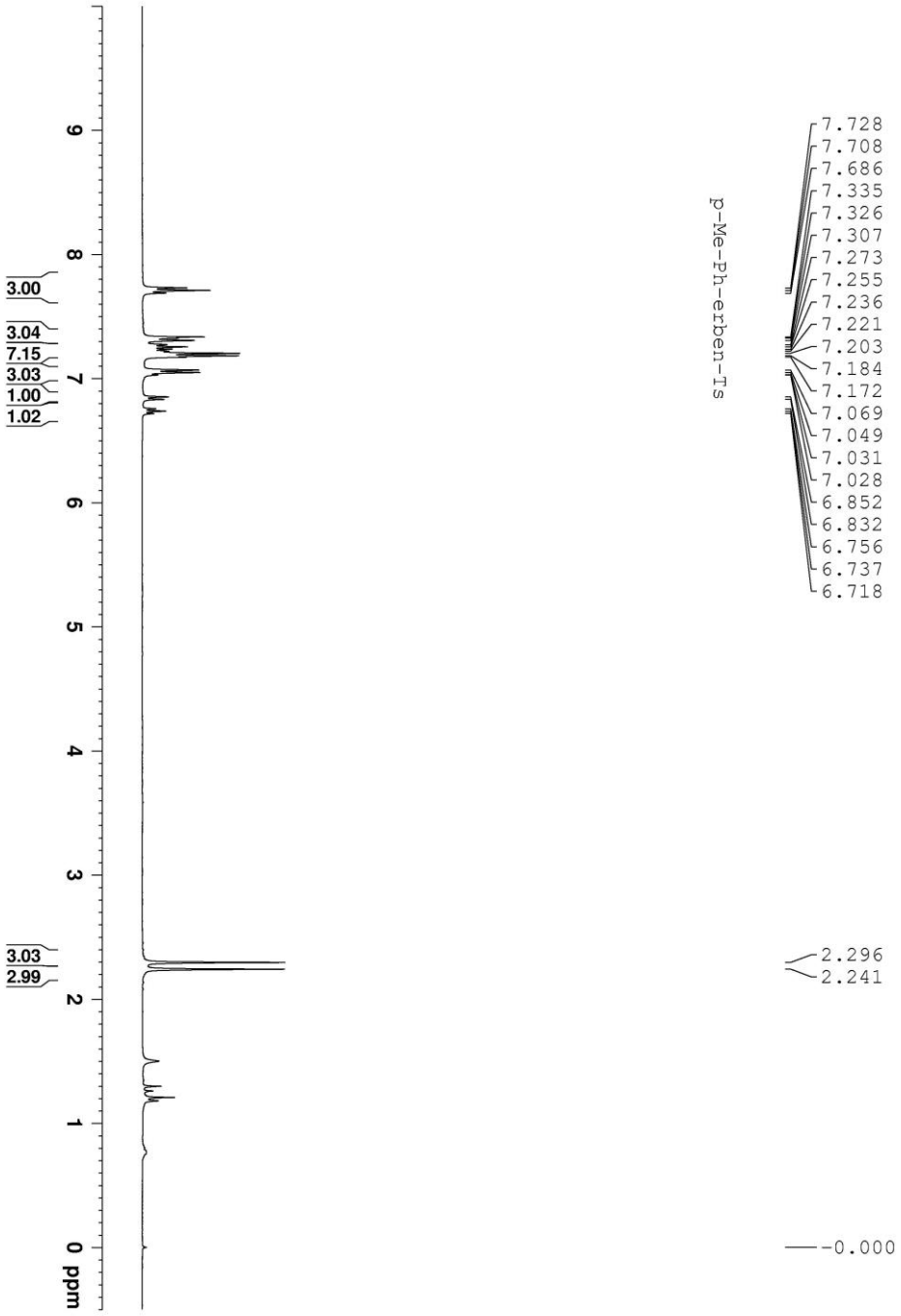
3f

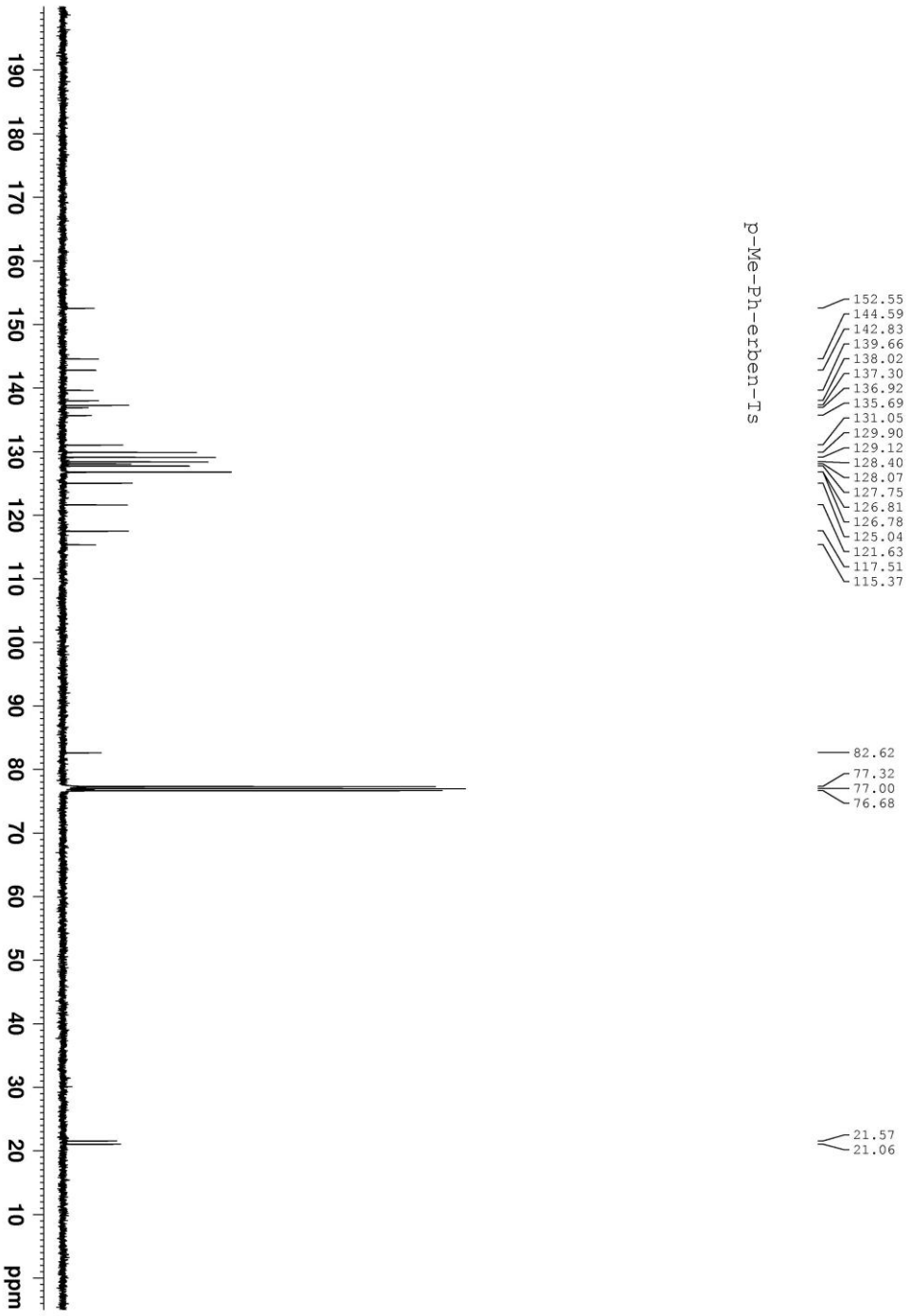

4-F-4-OMe-Ts-cw
7.722
7.702
7.298
7.285
7.276
7.268
7.262
7.257
7.204
7.182
7.165
7.069
7.066
7.047
7.030
7.027
6.956
6.934
6.912
6.820
6.800
6.790
6.783
6.766
6.761
6.748
6.731
6.729
3.692
2.289
-0.000
3.01
3.10
4.05
1.10
2.03
4.00
3.02
3.01
ppm

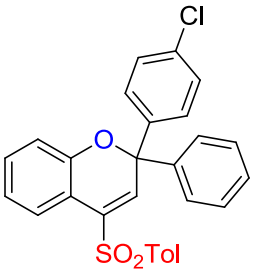

4-F-4-OMe-erben-Ts
163.72
161.21
152.35
144.70
138.71
136.88
136.80
135.91
134.40
131.17
129.94
128.74
128.66
128.21
127.76
125.07
121.78
117.49
115.45
115.31
115.23
113.85
82.13
77.31
77.00
76.68
55.27
21.58
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
SO2Tol

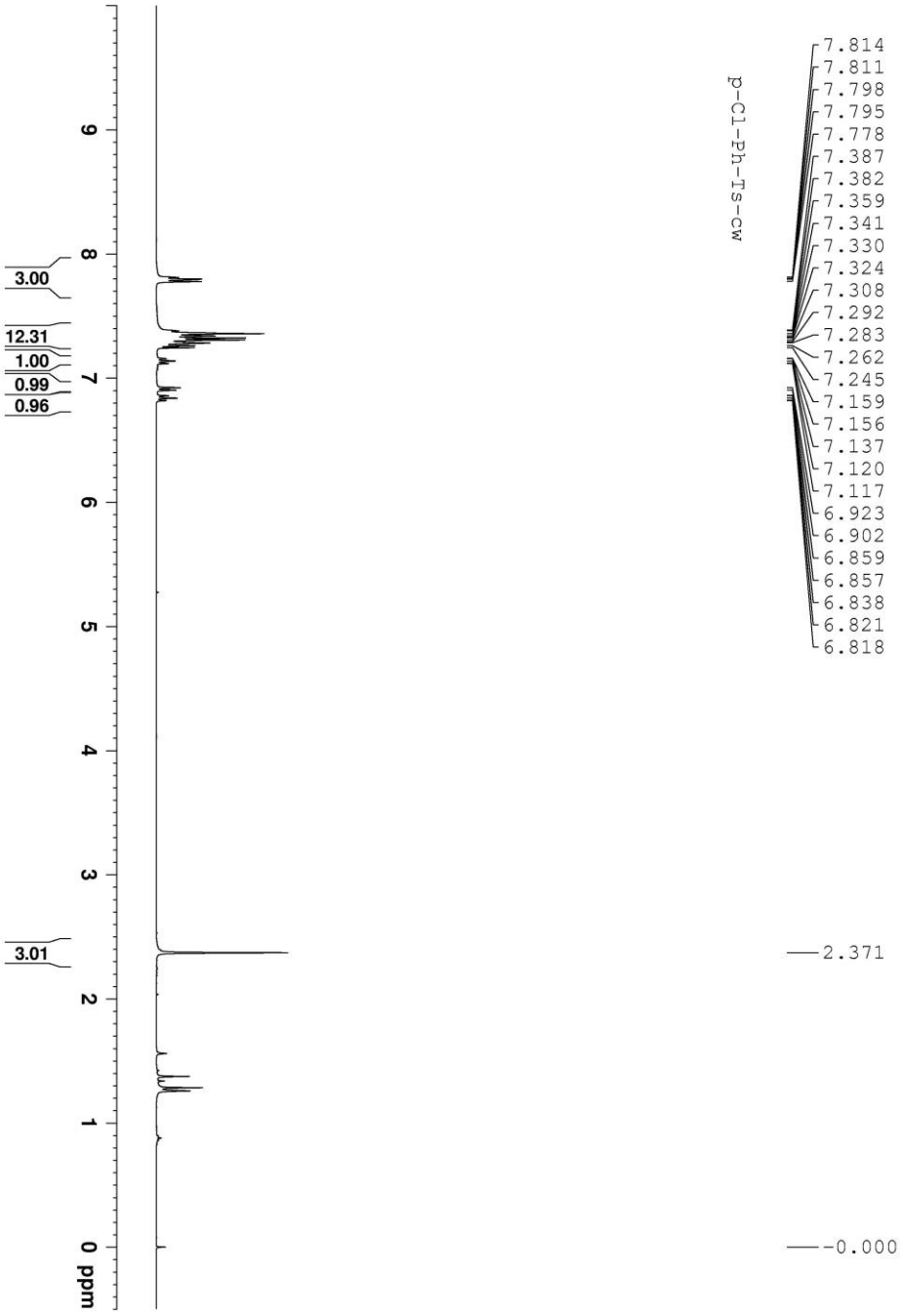
3g

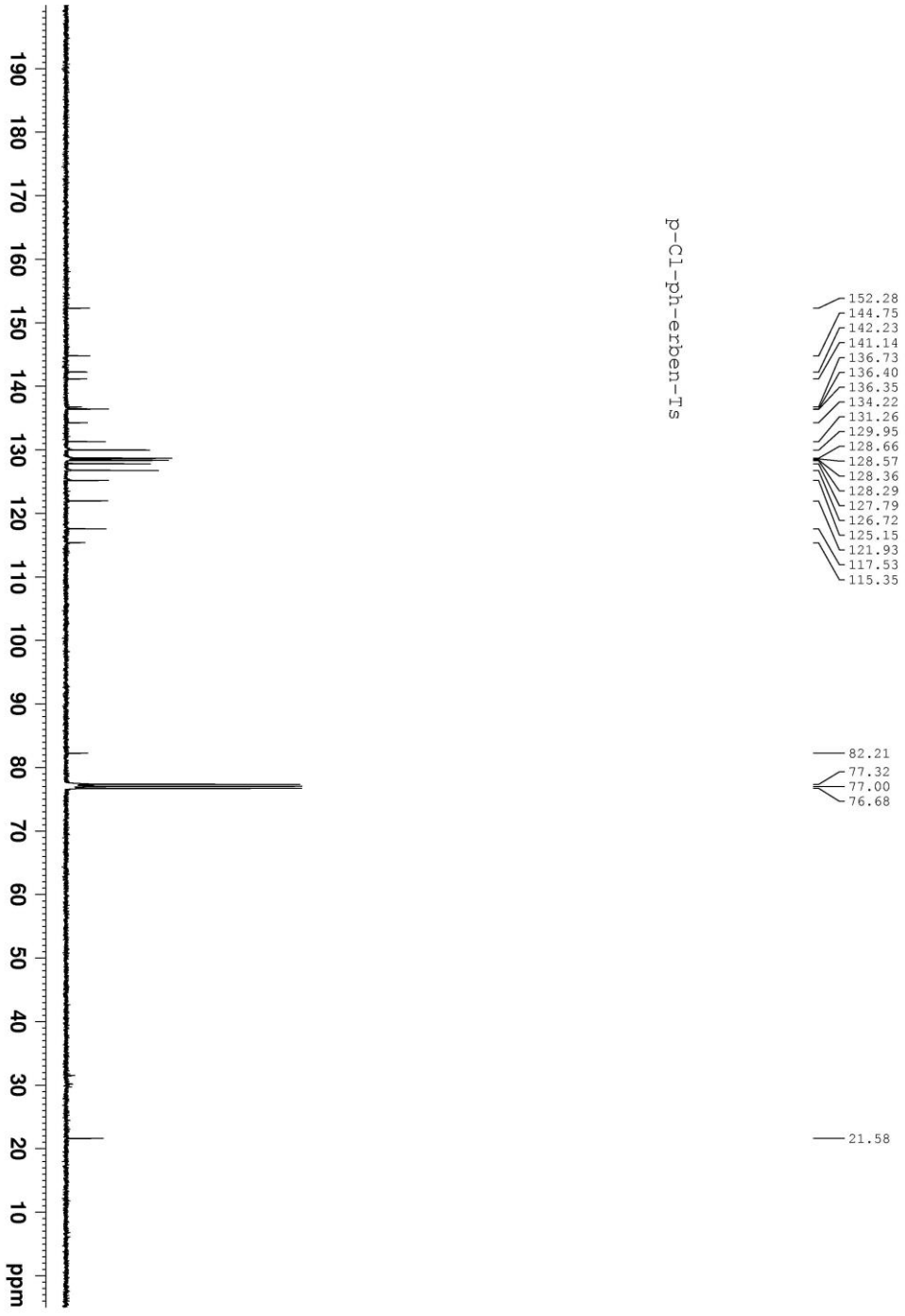

p-Me-Ph-erben-Ts
7.728
7.708
7.686
7.335
7.326
7.307
7.273
7.255
7.236
7.221
7.203
7.184
7.172
7.069
7.049
7.031
7.028
6.852
6.832
6.756
6.737
6.718
2.296
2.241
-0.000
3.00
3.04
7.15
3.03
1.00
1.02
3.03
2.99
9
8
7
6
5
4
3
2
1
0 ppm

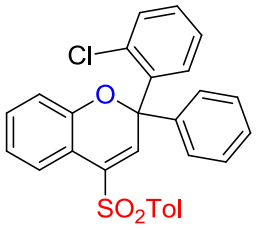

p-Me-Ph-erben-Ts
152.55
144.59
142.83
139.66
138.02
137.30
136.92
135.69
131.05
129.90
129.12
128.40
128.07
127.75
126.81
126.78
125.04
121.63
117.51
115.37
82.62
77.32
77.00
76.68
21.57
21.06
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
O
SO2Tol

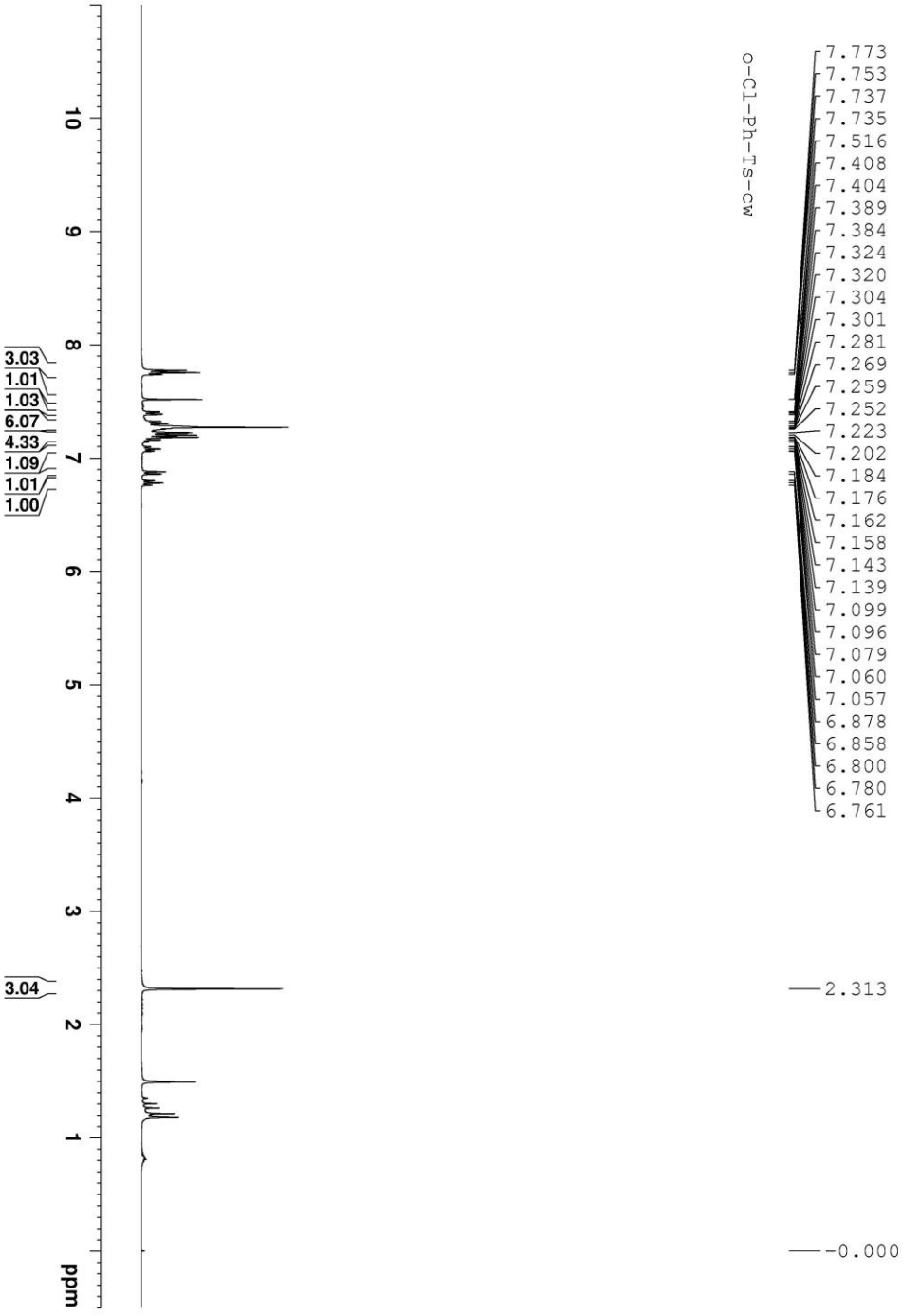
3h

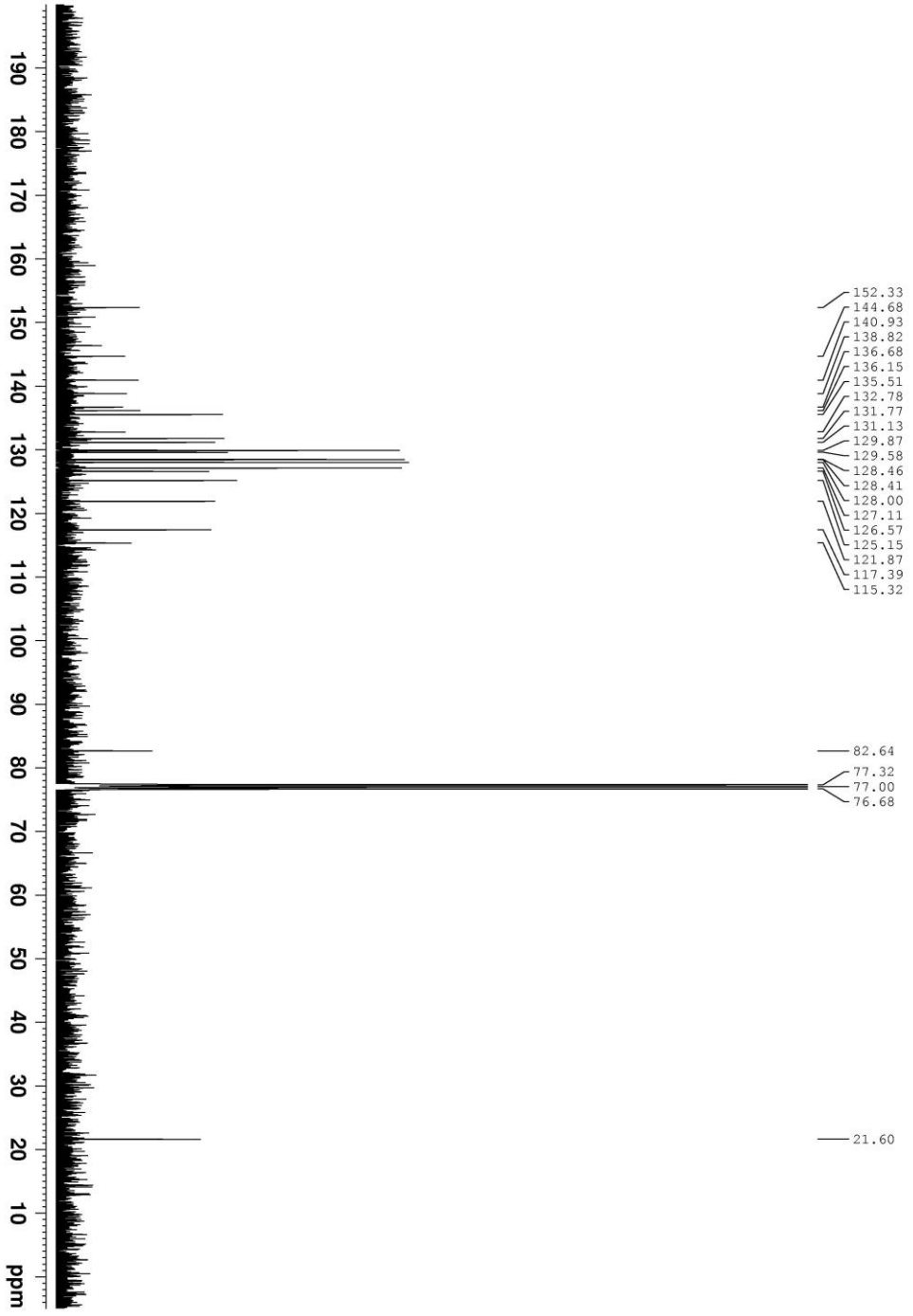

3.00
12.31
1.00
0.99
0.96
3.01
9
8
7
6
5
4
3
2
1
0 ppm
p-Cl-Ph-Ts-cw
7.814
7.811
7.798
7.795
7.778
7.387
7.382
7.359
7.341
7.330
7.324
7.308
7.292
7.283
7.262
7.245
7.159
7.156
7.137
7.120
7.117
6.923
6.902
6.859
6.857
6.838
6.821
6.818
2.371
-0.000

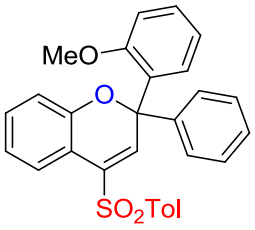

p-Cl-ph-erben-Ts
152.28
144.75
142.23
141.14
136.73
136.40
136.35
134.22
131.26
129.95
128.66
128.57
128.36
128.29
127.79
126.72
125.15
121.93
117.53
115.35
82.21
77.32
77.00
76.68
21.58
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Cl
O
SO2Tol

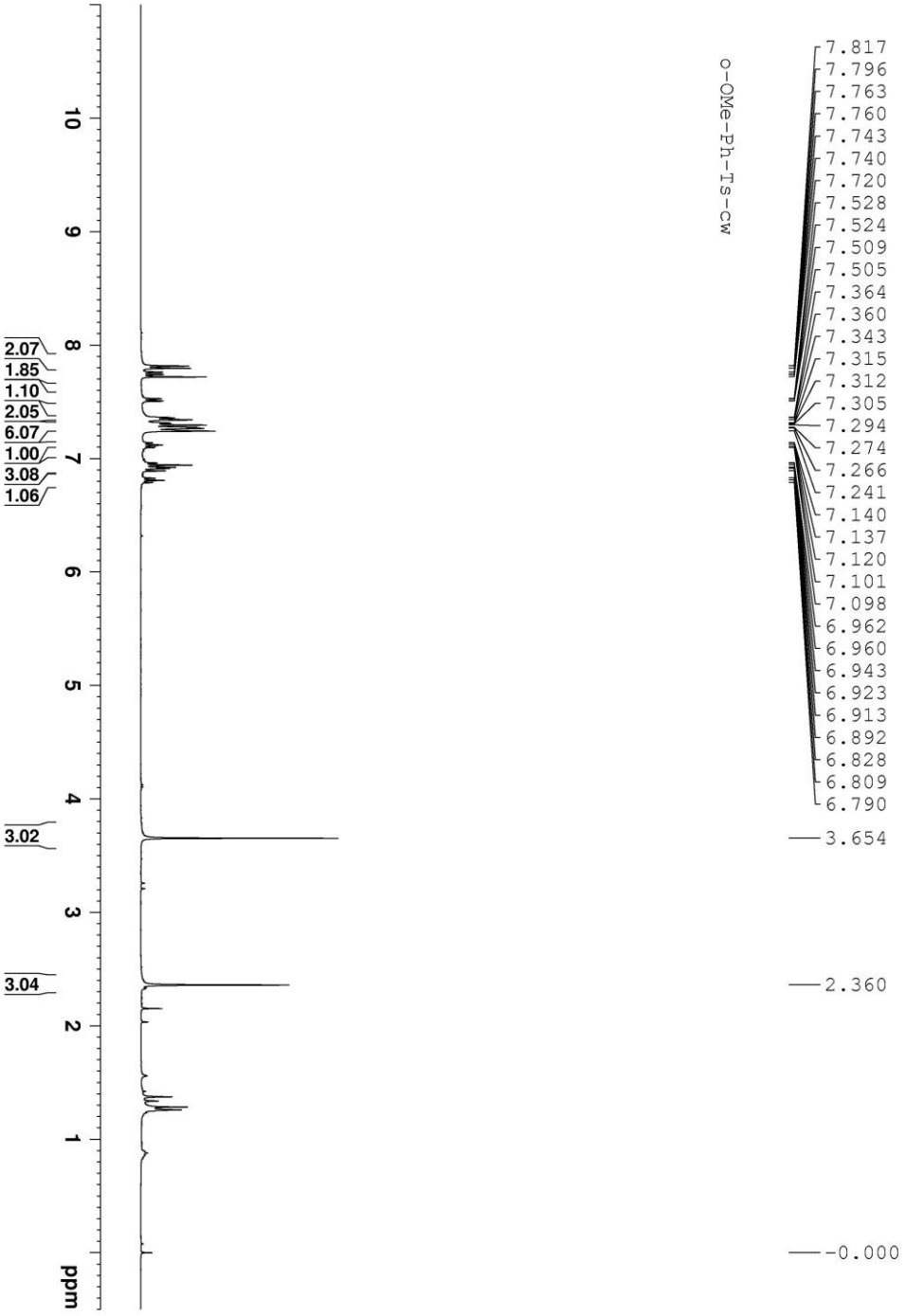
3i

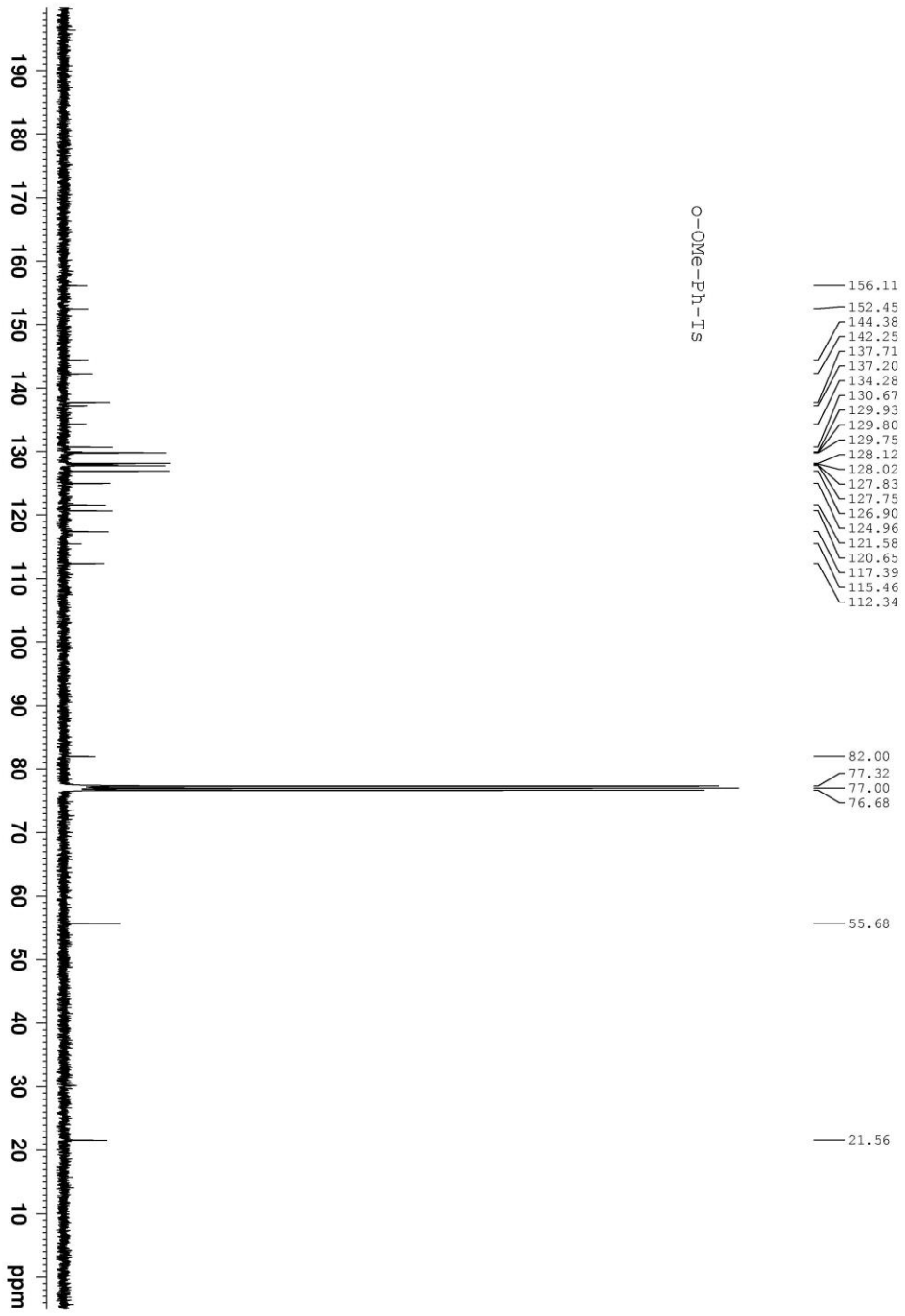

o-Cl-Ph-Ts-cw
7.773
7.753
7.737
7.735
7.516
7.408
7.404
7.389
7.384
7.324
7.320
7.304
7.301
7.281
7.269
7.259
7.252
7.223
7.202
7.184
7.176
7.162
7.158
7.143
7.139
7.099
7.096
7.079
7.060
7.057
6.878
6.858
6.800
6.780
6.761
2.313
-0.000
3.03
1.01
1.03
6.07
4.33
1.09
1.01
1.00
3.04
ppm

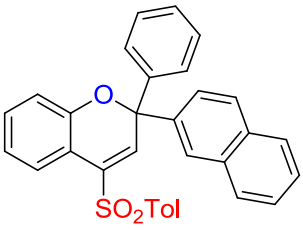

152.33
144.68
140.93
138.82
136.68
136.15
135.51
132.78
131.77
131.13
129.87
129.58
128.46
128.41
128.00
127.11
126.57
125.15
121.87
117.39
115.32
82.64
77.32
77.00
76.68
21.60
ppm


MeO
O
SO2Tol

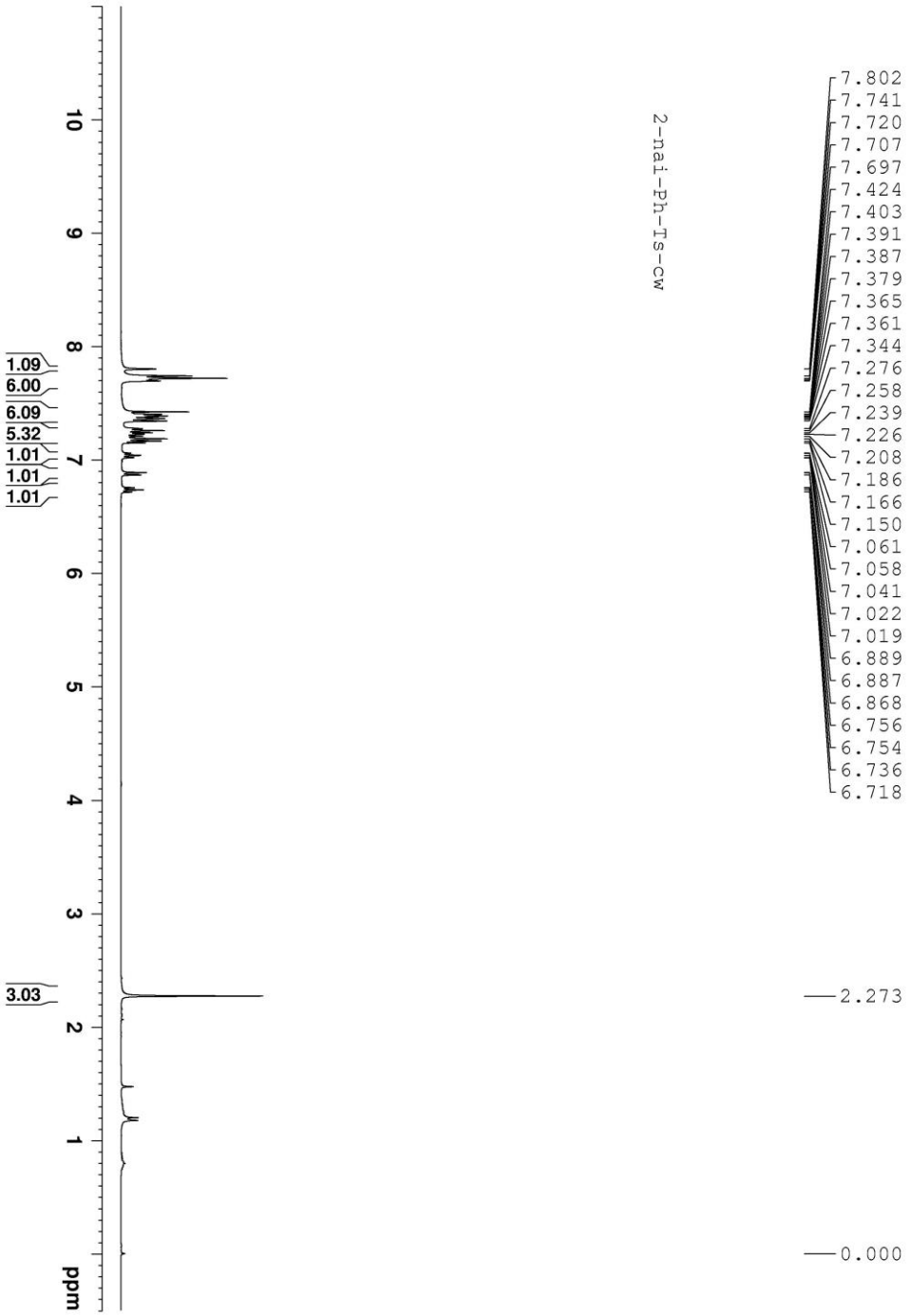
3j

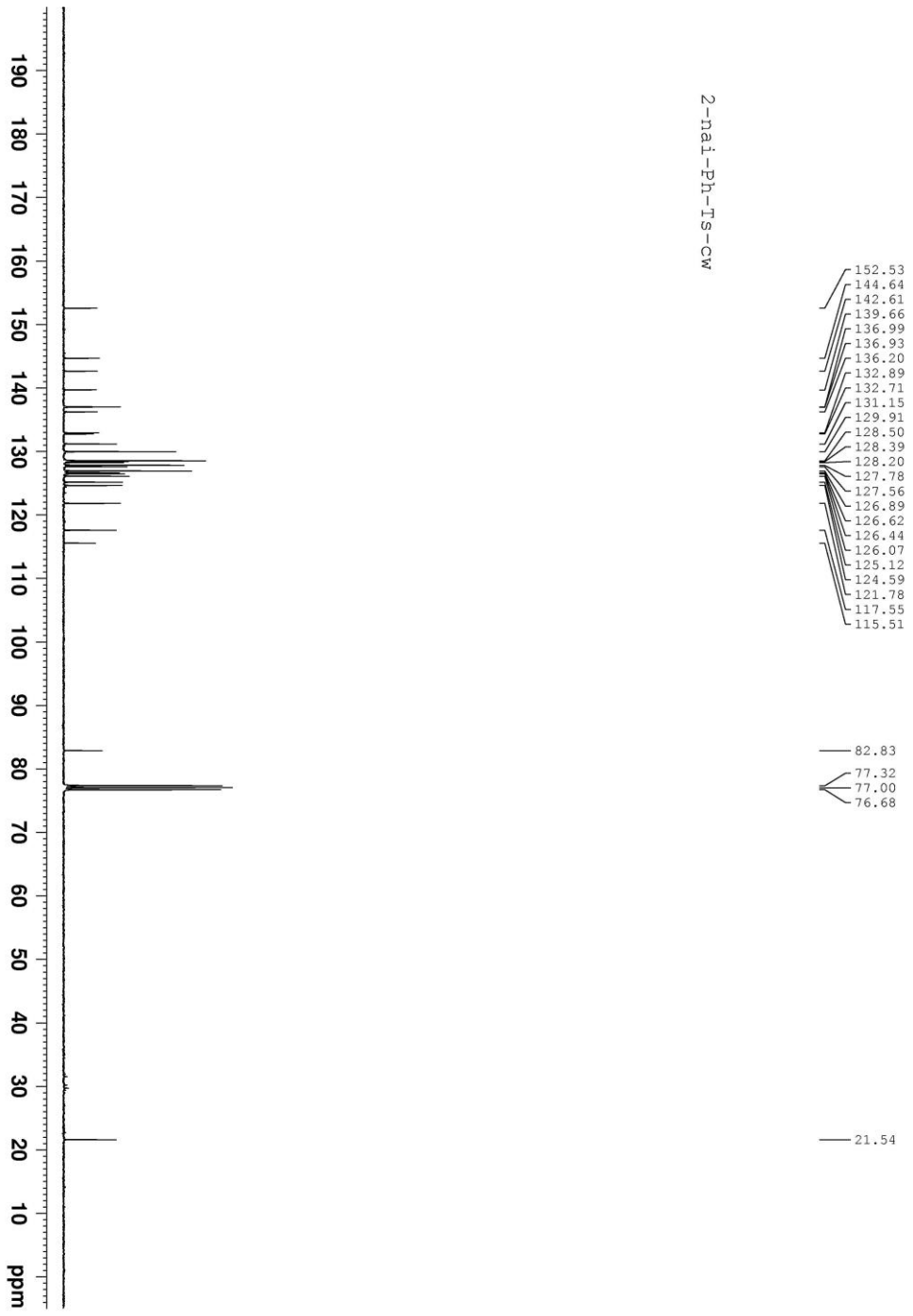

o-OMe-Ph-Ts-cw
7.817
7.796
7.763
7.760
7.743
7.740
7.720
7.528
7.524
7.509
7.505
7.364
7.360
7.343
7.315
7.312
7.305
7.294
7.274
7.266
7.241
7.140
7.137
7.120
7.101
7.098
6.962
6.960
6.943
6.923
6.913
6.892
6.828
6.809
6.790
3.654
2.360
-0.000
2.07
1.85
1.10
2.05
6.07
1.00
3.08
1.06
3.02
3.04
ppm

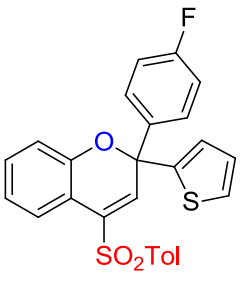

o-OMe-Ph-Ts
156.11
152.45
144.38
142.25
137.71
137.20
134.28
130.67
129.93
129.80
129.75
128.12
128.02
127.83
127.75
126.90
124.96
121.58
120.65
117.39
115.46
112.34
82.00
77.32
77.00
76.68
55.68
21.56
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
SO2Tol

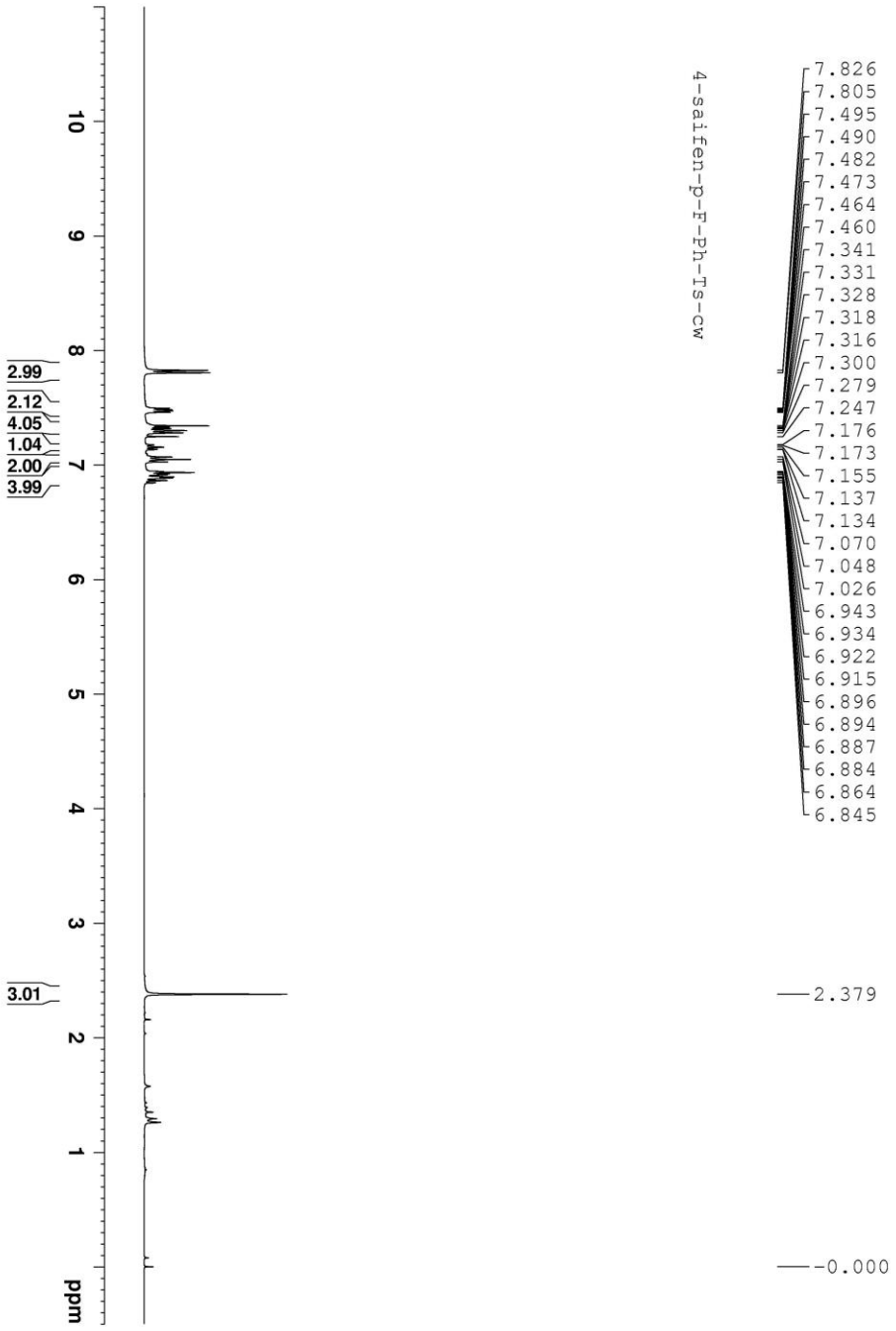
3k

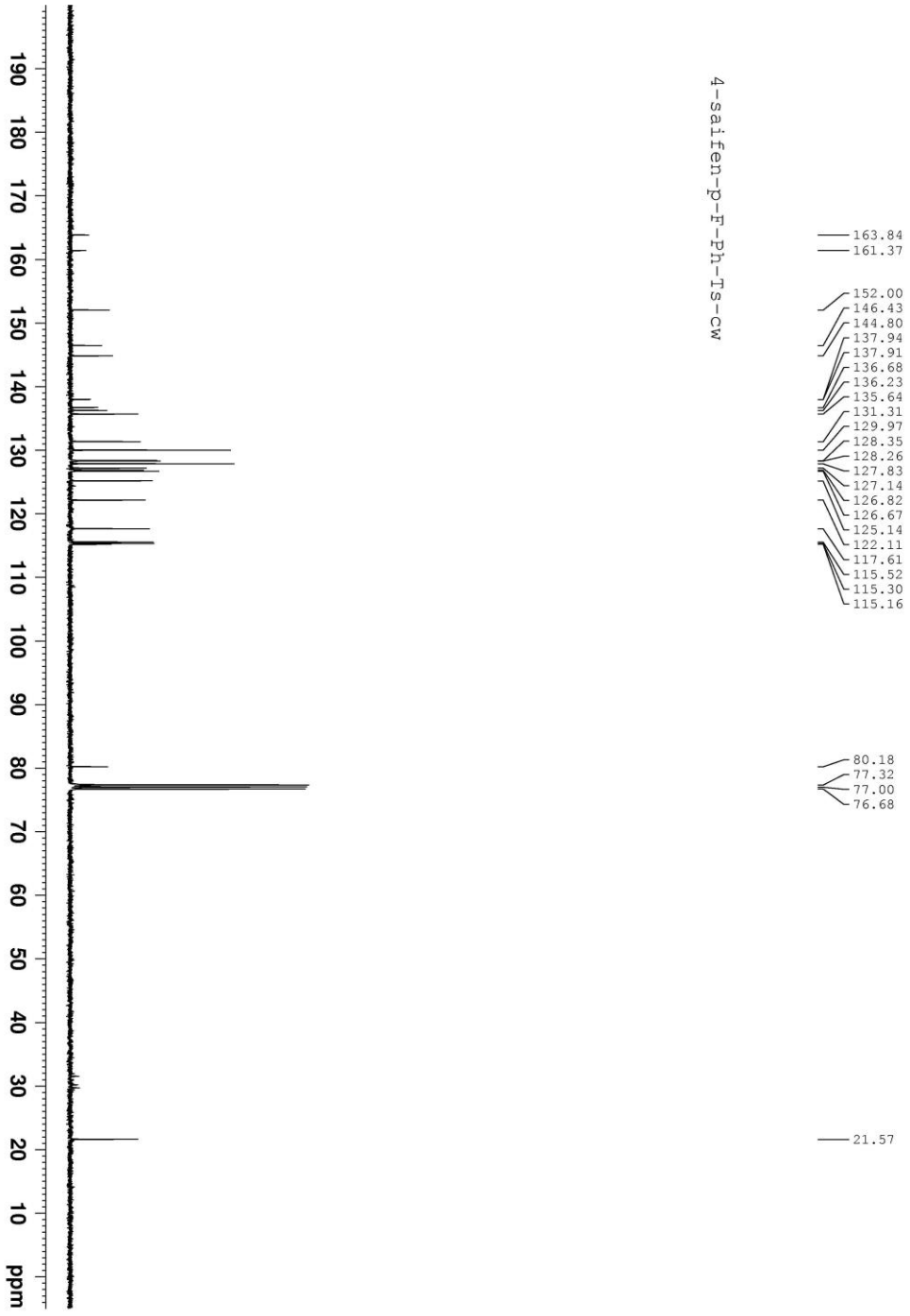

2-nai-Ph-Ts-cw
7.802
7.741
7.720
7.707
7.697
7.424
7.403
7.391
7.387
7.379
7.365
7.361
7.344
7.276
7.258
7.239
7.226
7.208
7.186
7.166
7.150
7.061
7.058
7.041
7.022
7.019
6.889
6.887
6.868
6.756
6.754
6.736
6.718
1.09
6.00
6.09
5.32
1.01
1.01
1.01
3.03
2.273
0.000
ppm

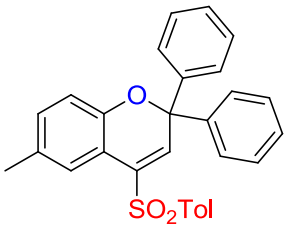

2-nai-Ph-Ts-cw
152.53
144.64
142.61
139.66
136.99
136.93
136.20
132.89
132.71
131.15
129.91
128.50
128.39
128.20
127.78
127.56
126.89
126.62
126.44
126.07
125.12
124.59
121.78
117.55
115.51
82.83
77.32
77.00
76.68
21.54
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


F
O
S
SO2Tol

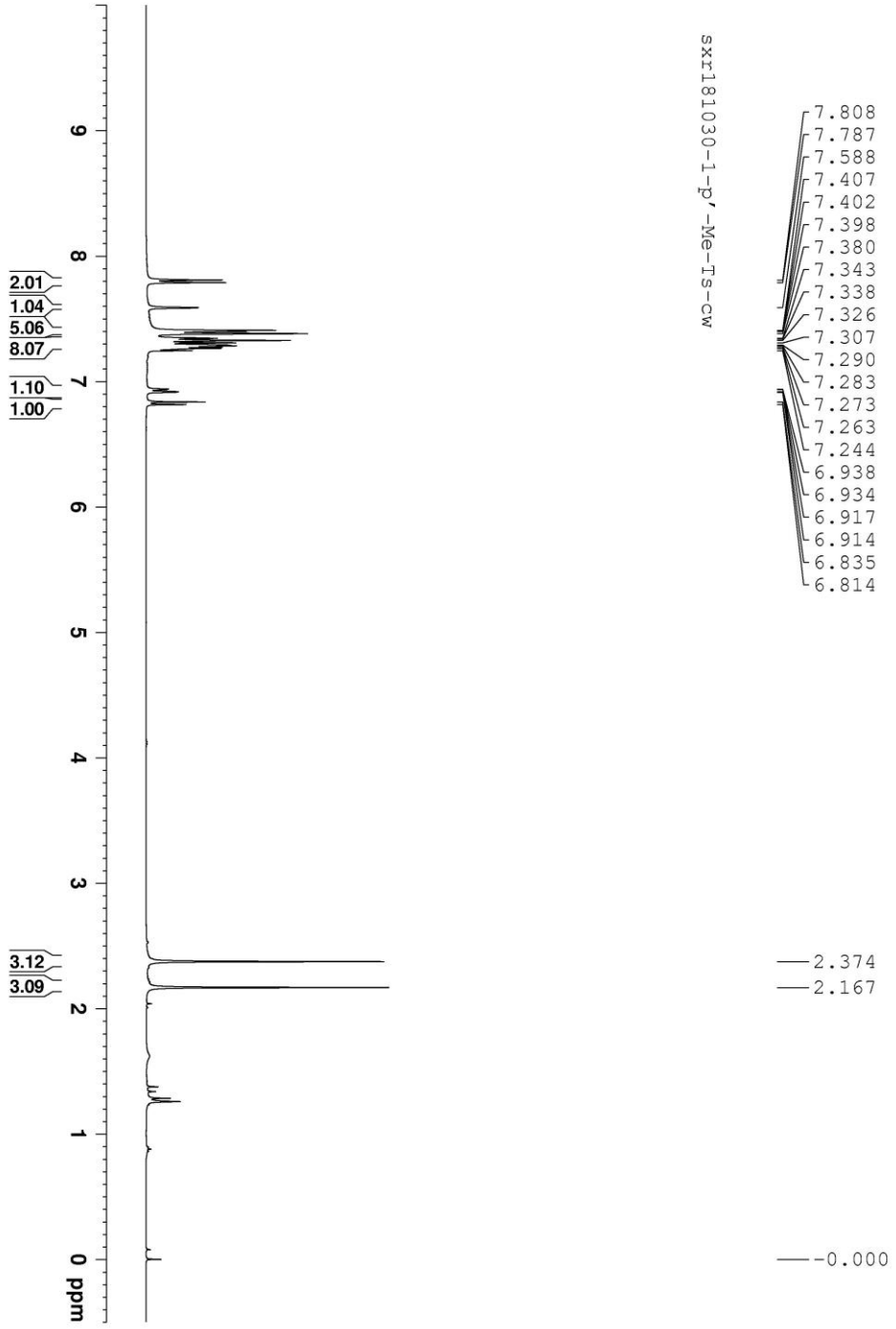
3l

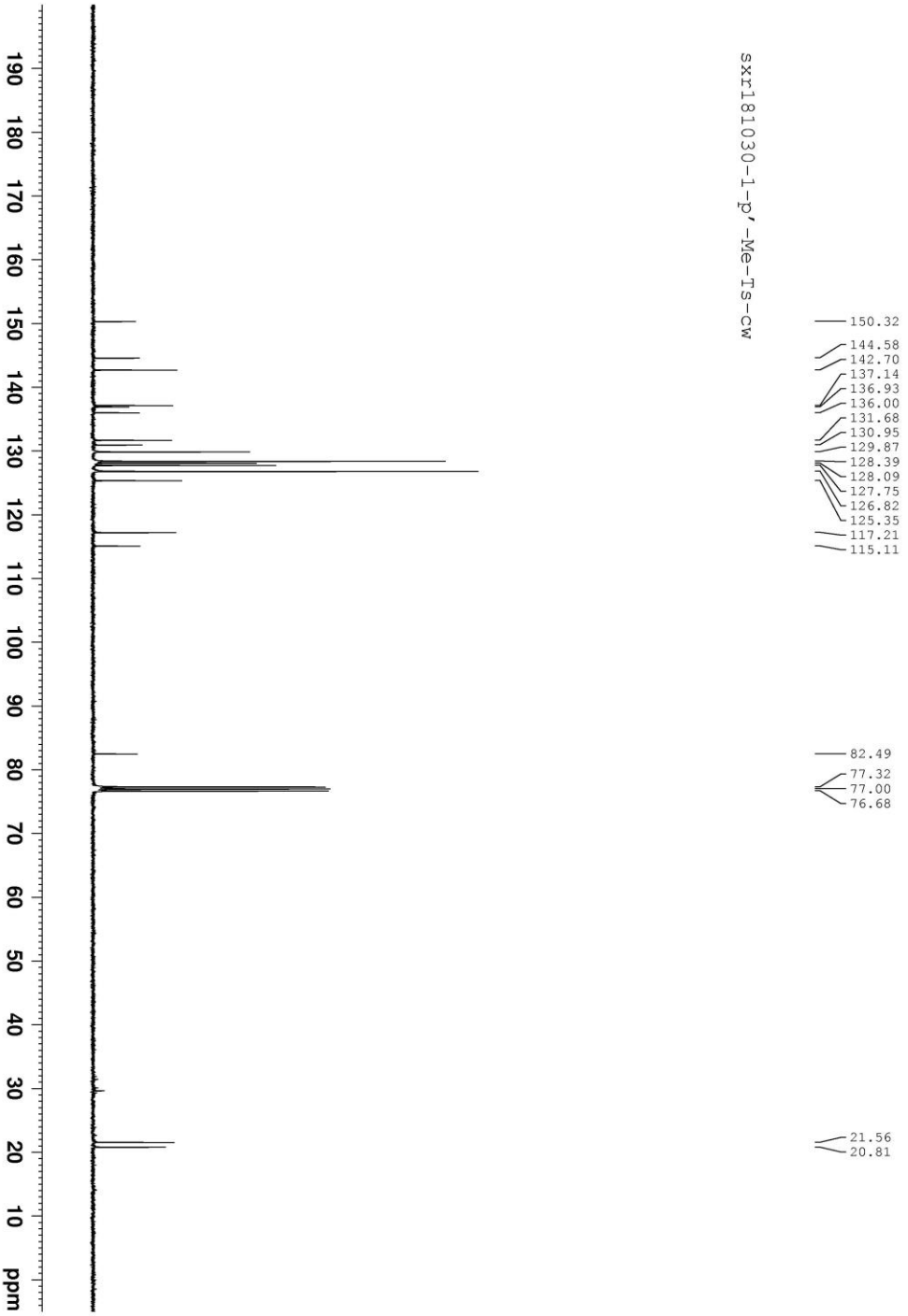

4-saifen-p-F-Ph-Ts-cw
7.826
7.805
7.495
7.490
7.482
7.473
7.464
7.460
7.341
7.331
7.328
7.318
7.316
7.300
7.279
7.247
7.176
7.173
7.155
7.137
7.134
7.070
7.048
7.026
6.943
6.934
6.922
6.915
6.896
6.894
6.887
6.884
6.864
6.845
2.379
-0.000
2.99
2.12
4.05
1.04
2.00
3.99
3.01
ppm

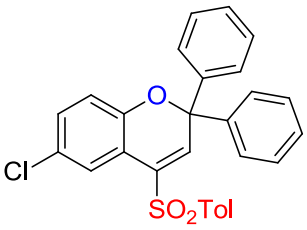

4-saifen-p-F-Ph-Ts-cw
163.84
161.37
152.00
146.43
144.80
137.94
137.91
136.68
136.23
135.64
131.31
129.97
128.35
128.26
127.83
127.14
126.82
126.67
125.14
122.11
117.61
115.52
115.30
115.16
80.18
77.32
77.00
76.68
21.57
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
SO2Tol

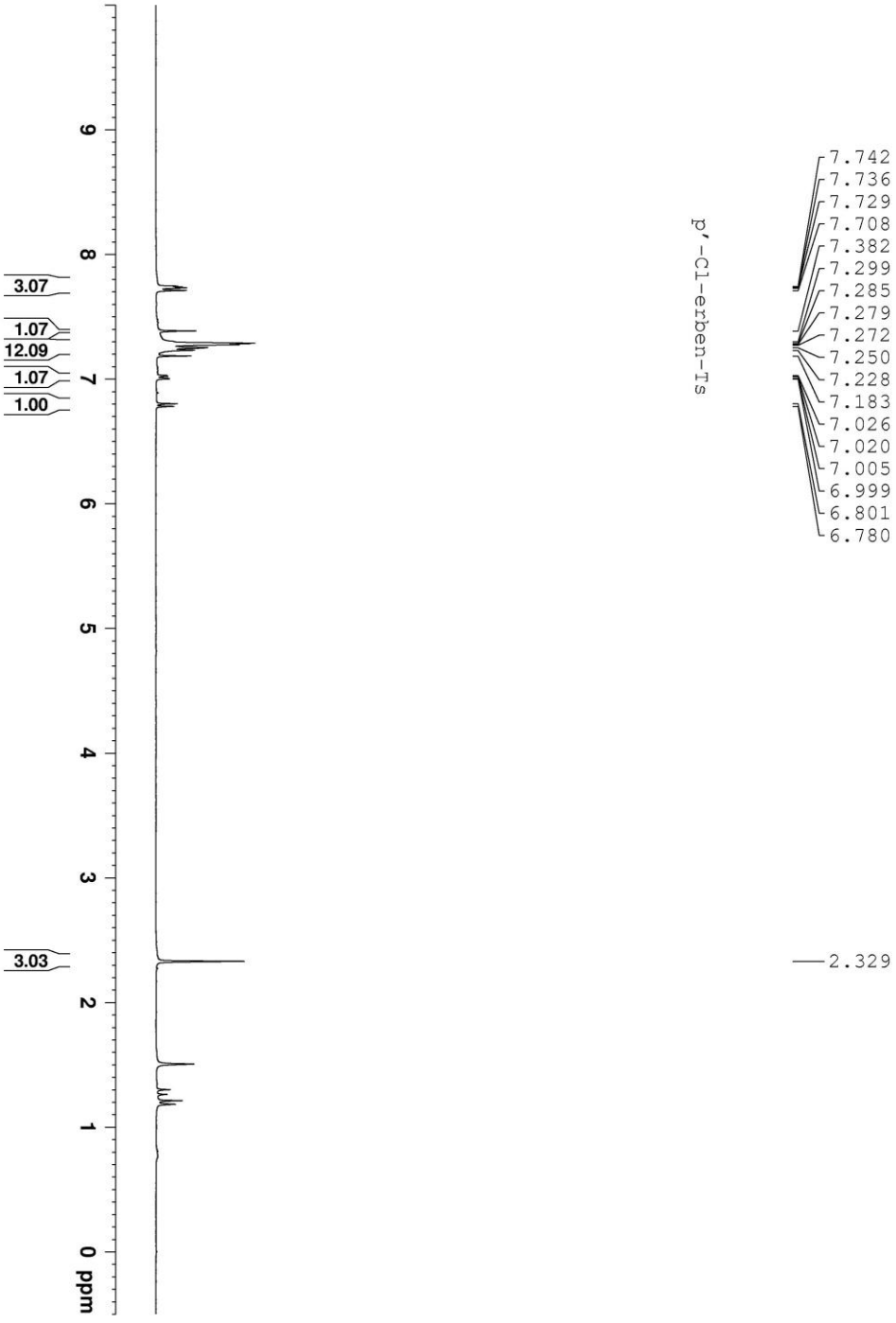
3m

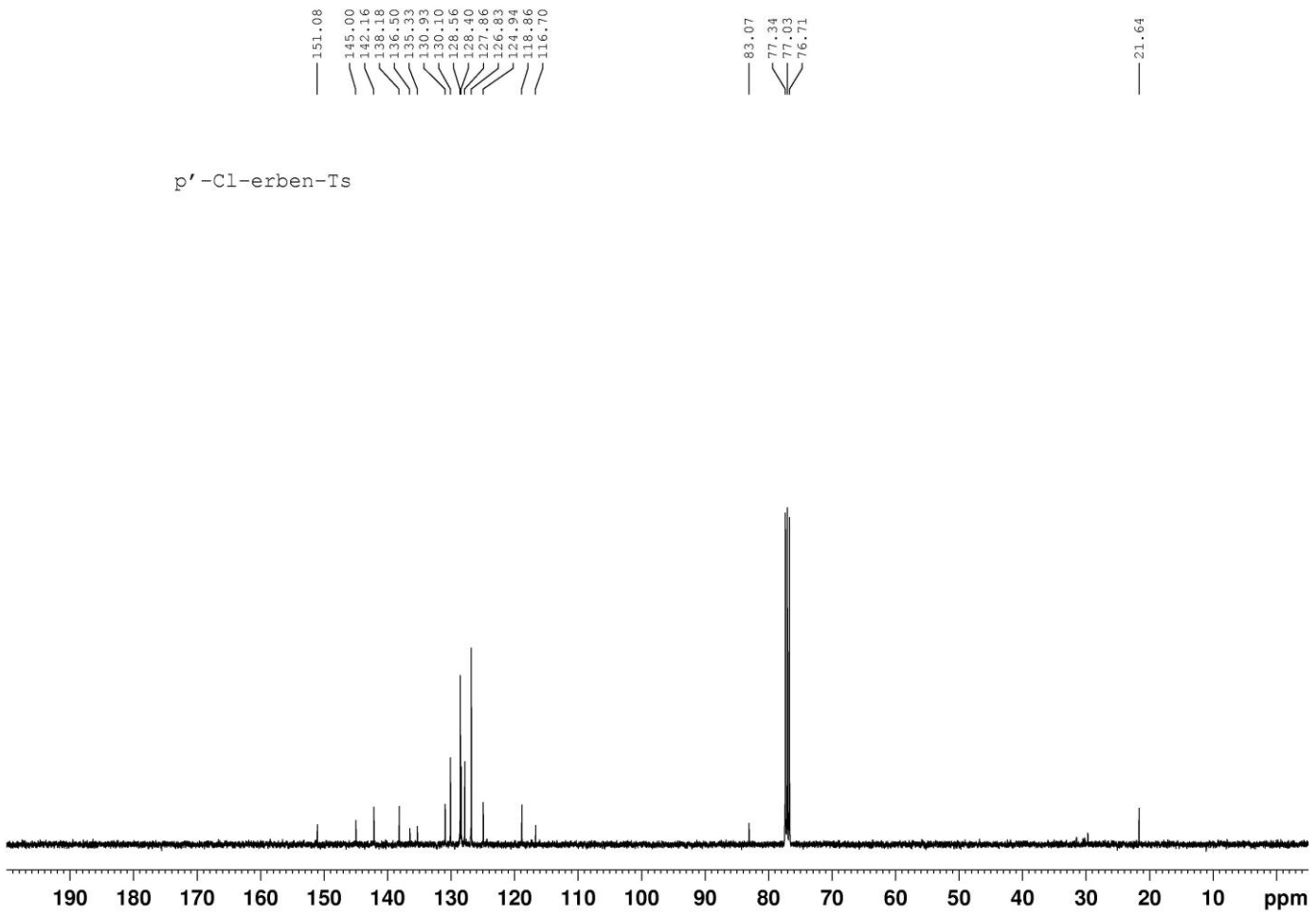

sxr181030-1-p'-Me-Ts-cw
7.808
7.787
7.588
7.407
7.402
7.398
7.380
7.343
7.338
7.326
7.307
7.290
7.283
7.273
7.263
7.244
6.938
6.934
6.917
6.914
6.835
6.814
2.374
2.167
-0.000
2.01
1.04
5.06
8.07
1.10
1.00
3.12
3.09
ppm

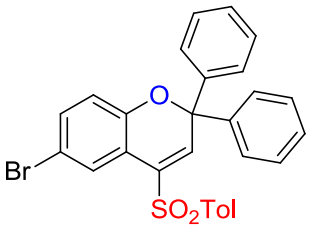

sxr181030-1-p'-Me-Ts-cw
150.32
144.58
142.70
137.14
136.93
136.00
131.68
130.95
129.87
128.39
128.09
127.75
126.82
125.35
117.21
115.11
82.49
77.32
77.00
76.68
21.56
20.81
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
Cl
SO2Tol

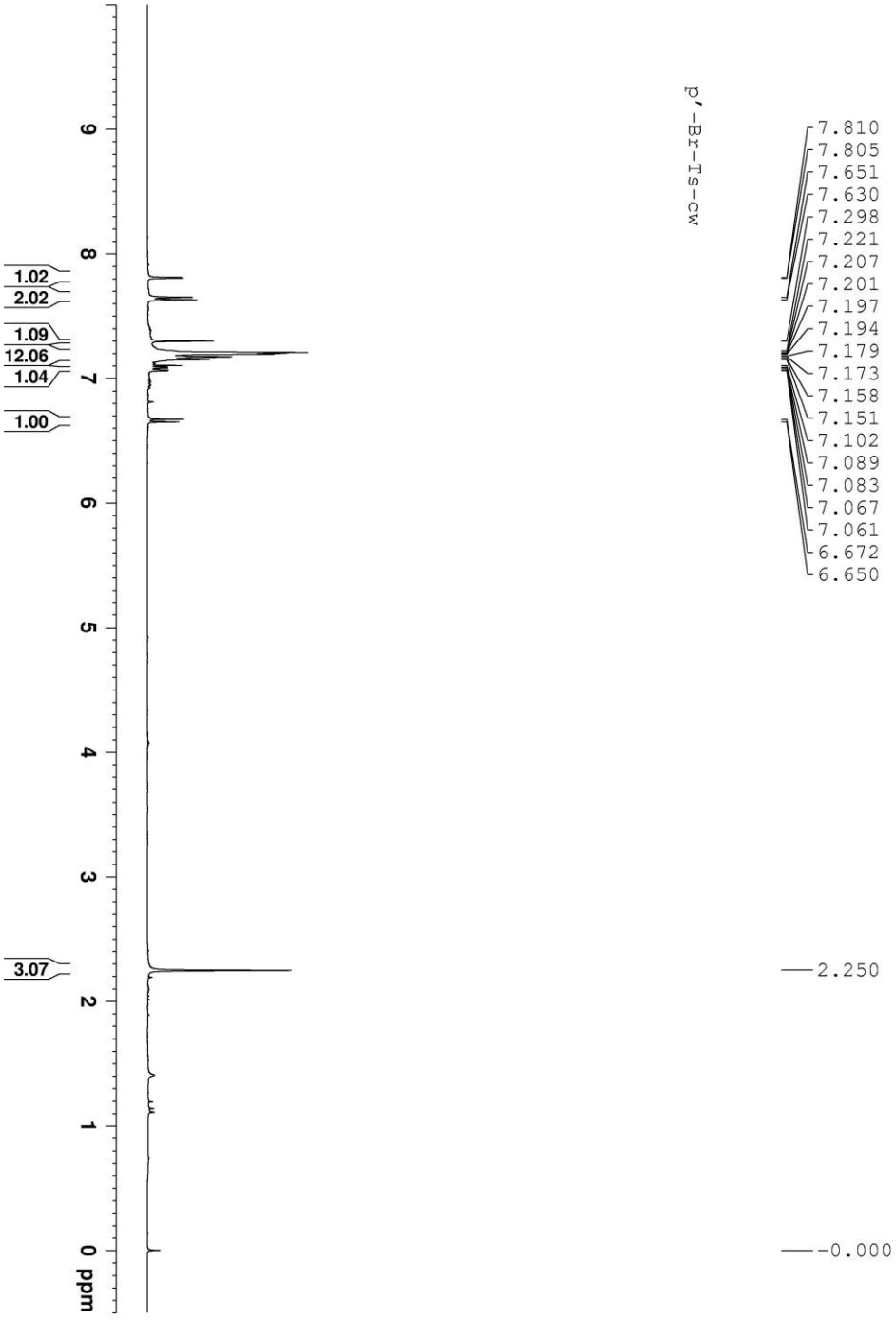
3n

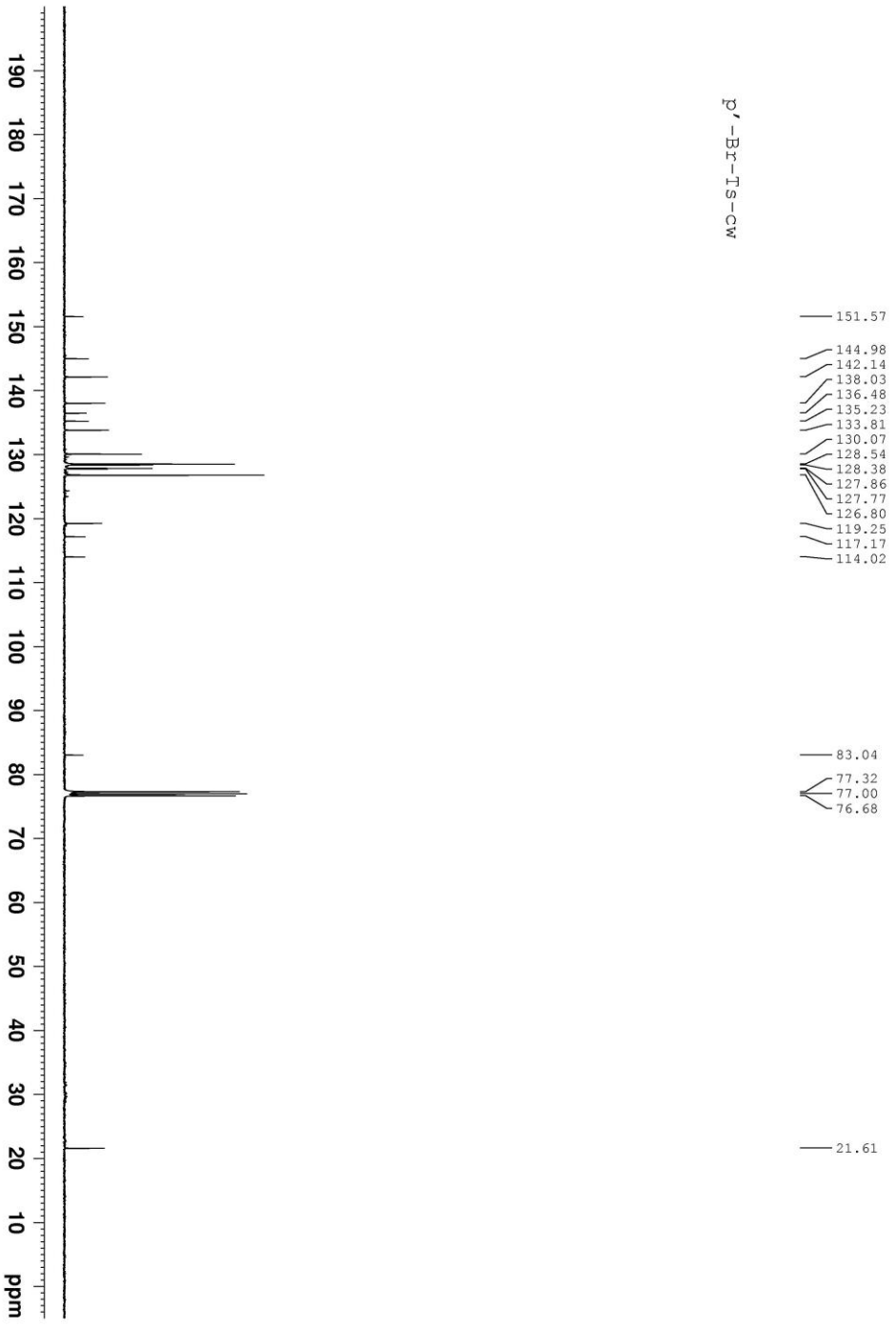

p'-Cl-erben-Ts
7.742
7.736
7.729
7.708
7.382
7.299
7.285
7.279
7.272
7.250
7.228
7.183
7.026
7.020
7.005
6.999
6.801
6.780
2.329
3.07
1.07
12.09
1.07
1.00
3.03
9
8
7
6
5
4
3
2
1
0 ppm

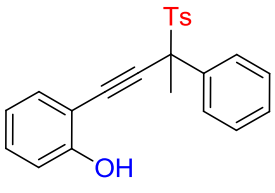

151.08
145.00
142.16
138.18
136.50
135.33
130.93
130.10
128.56
128.40
127.86
126.83
124.94
118.86
116.70
83.07
77.34
77.03
76.71
21.64
p'-Cl-erben-Ts
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
Br
SO2Tol

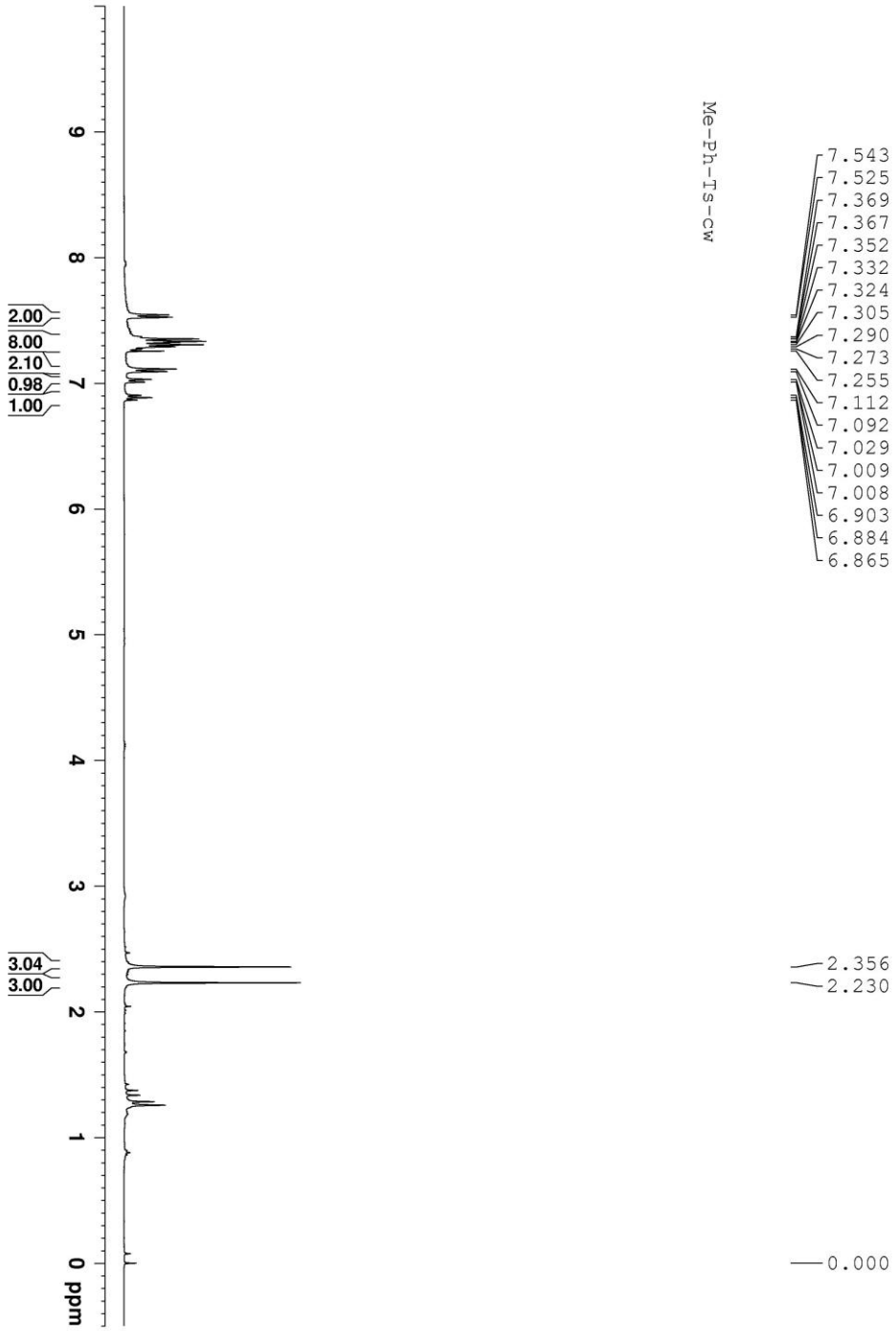
3o

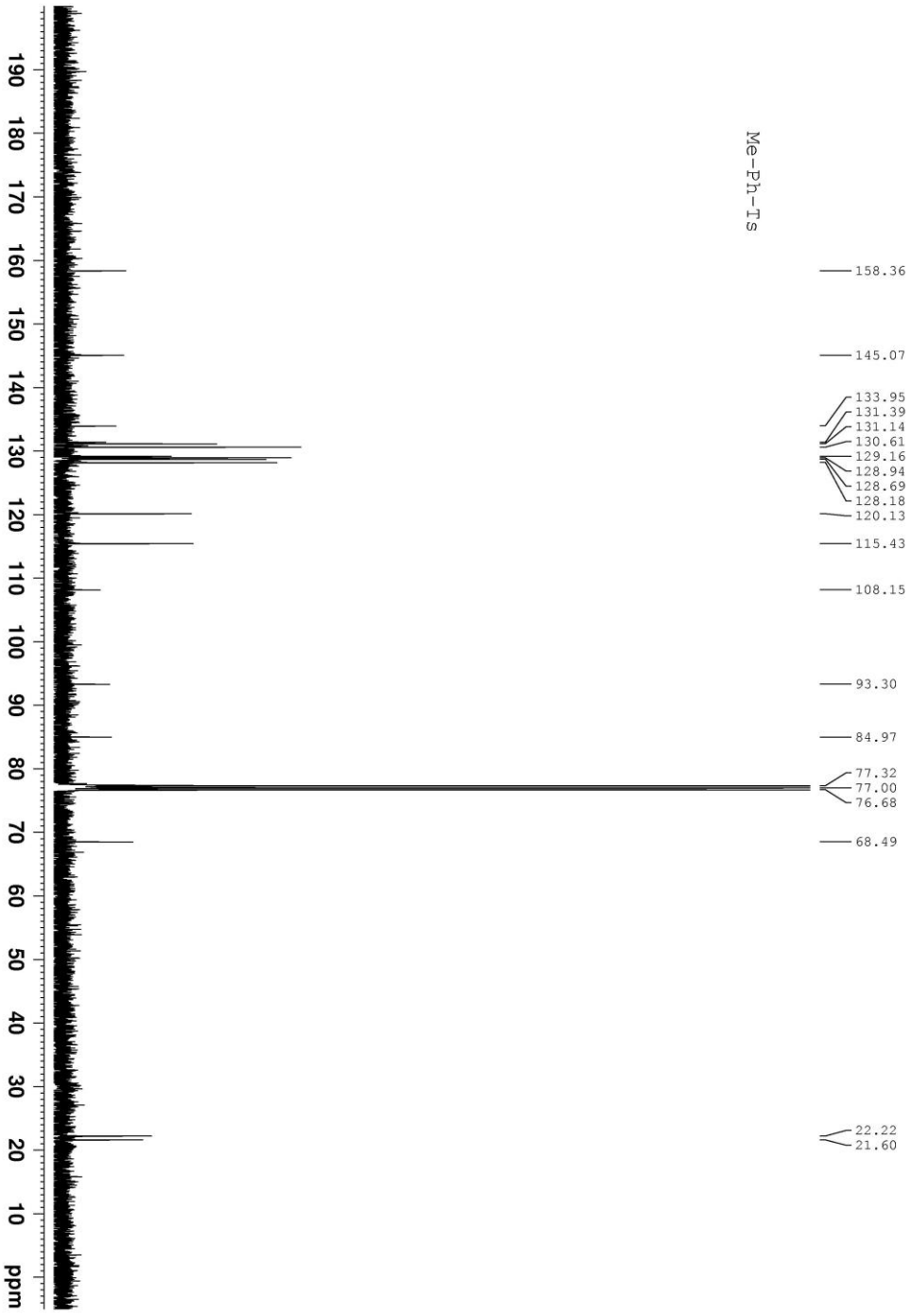

p,Br-Ts-cm
7.810
7.805
7.651
7.630
7.298
7.221
7.207
7.201
7.197
7.194
7.179
7.173
7.158
7.151
7.102
7.089
7.083
7.067
7.061
6.672
6.650
1.02
2.02
1.09
12.06
1.04
1.00
3.07
2.250
-0.000
ppm

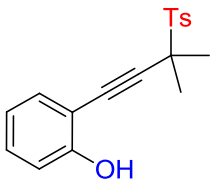

p'-Br-Is-cm
151.57
144.98
142.14
138.03
136.48
135.23
133.81
130.07
128.54
128.38
127.86
127.77
126.80
119.25
117.17
114.02
83.04
77.32
77.00
76.68
21.61
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Ts
OH

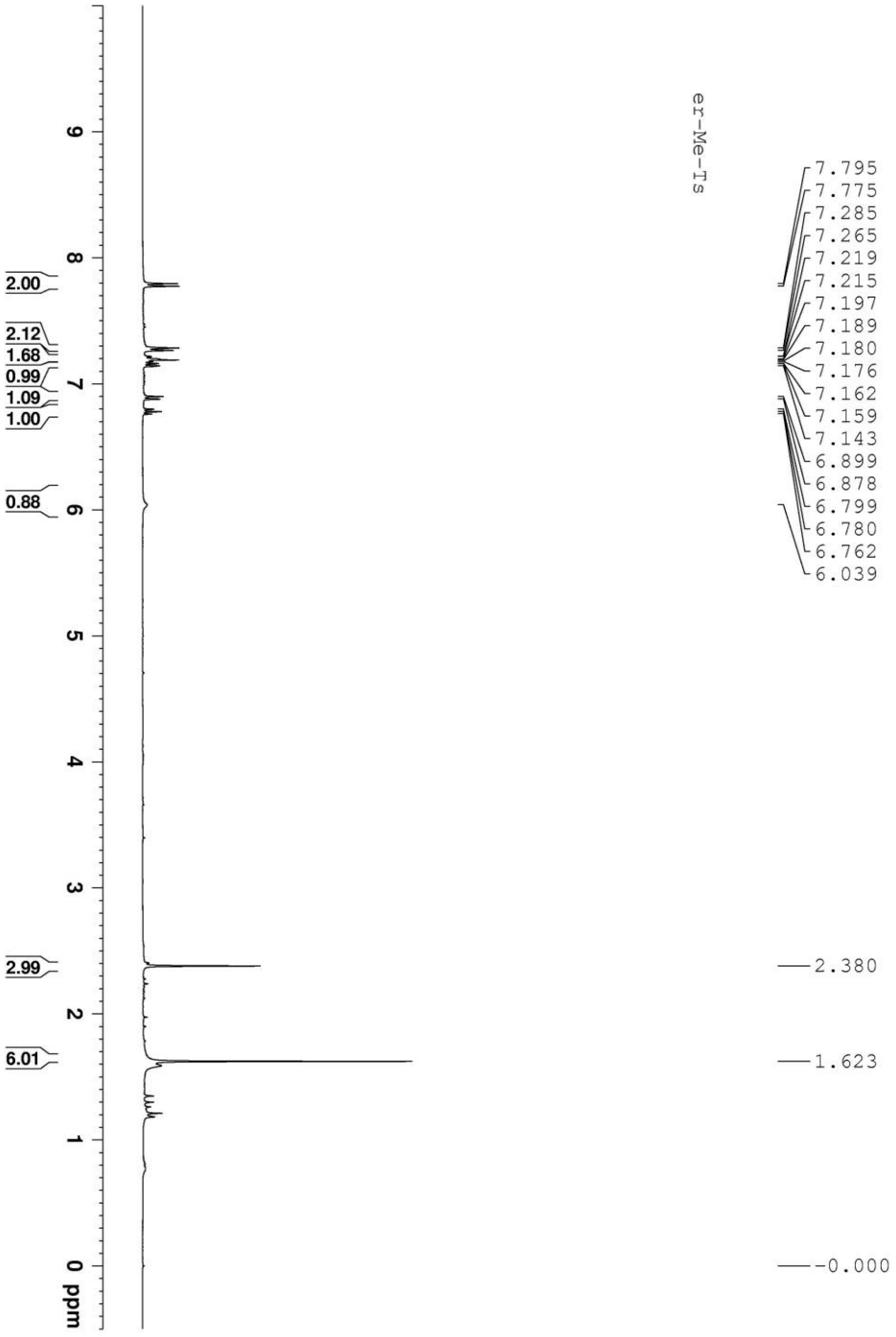
3p’

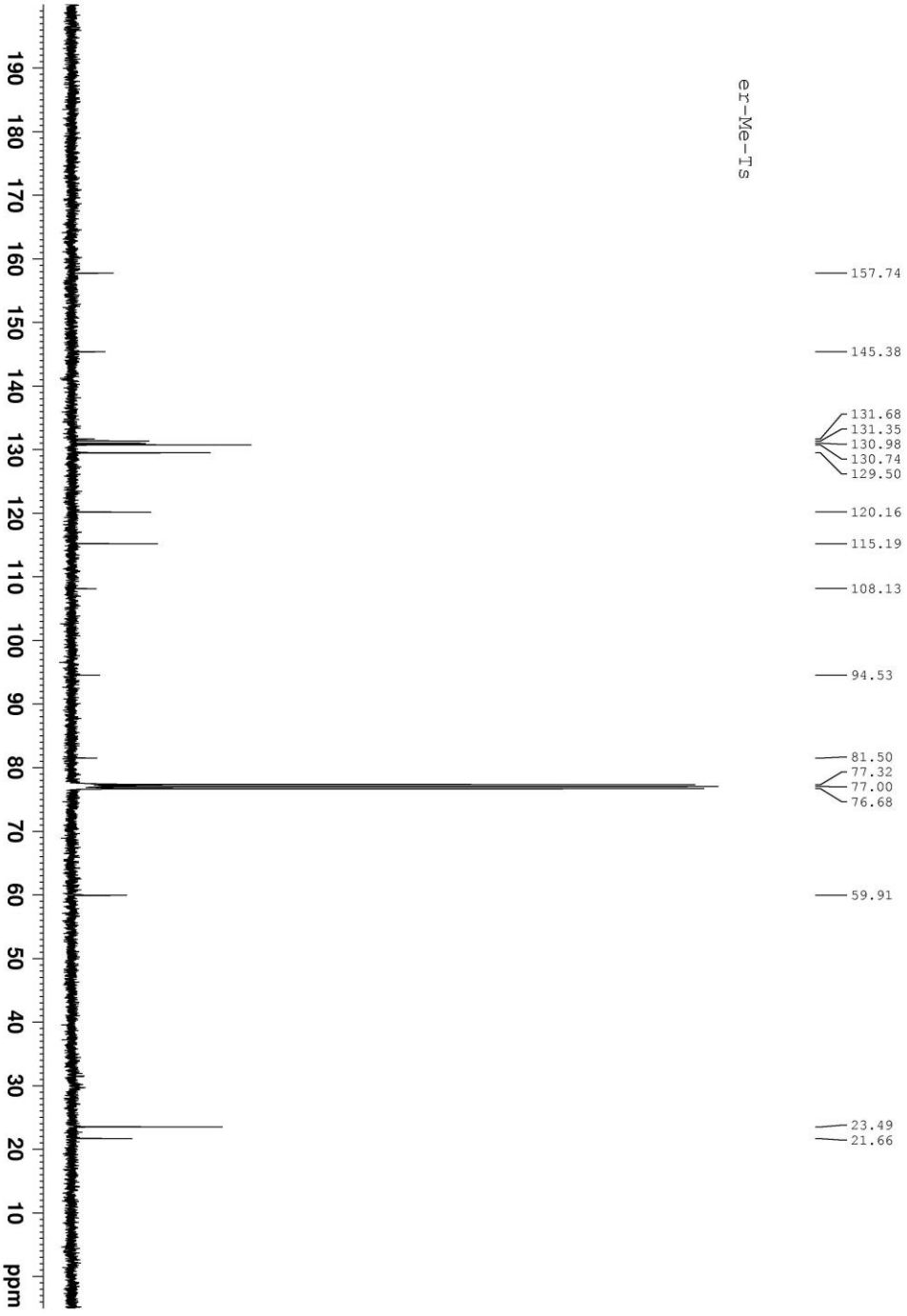

Me-Ph-Ts-cw
7.543
7.525
7.369
7.367
7.352
7.332
7.324
7.305
7.290
7.273
7.255
7.112
7.092
7.029
7.009
7.008
6.903
6.884
6.865
2.356
2.230
0.000
2.00
8.00
2.10
0.98
1.00
3.04
3.00
9
8
7
6
5
4
3
2
1
0 ppm

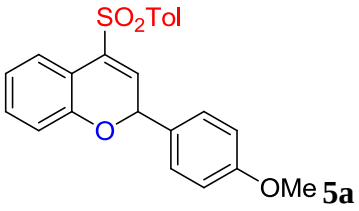

Me-Ph-Ts
158.36
145.07
133.95
131.39
131.14
130.61
129.16
128.94
128.69
128.18
120.13
115.43
108.15
93.30
84.97
77.32
77.00
76.68
68.49
22.22
21.60
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Ts
OH

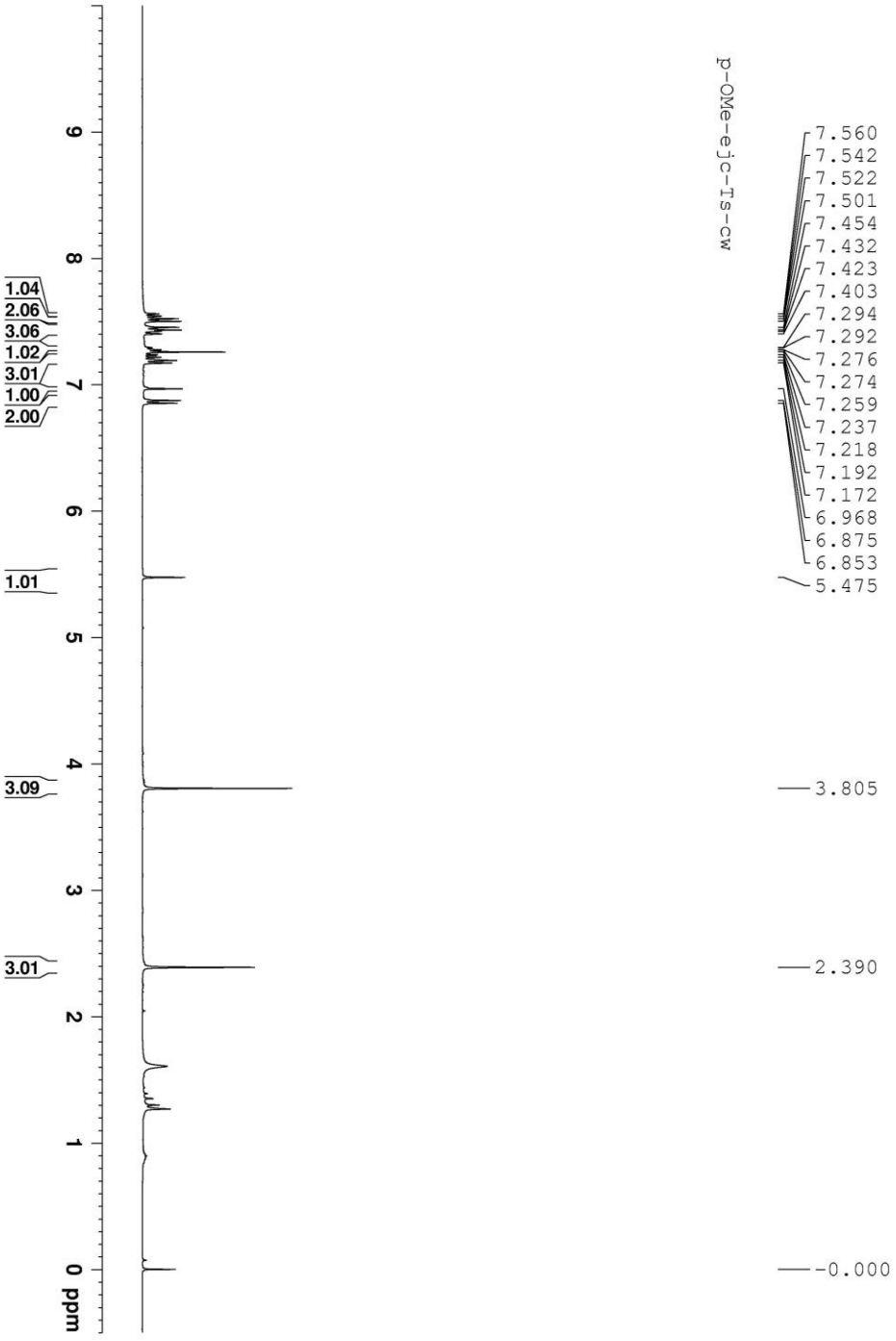
3q'

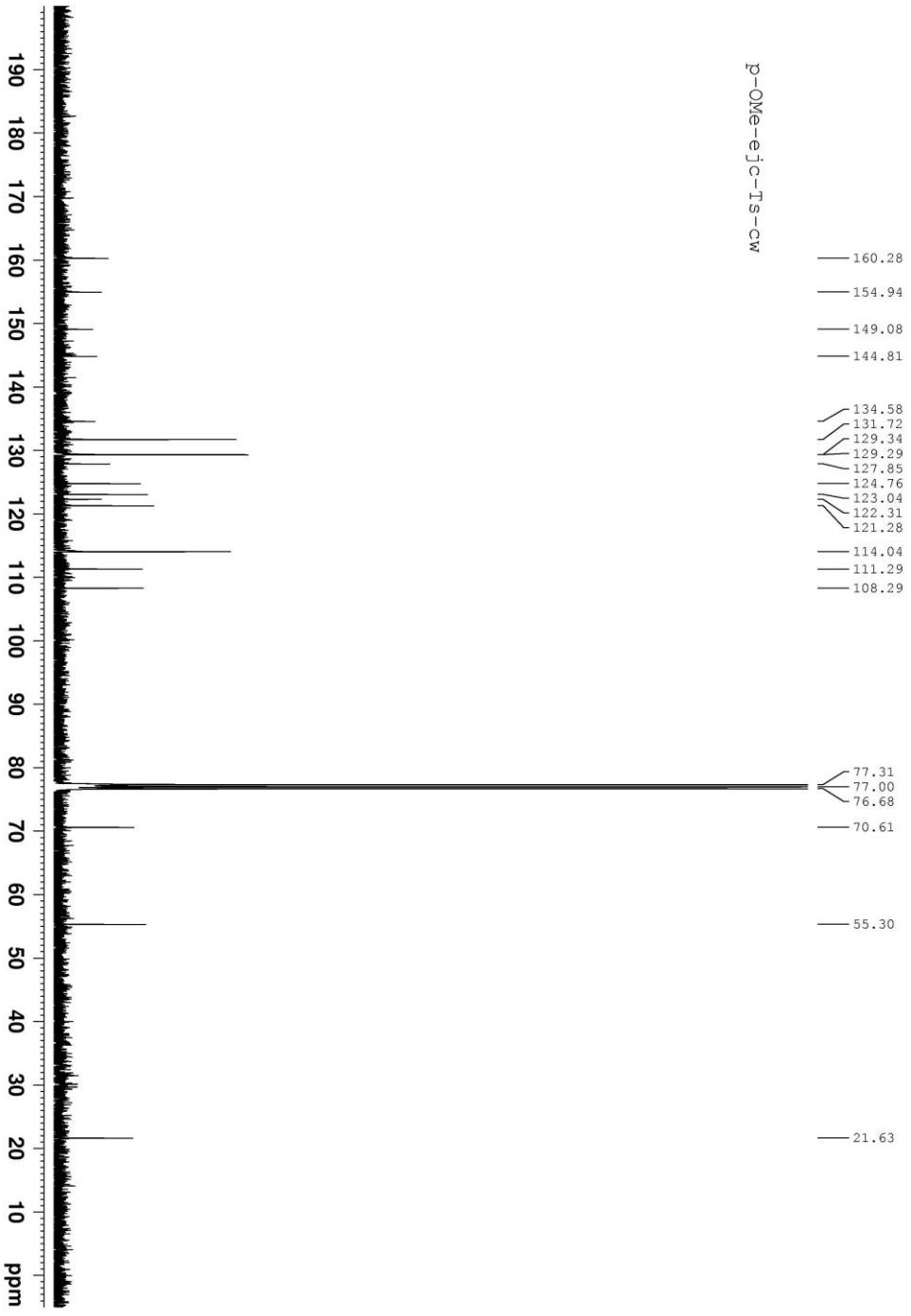

er-Me-Ts
7.795
7.775
7.285
7.265
7.219
7.215
7.197
7.189
7.180
7.176
7.162
7.159
7.143
6.899
6.878
6.799
6.780
6.762
6.039
2.380
1.623
-0.000
2.00
2.12
1.68
0.99
1.09
1.00
0.88
2.99
6.01
9
8
7
6
5
4
3
2
1
0 ppm

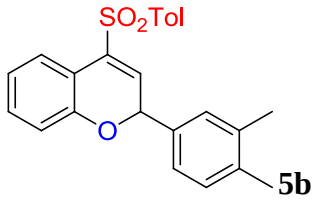

er-Me-Is
157.74
145.38
131.68
131.35
130.98
130.74
129.50
120.16
115.19
108.13
94.53
81.50
77.32
77.00
76.68
59.91
23.49
21.66
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SO2Tol
O
OMe

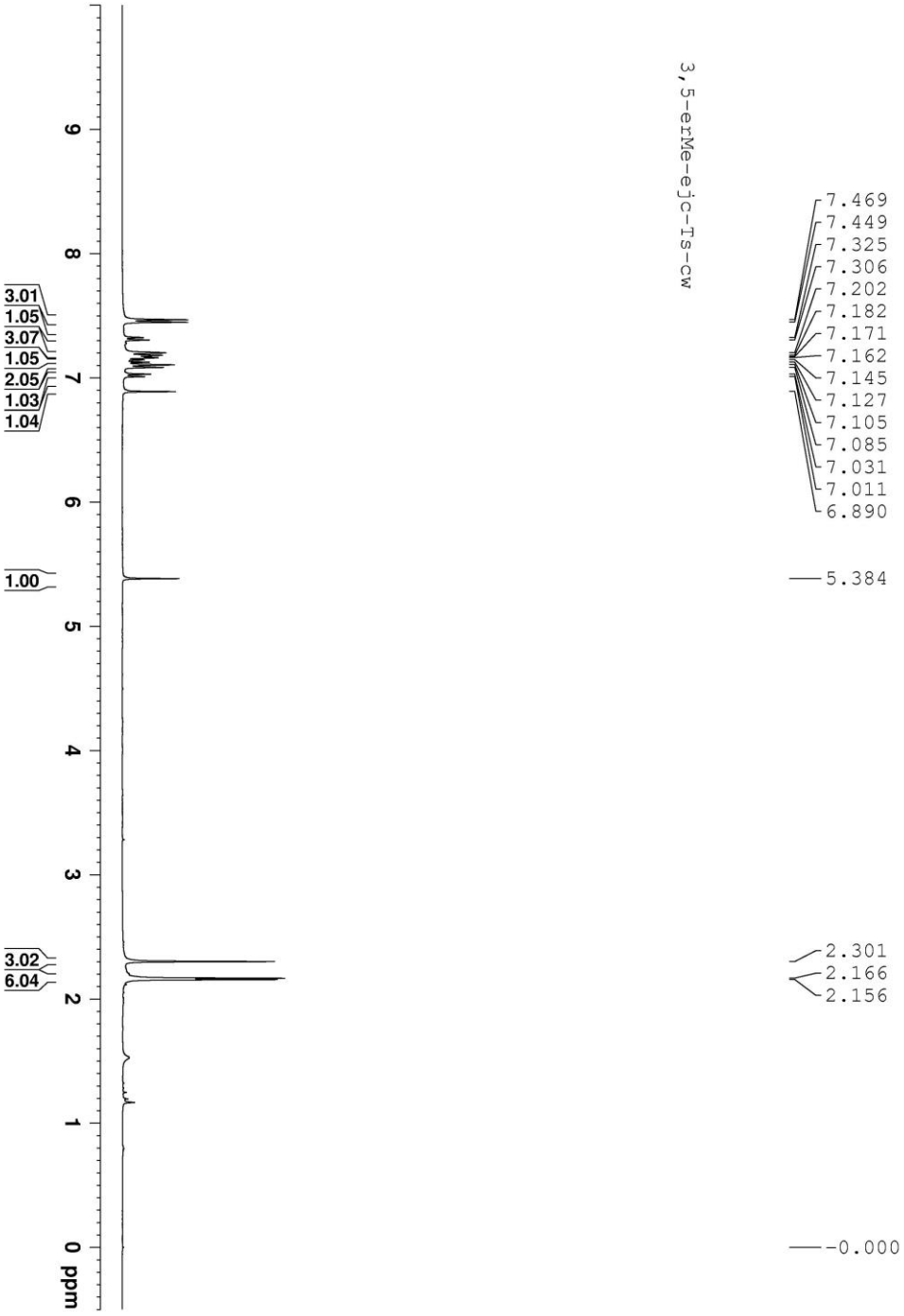
5a

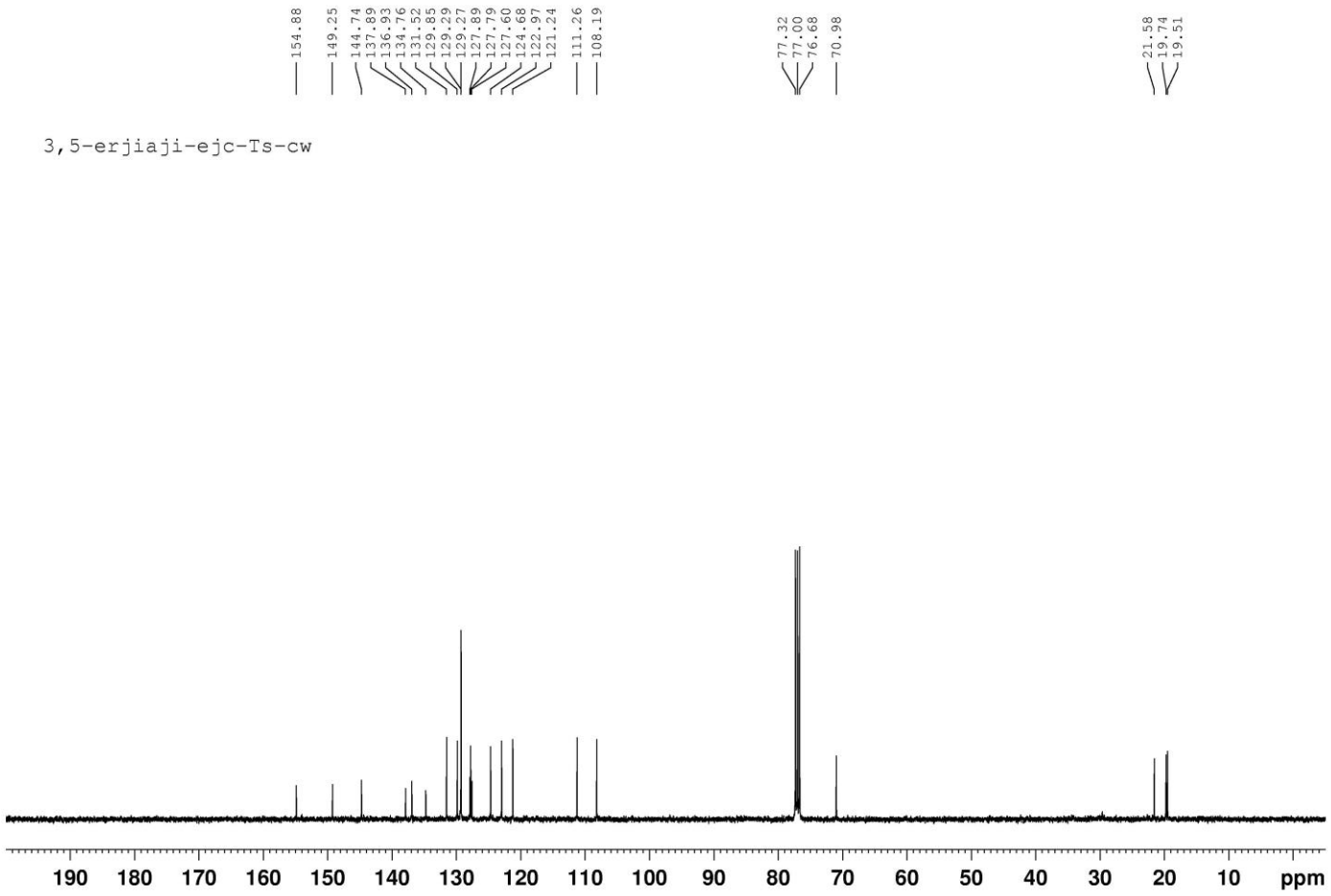

p-OMe-ejc-Ts-cw
1.04
2.06
3.06
1.02
3.01
1.00
2.00
1.01
3.09
3.01
ppm
7.560
7.542
7.522
7.501
7.454
7.432
7.423
7.403
7.294
7.292
7.276
7.274
7.259
7.237
7.218
7.192
7.172
6.968
6.875
6.853
5.475
3.805
2.390
-0.000

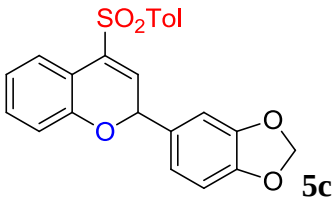

p-OMe-ejc-Is-cw
160.28
154.94
149.08
144.81
134.58
131.72
129.34
129.29
127.85
124.76
123.04
122.31
121.28
114.04
111.29
108.29
77.31
77.00
76.68
70.61
55.30
21.63
ppm


SO2Tol
O

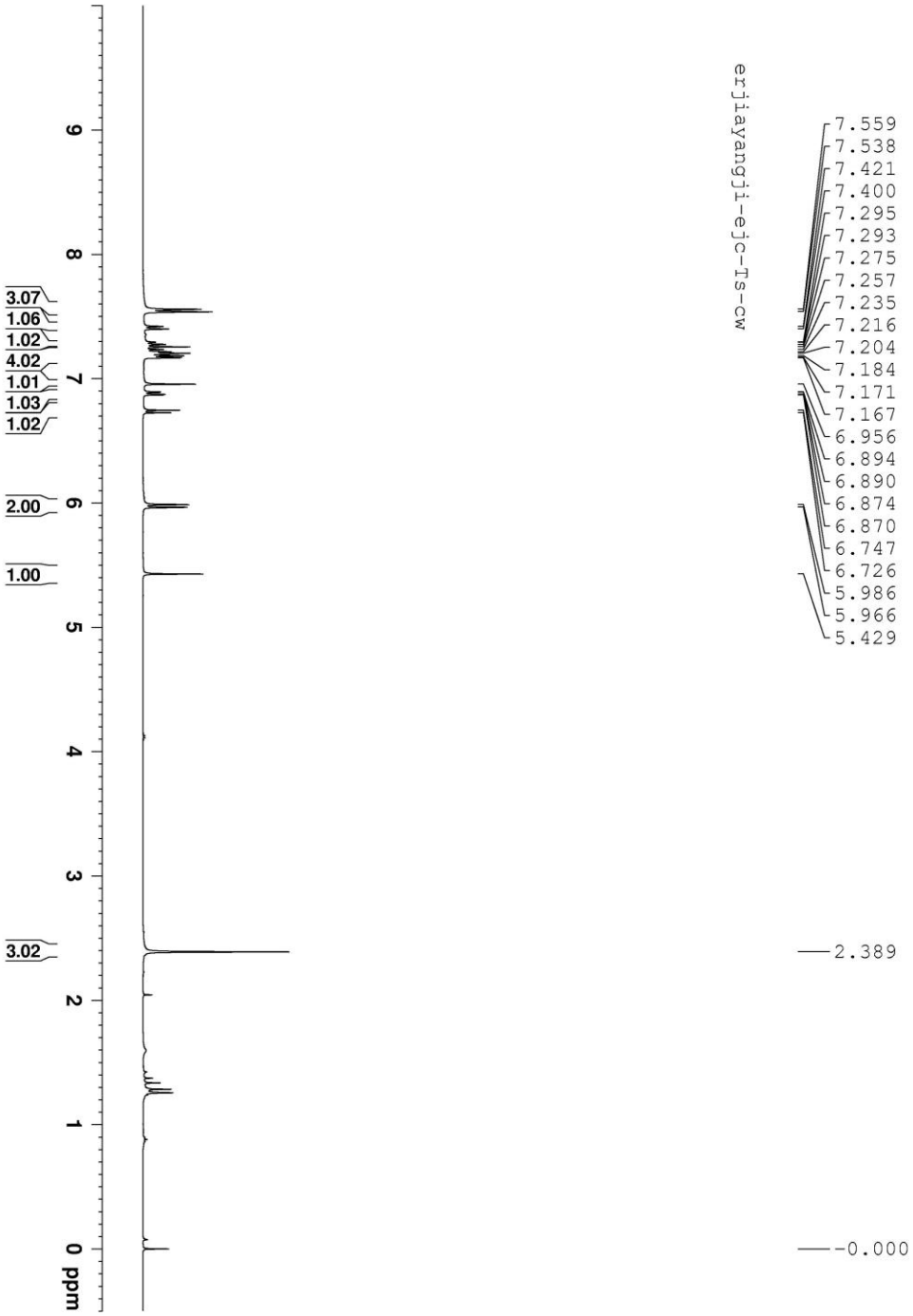
5b

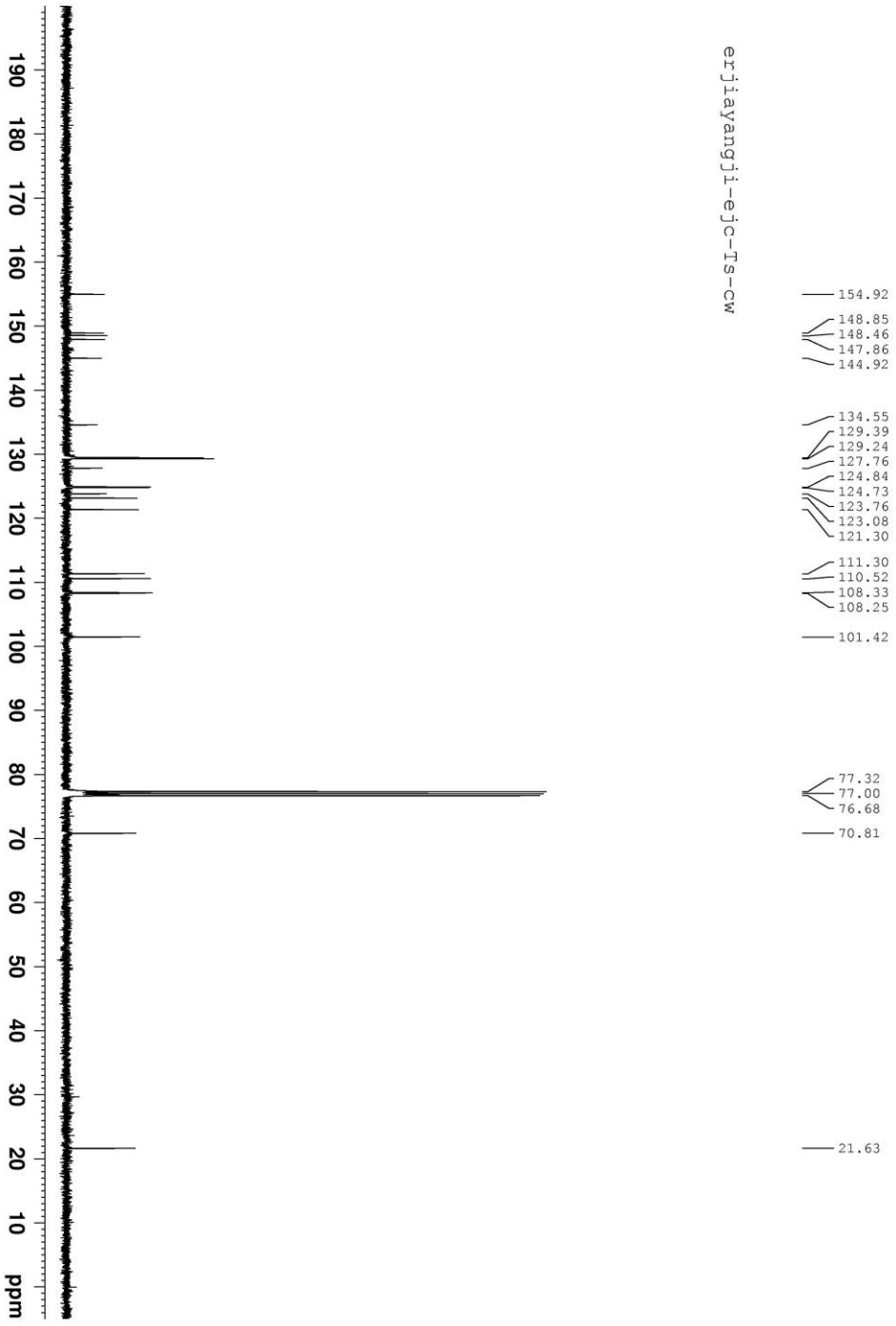

3,5-erMe-ejc-Ts-cw
7.469
7.449
7.325
7.306
7.202
7.182
7.171
7.162
7.145
7.127
7.105
7.085
7.031
7.011
6.890
5.384
2.301
2.166
2.156
-0.000
3.01
1.05
3.07
1.05
2.05
1.03
1.04
1.00
3.02
6.04
ppm

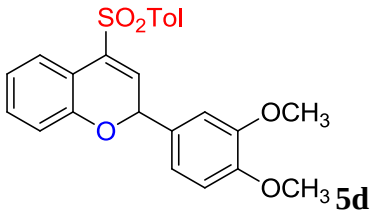

154.88
149.25
144.74
137.89
136.93
134.76
131.52
129.85
129.29
129.27
127.89
127.79
127.60
124.68
122.97
121.24
111.26
108.19
77.32
77.00
76.68
70.98
21.58
19.74
19.51
3,5-erjiaji-ejc-Ts-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SO2Tol
O
O
O

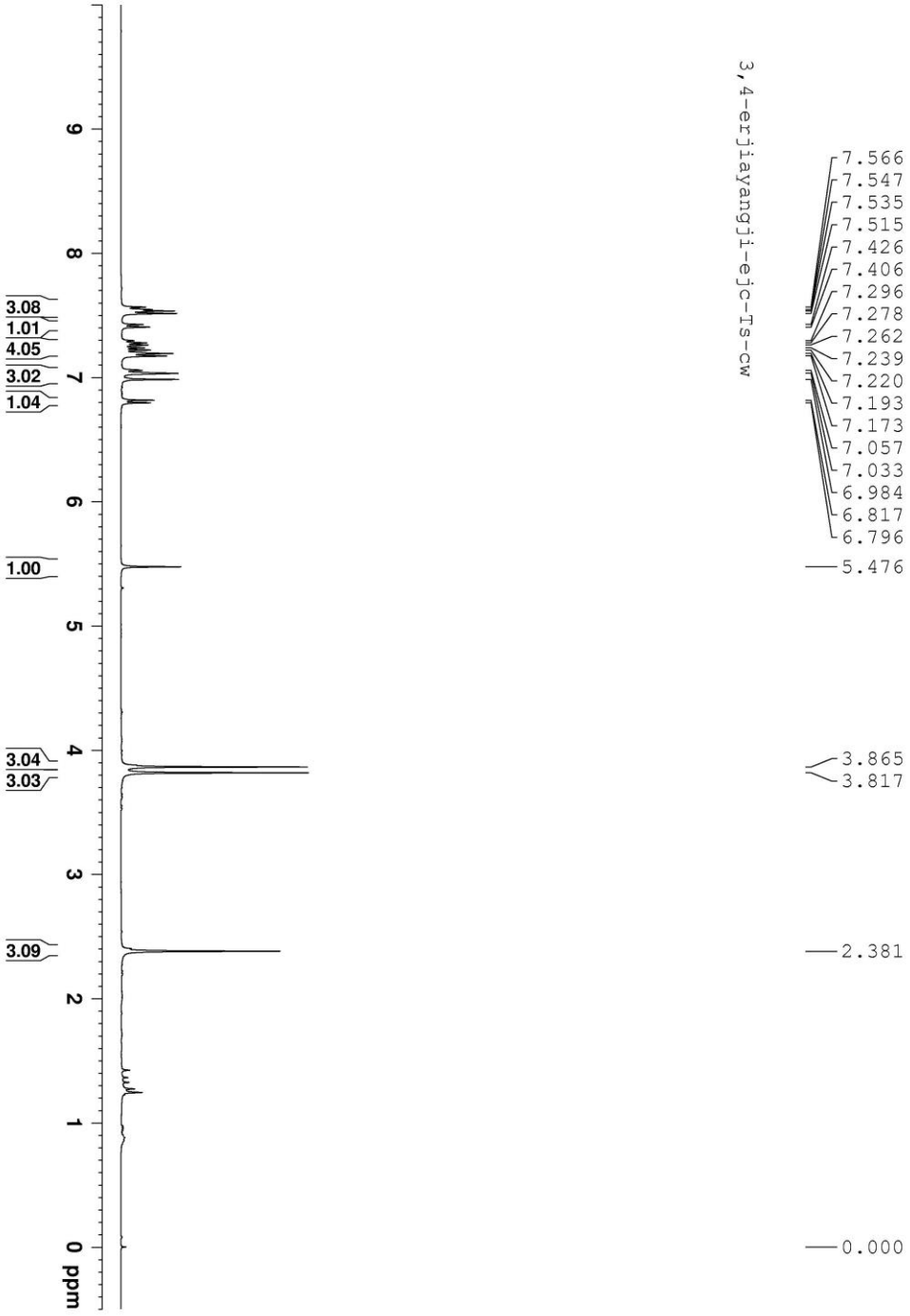
5c

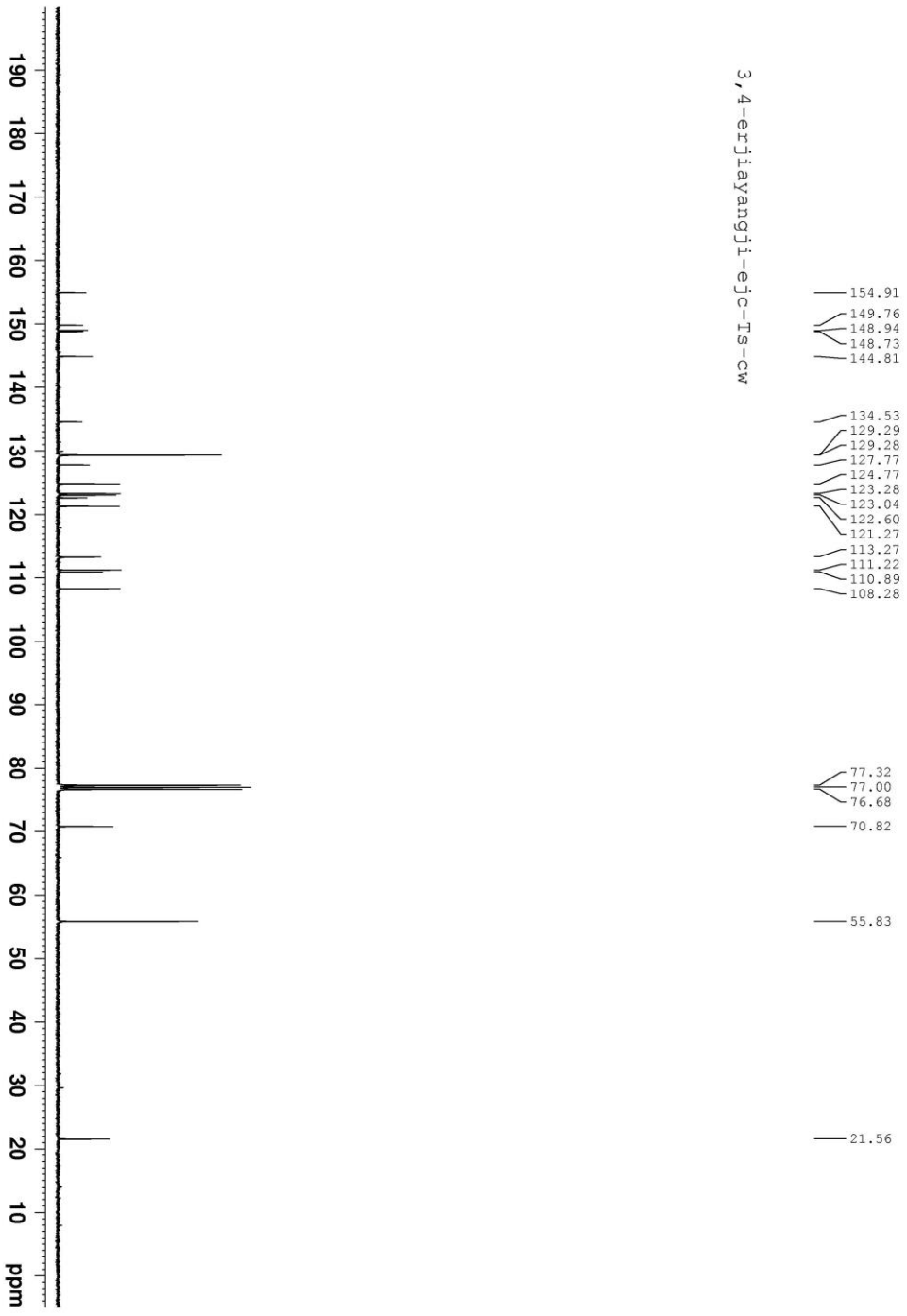

erjiayangji-ejc-Ts-cw
7.559
7.538
7.421
7.400
7.295
7.293
7.275
7.257
7.235
7.216
7.204
7.184
7.171
7.167
6.956
6.894
6.890
6.874
6.870
6.747
6.726
5.986
5.966
5.429
2.389
-0.000
3.07
1.06
1.02
4.02
1.01
1.03
1.02
2.00
1.00
3.02
9
8
7
6
5
4
3
2
1
0 ppm

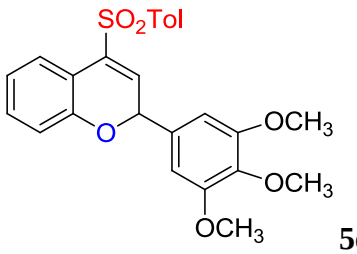

erjiayangji-ejc-Ts-cw
154.92
148.85
148.46
147.86
144.92
134.55
129.39
129.24
127.76
124.84
124.73
123.76
123.08
121.30
111.30
110.52
108.33
108.25
101.42
77.32
77.00
76.68
70.81
21.63
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SO2Tol
O
OCH3
OCH3

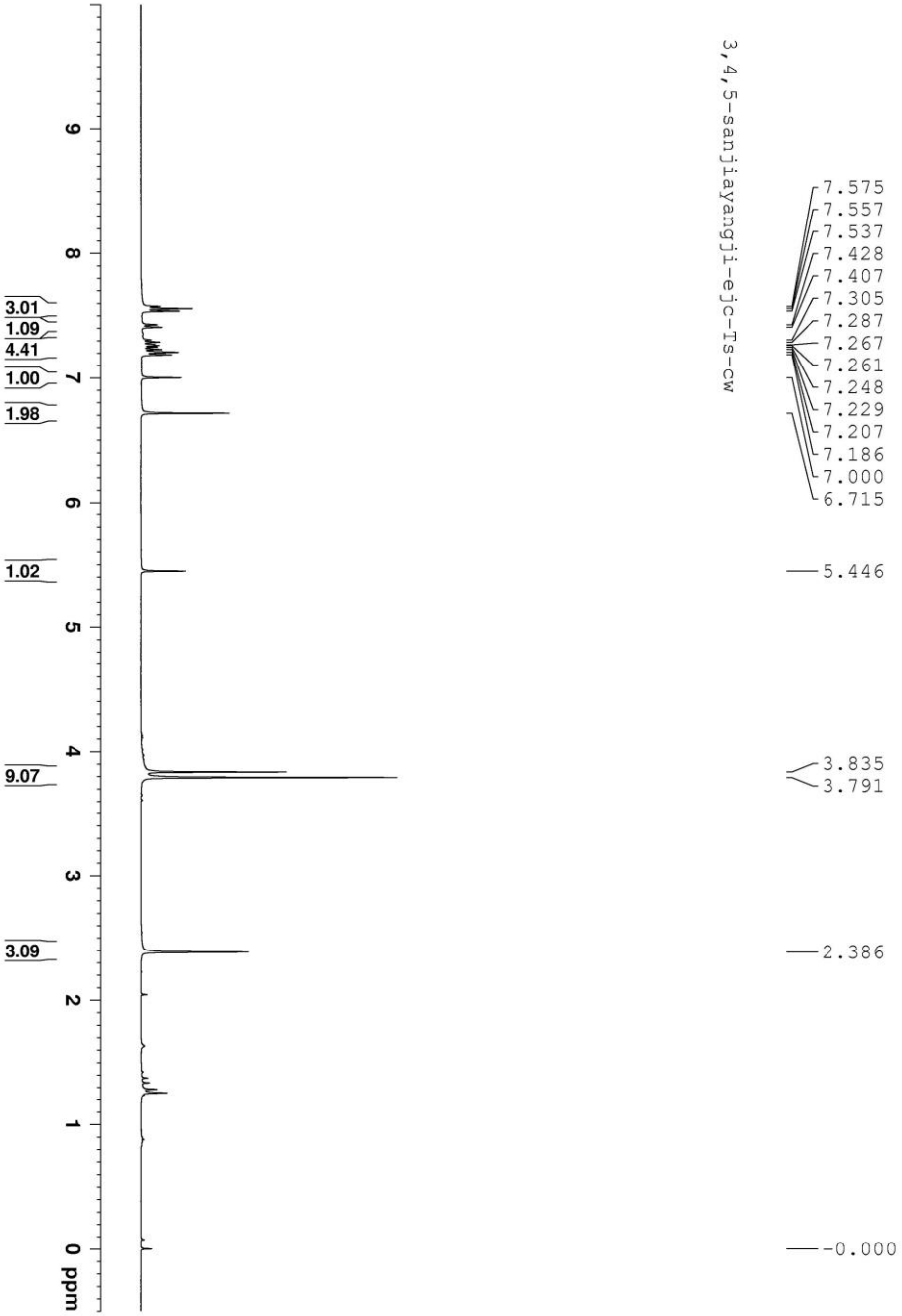
5d

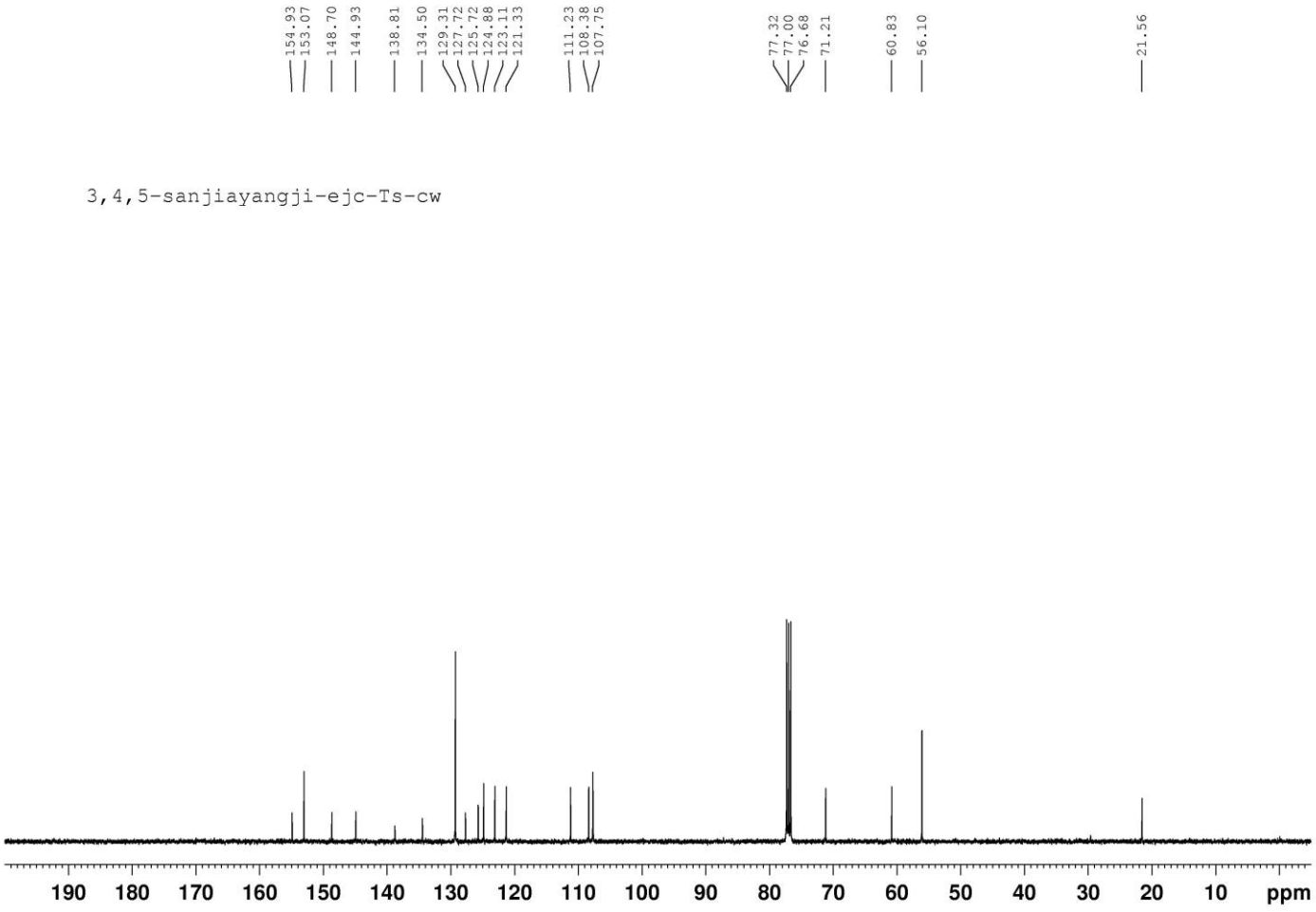

3,4-erjiayangji-ejc-Ts-cw
7.566
7.547
7.535
7.515
7.426
7.406
7.296
7.278
7.262
7.239
7.220
7.193
7.173
7.057
7.033
6.984
6.817
6.796
5.476
3.865
3.817
2.381
0.000
3.08
1.01
4.05
3.02
1.04
1.00
3.04
3.03
3.09
ppm

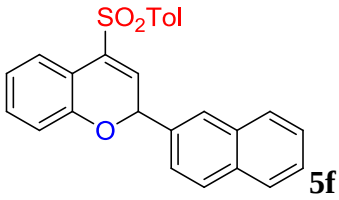

3,4-erjiayangji-ejc-Ts-cw
154.91
149.76
148.94
148.73
144.81
134.53
129.29
129.28
127.77
124.77
123.28
123.04
122.60
121.27
113.27
111.22
110.89
108.28
77.32
77.00
76.68
70.82
55.83
21.56
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SO2Tol
O
OCH3
OCH3
OCH3

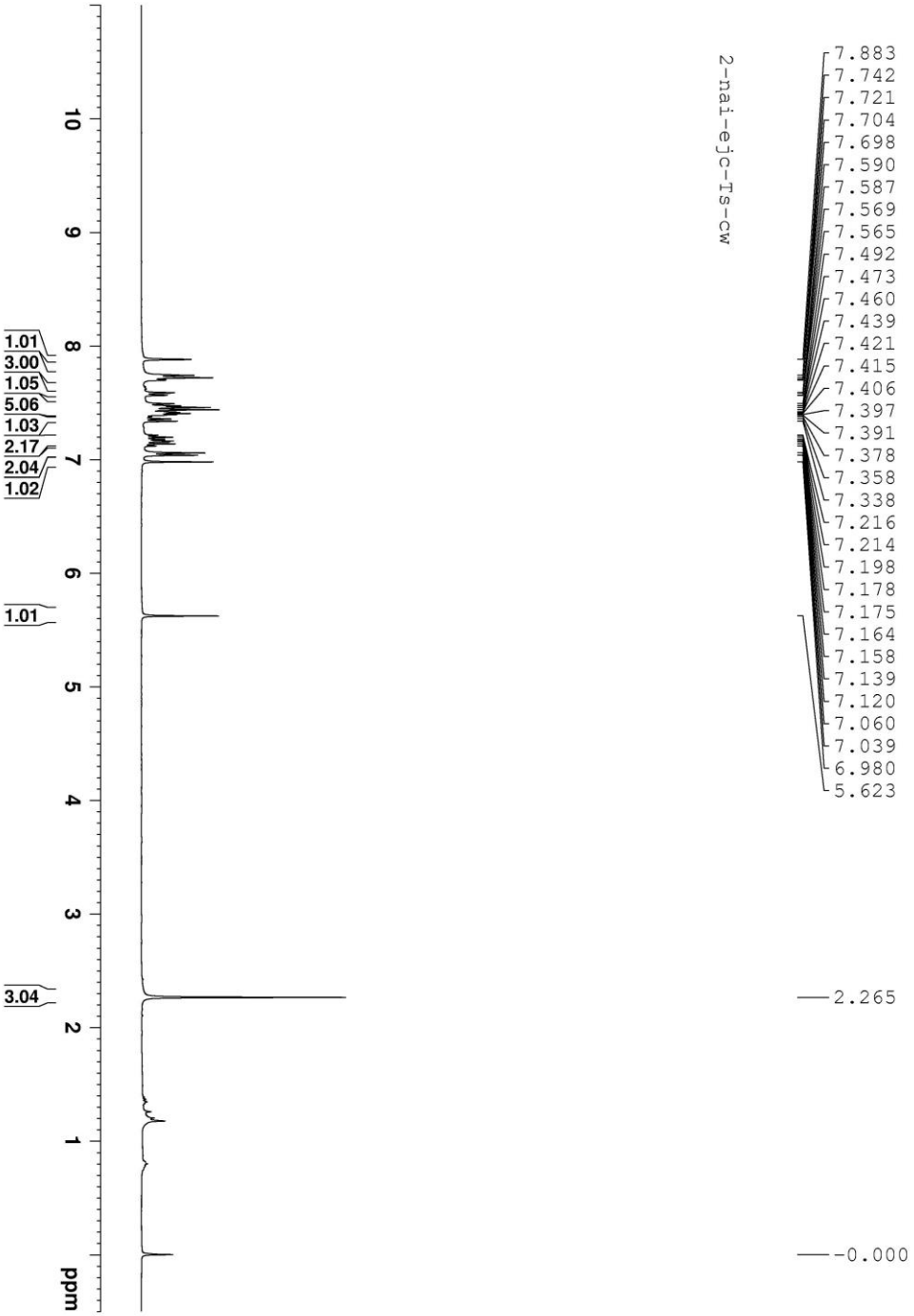
5e

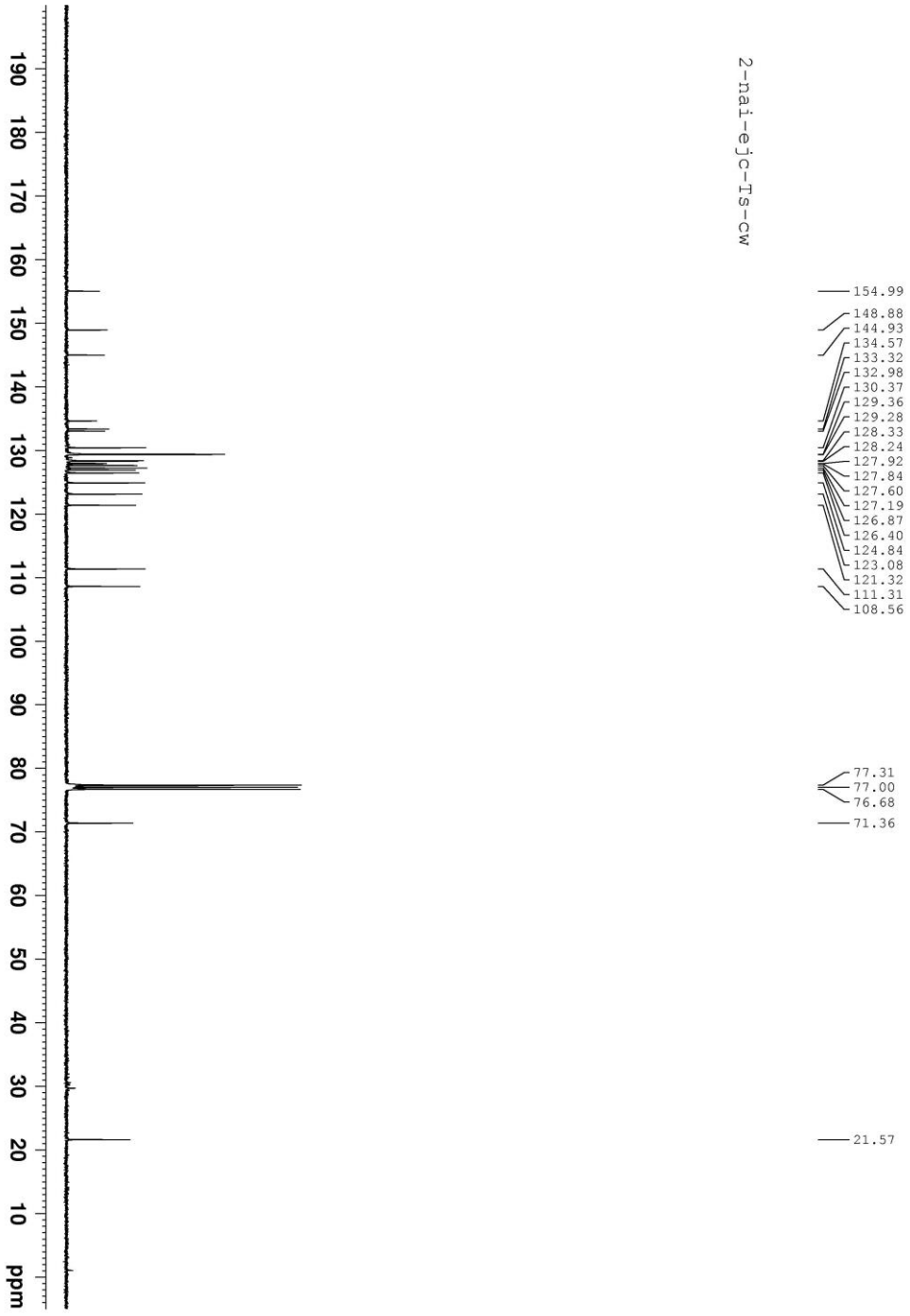

3,4,5-sanjiayangji-ejc-Ts-cw
7.575
7.557
7.537
7.428
7.407
7.305
7.287
7.267
7.261
7.248
7.229
7.207
7.186
7.000
6.715
5.446
3.835
3.791
2.386
-0.000
3.01
1.09
4.41
1.00
1.98
1.02
9.07
3.09
ppm

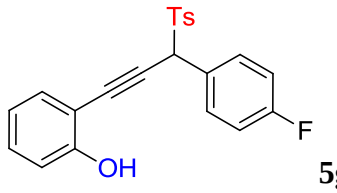

154.93
153.07
148.70
144.93
138.81
134.50
129.31
127.72
125.72
124.88
123.11
121.33
111.23
108.38
107.75
77.32
77.00
76.68
71.21
60.83
56.10
21.56
3,4,5-sanjiayangji-ejc-Ts-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


SO2Tol
O

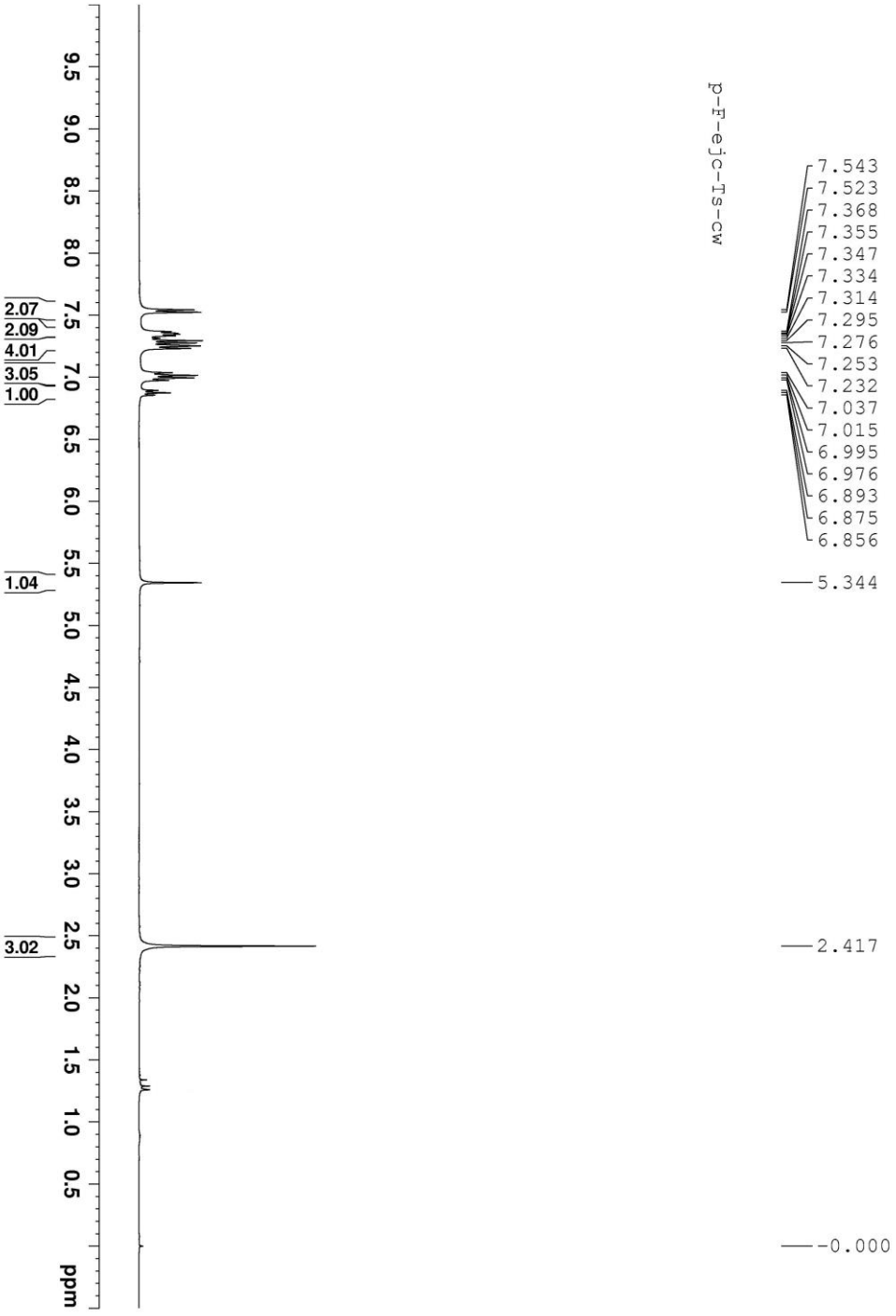
5f

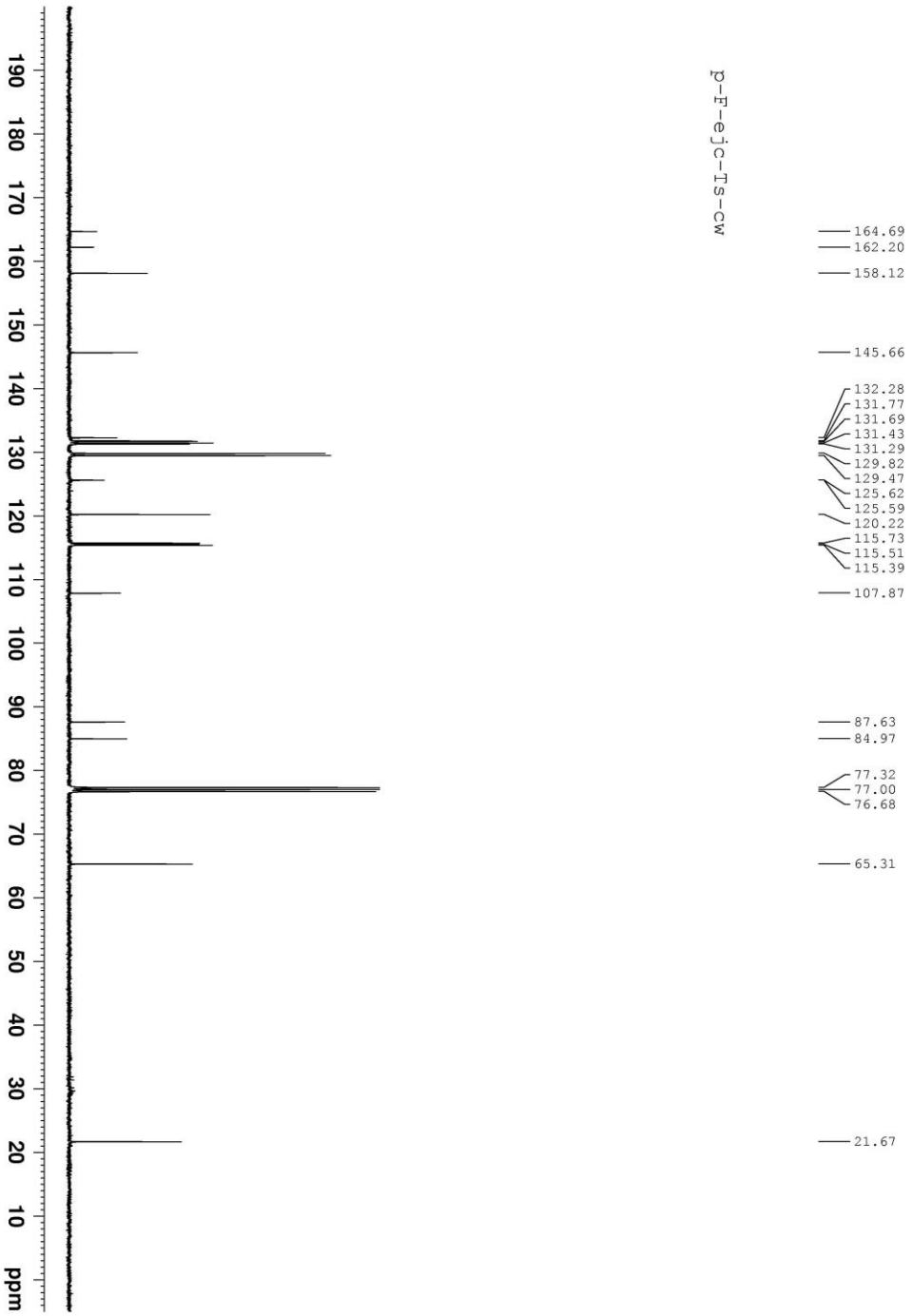

2-nai-ejc-Ts-cw
7.883
7.742
7.721
7.704
7.698
7.590
7.587
7.569
7.565
7.492
7.473
7.460
7.439
7.421
7.415
7.406
7.397
7.391
7.378
7.358
7.338
7.216
7.214
7.198
7.178
7.175
7.164
7.158
7.139
7.120
7.060
7.039
6.980
5.623
2.265
-0.000
1.01
3.00
1.05
5.06
1.03
2.17
2.04
1.02
1.01
3.04
ppm

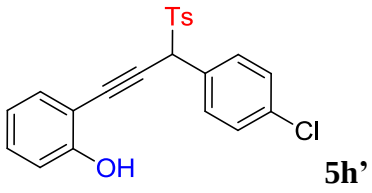

2-nai-ejc-Ts-cw
154.99
148.88
144.93
134.57
133.32
132.98
130.37
129.36
129.28
128.33
128.24
127.92
127.84
127.60
127.19
126.87
126.40
124.84
123.08
121.32
111.31
108.56
77.31
77.00
76.68
71.36
21.57
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Ts
F
OH

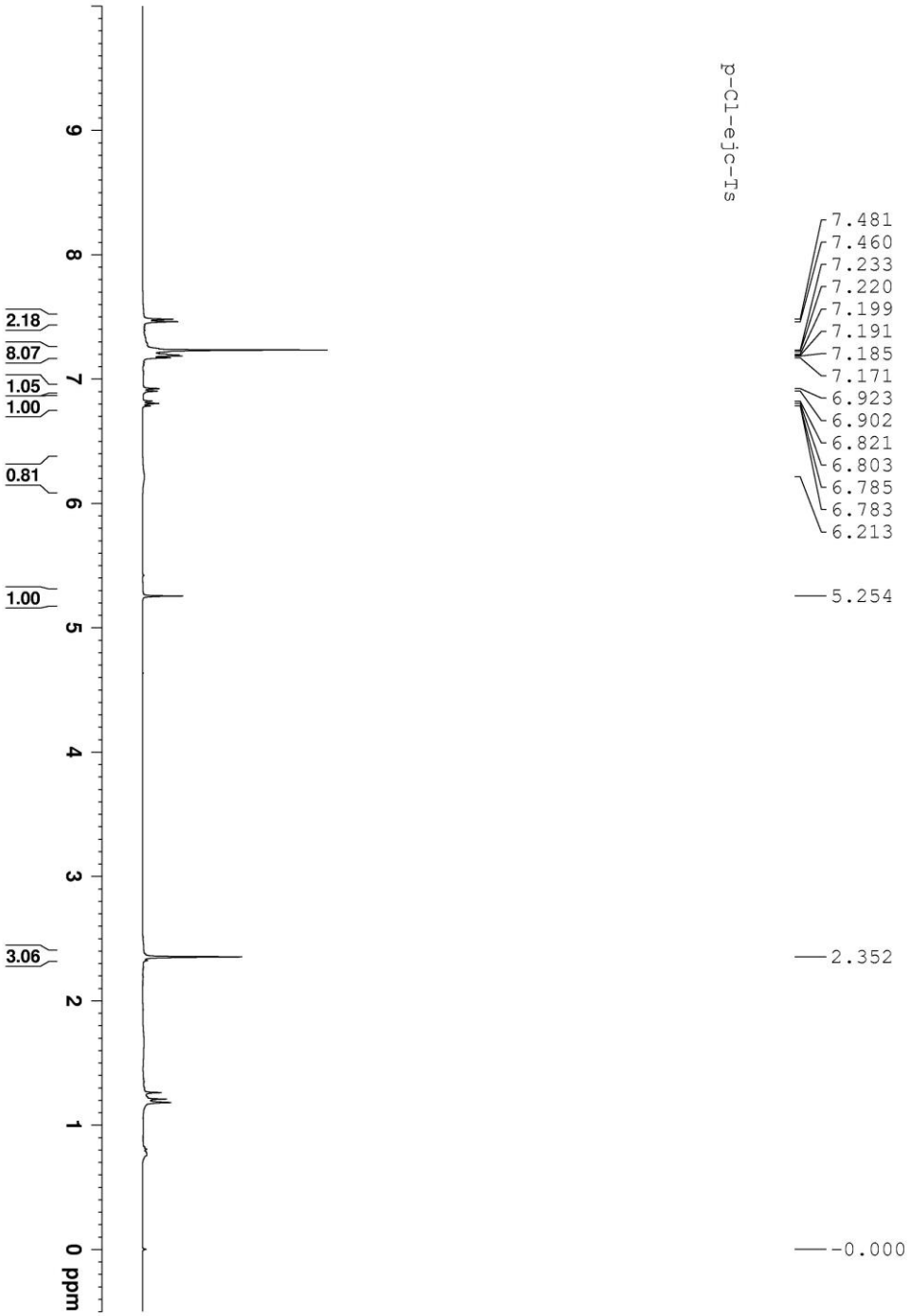
5g'

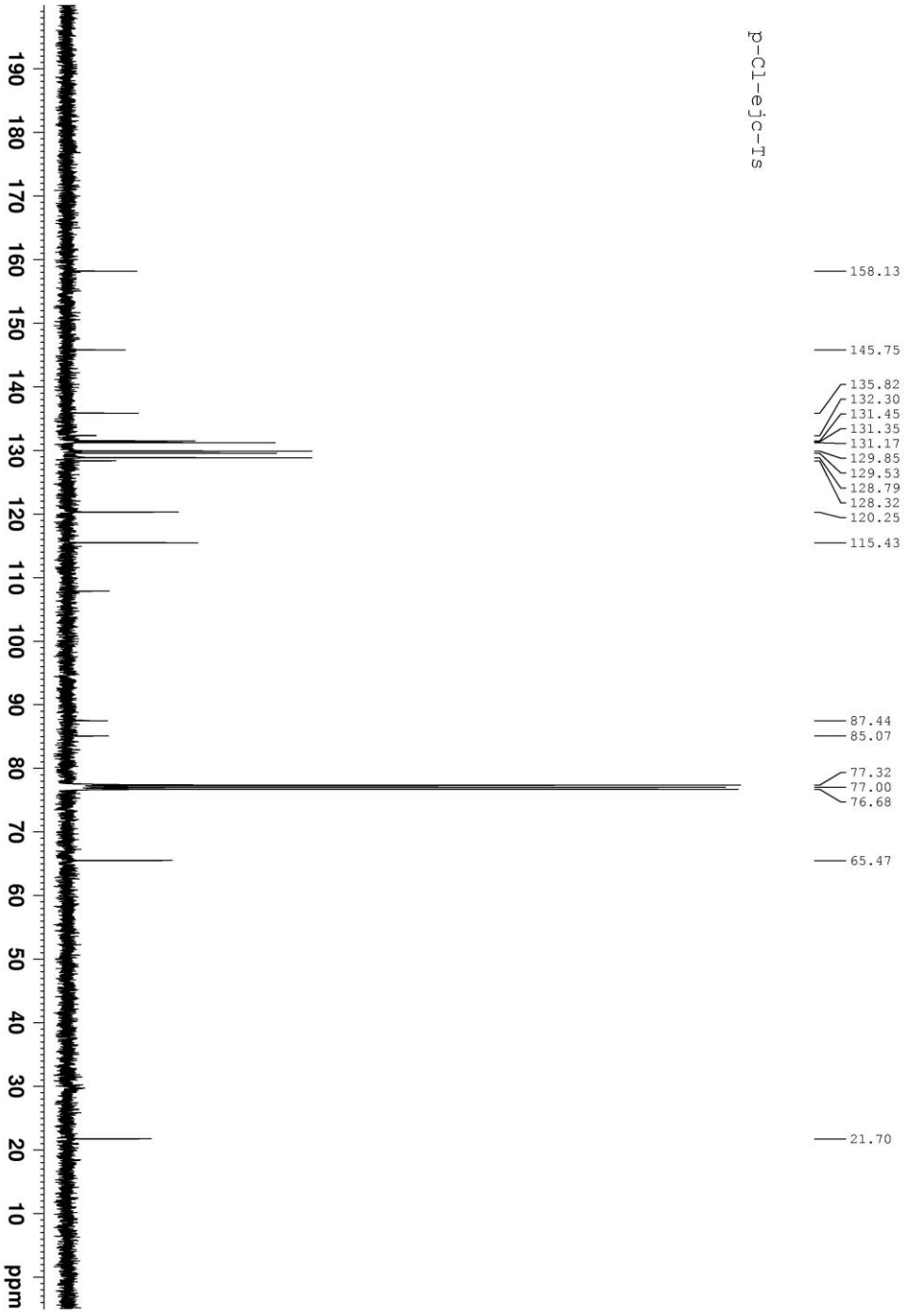

p-F-ejc-Ts-cw
7.543
7.523
7.368
7.355
7.347
7.334
7.314
7.295
7.276
7.253
7.232
7.037
7.015
6.995
6.976
6.893
6.875
6.856
5.344
2.417
-0.000
2.07
2.09
4.01
3.05
1.00
1.04
3.02
ppm

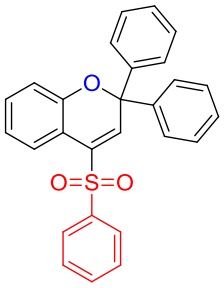

p-F-ejc-Ts-cw
164.69
162.20
158.12
145.66
132.28
131.77
131.69
131.43
131.29
129.82
129.47
125.62
125.59
120.22
115.73
115.51
115.39
107.87
87.63
84.97
77.32
77.00
76.68
65.31
21.67
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Ts
Cl
OH

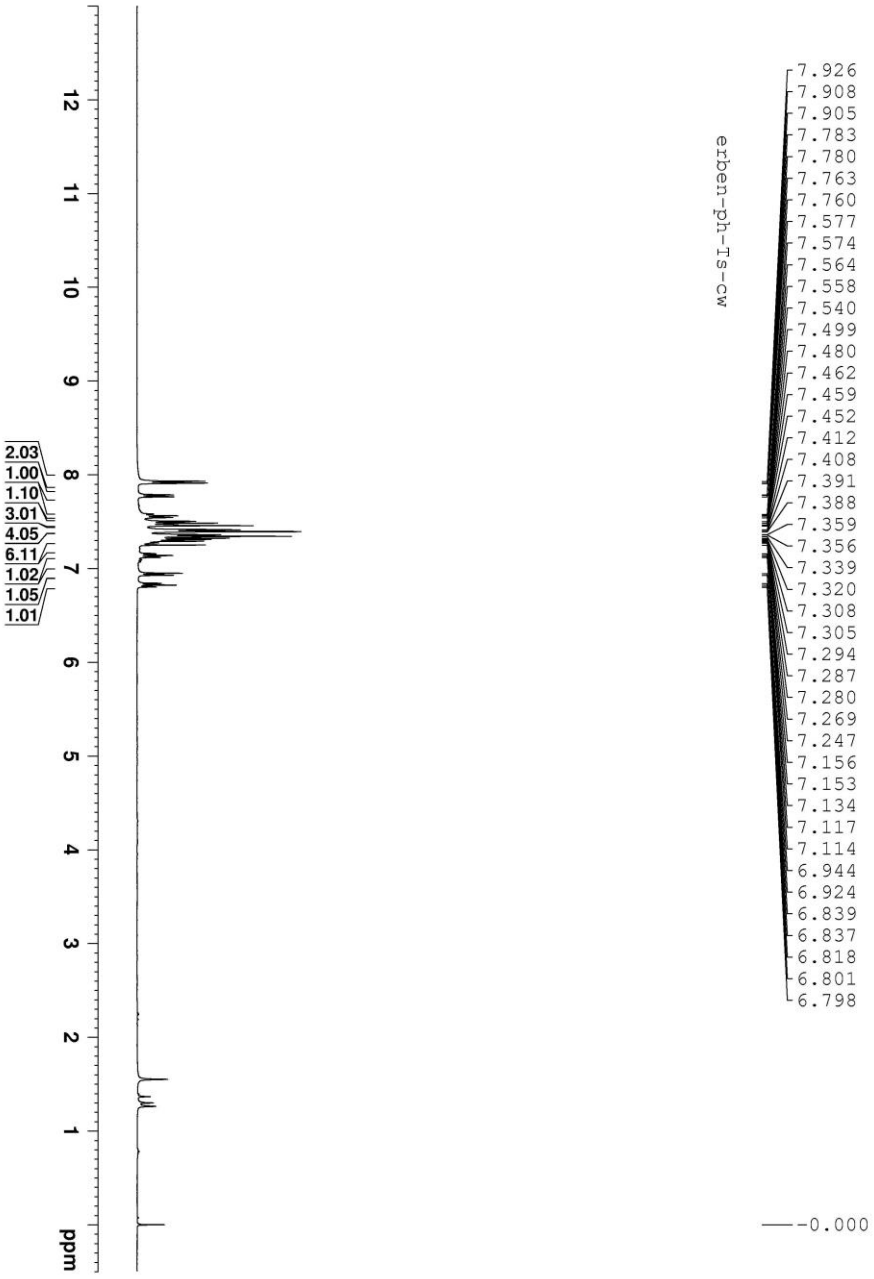
5h'

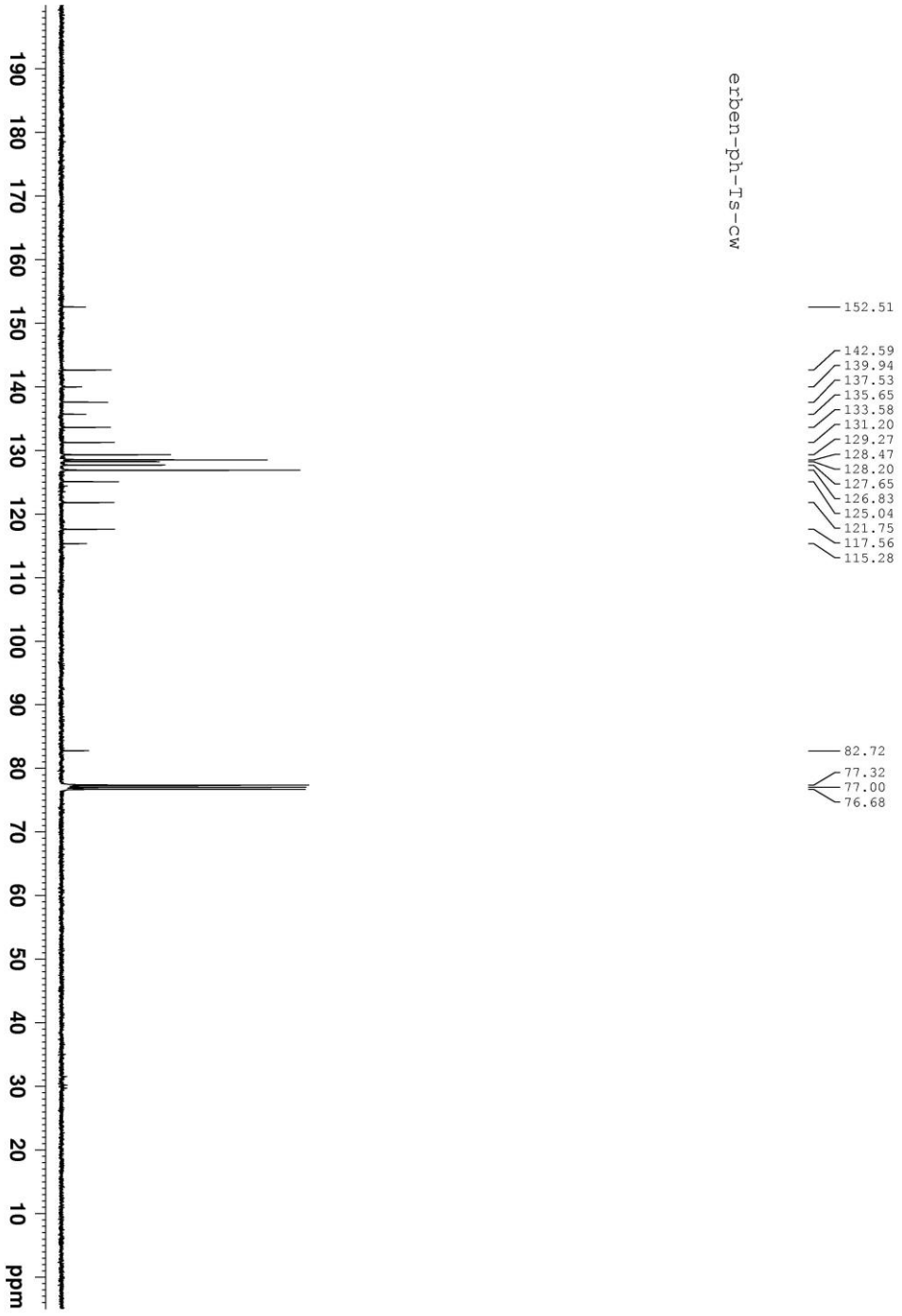

p-Cl-ejc-Ts
7.481
7.460
7.233
7.220
7.199
7.191
7.185
7.171
6.923
6.902
6.821
6.803
6.785
6.783
6.213
5.254
2.352
-0.000
2.18
8.07
1.05
1.00
0.81
1.00
3.06
ppm

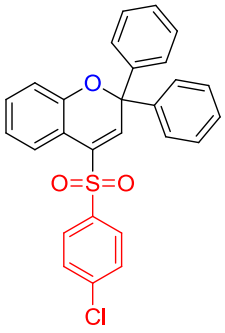

p-Cl-ejc-Ts
158.13
145.75
135.82
132.30
131.45
131.35
131.17
129.85
129.53
128.79
128.32
120.25
115.43
87.44
85.07
77.32
77.00
76.68
65.47
21.70
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
O=S=O

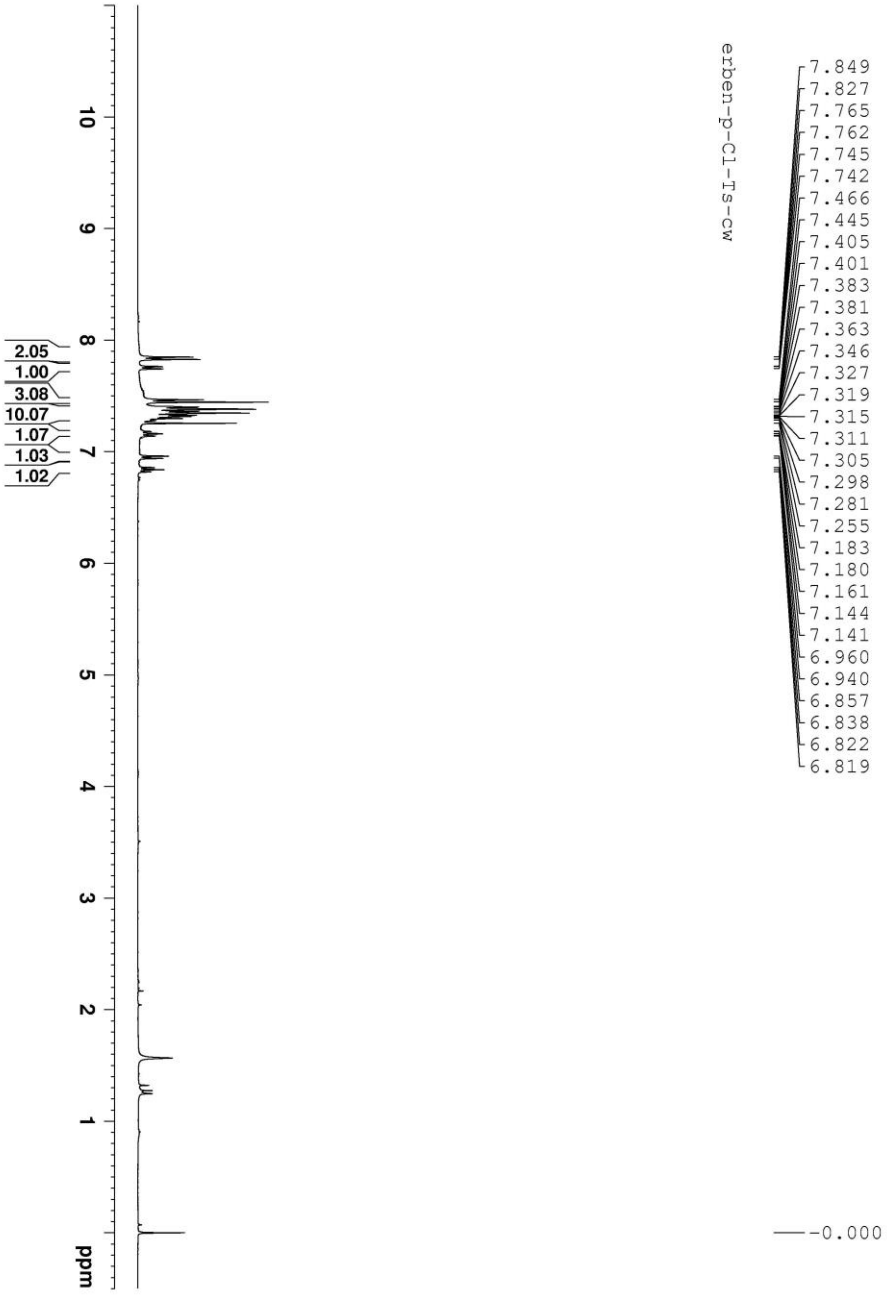
3aa

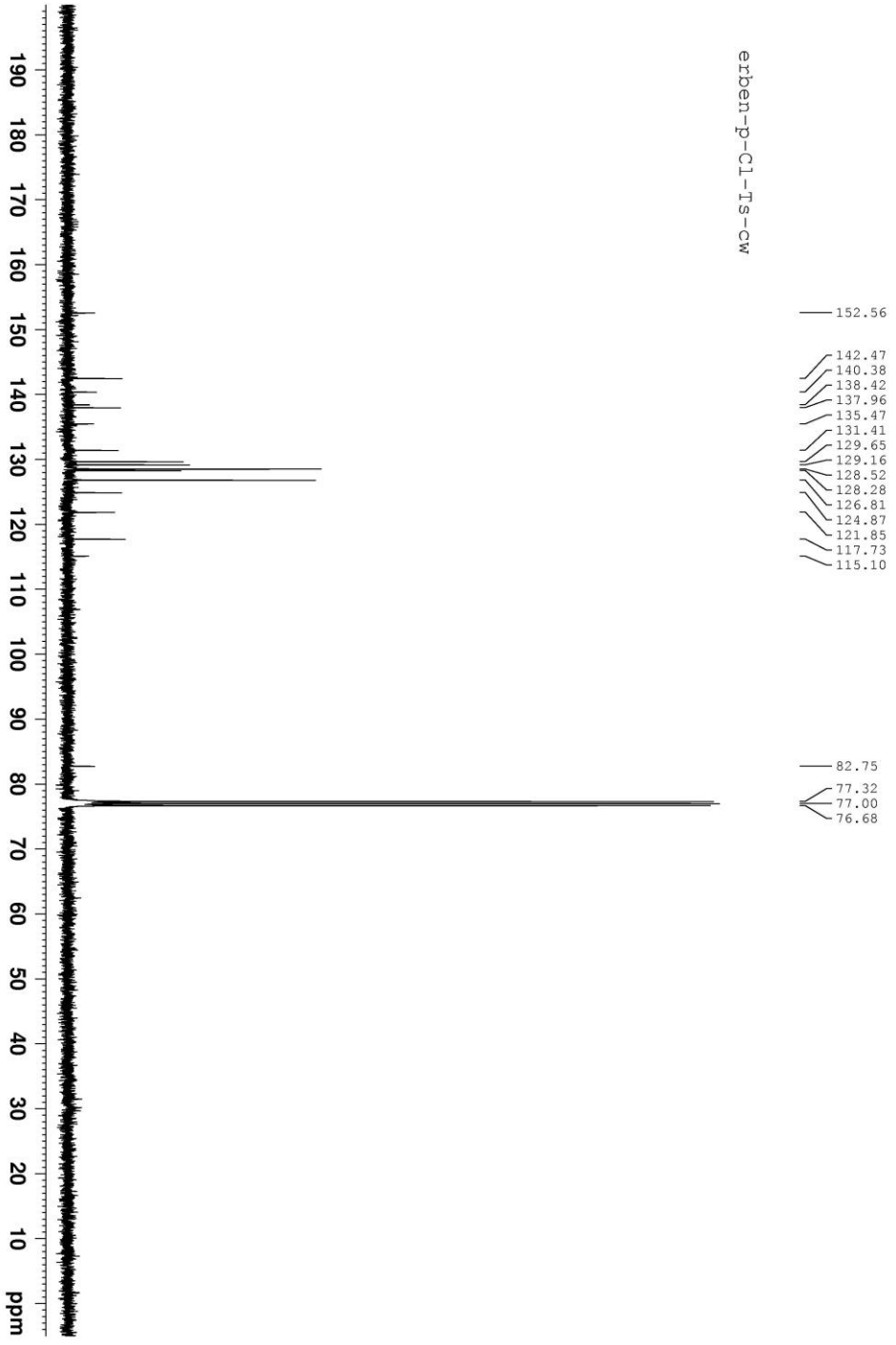

2.03
1.00
1.10
3.01
4.05
6.11
1.02
1.05
1.01
ppm
erben-ph-Ts-cw
7.926
7.908
7.905
7.783
7.780
7.763
7.760
7.577
7.574
7.564
7.558
7.540
7.499
7.480
7.462
7.459
7.452
7.412
7.408
7.391
7.388
7.359
7.356
7.339
7.320
7.308
7.305
7.294
7.287
7.280
7.269
7.247
7.156
7.153
7.134
7.117
7.114
6.944
6.924
6.839
6.837
6.818
6.801
6.798
-0.000

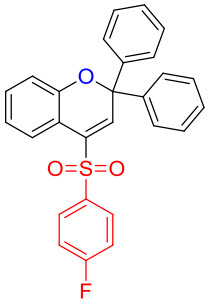

mc-1-ph-neqre
152.51
142.59
139.94
137.53
135.65
133.58
131.20
129.27
128.47
128.20
127.65
126.83
125.04
121.75
117.56
115.28
82.72
77.32
77.00
76.68
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


O
O=S=O
Cl

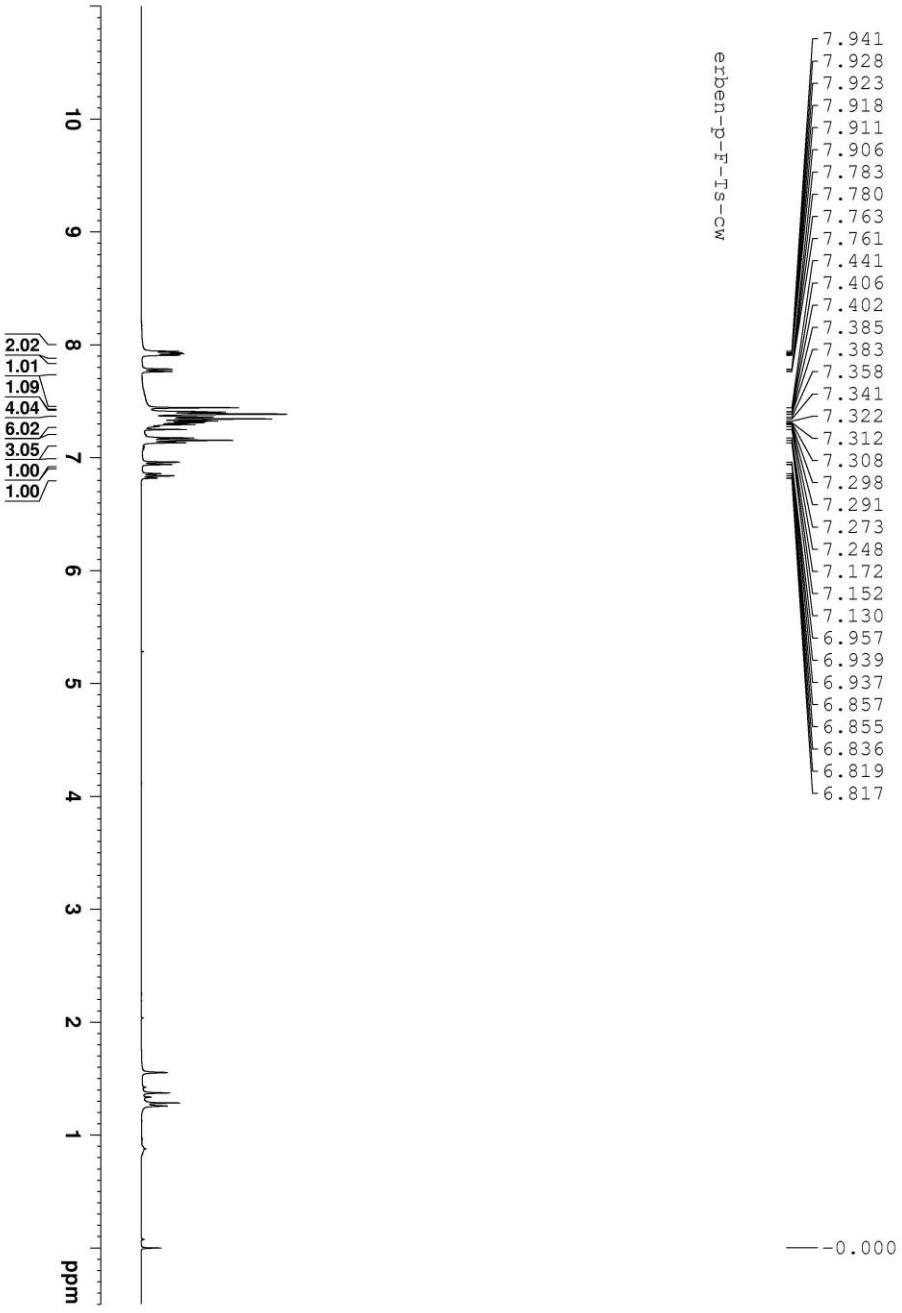
3ab

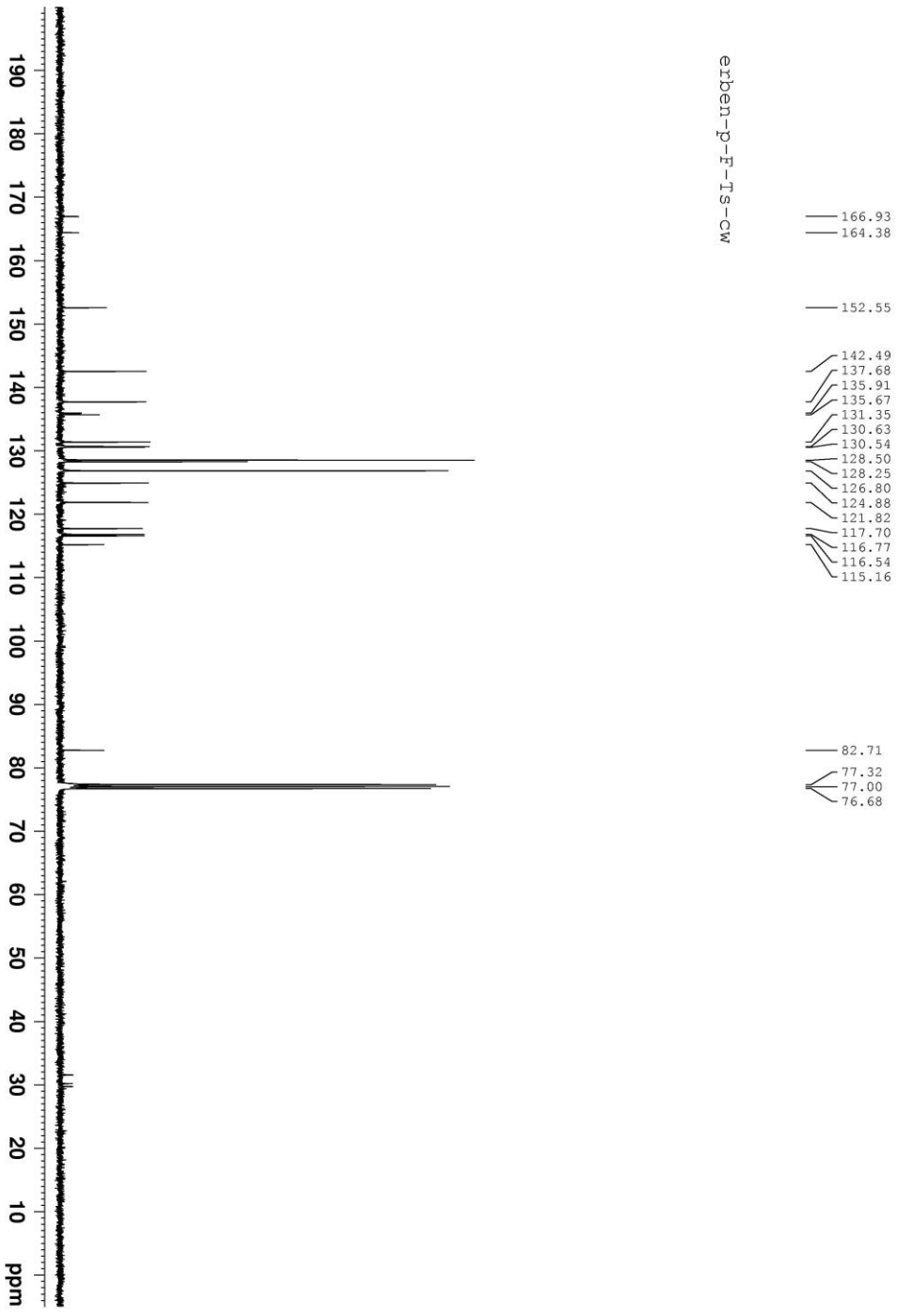

2.05
1.00
3.08
10.07
1.07
1.03
1.02
10
9
8
7
6
5
4
3
2
1
ppm
erben-p-Cl-Is-cw
7.849
7.827
7.765
7.762
7.745
7.742
7.466
7.445
7.405
7.401
7.383
7.381
7.363
7.346
7.327
7.319
7.315
7.311
7.305
7.298
7.281
7.255
7.183
7.180
7.161
7.144
7.141
6.960
6.940
6.857
6.838
6.822
6.819
-0.000

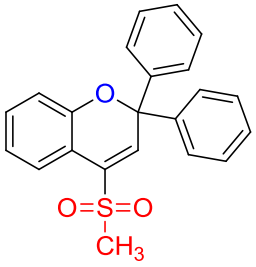

erben-p-Cl-1s-cm
152.56
142.47
140.38
138.42
137.96
135.47
131.41
129.65
129.16
128.52
128.28
126.81
124.87
121.85
117.73
115.10
82.75
77.32
77.00
76.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
O=S=O
F

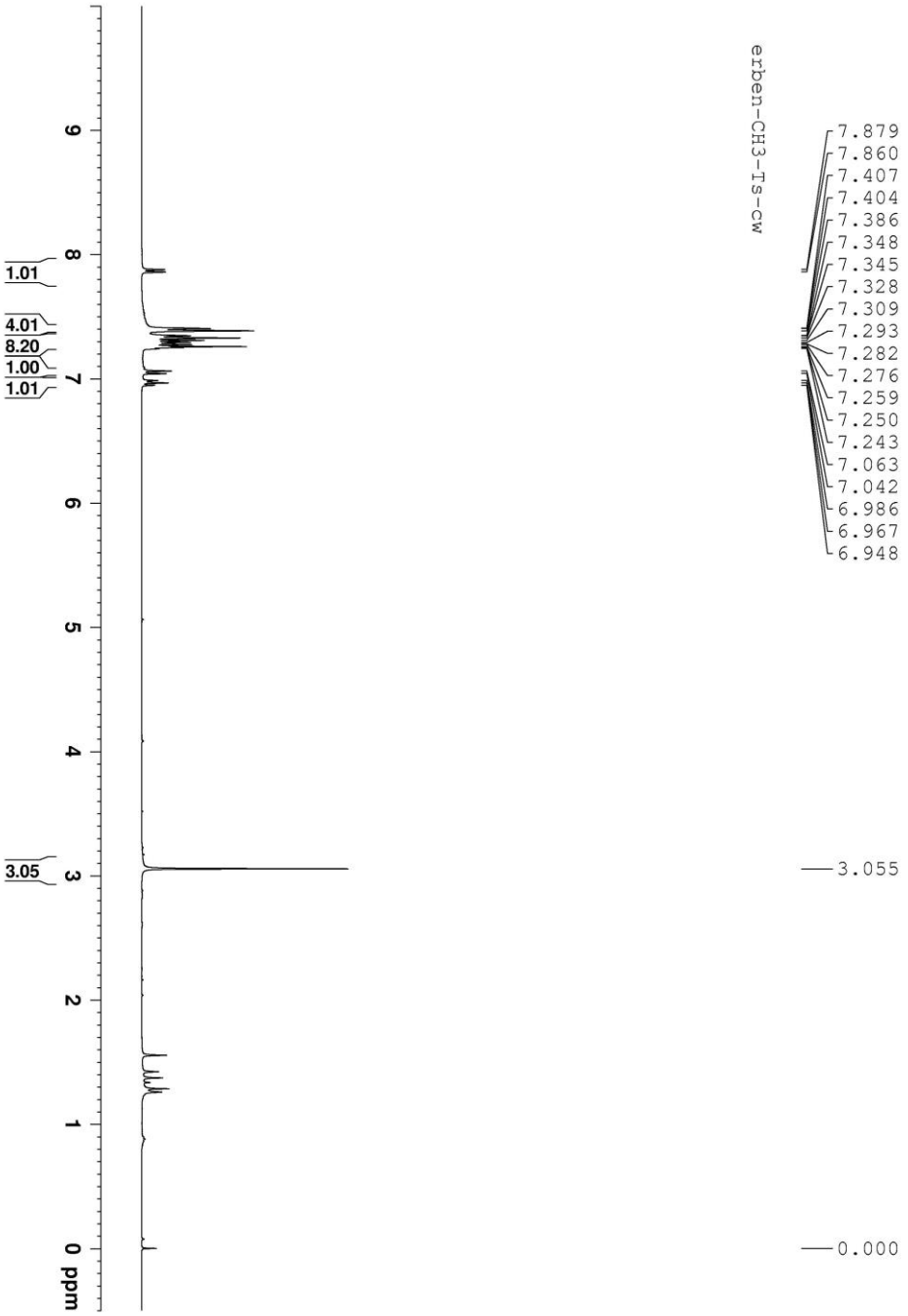
3ac

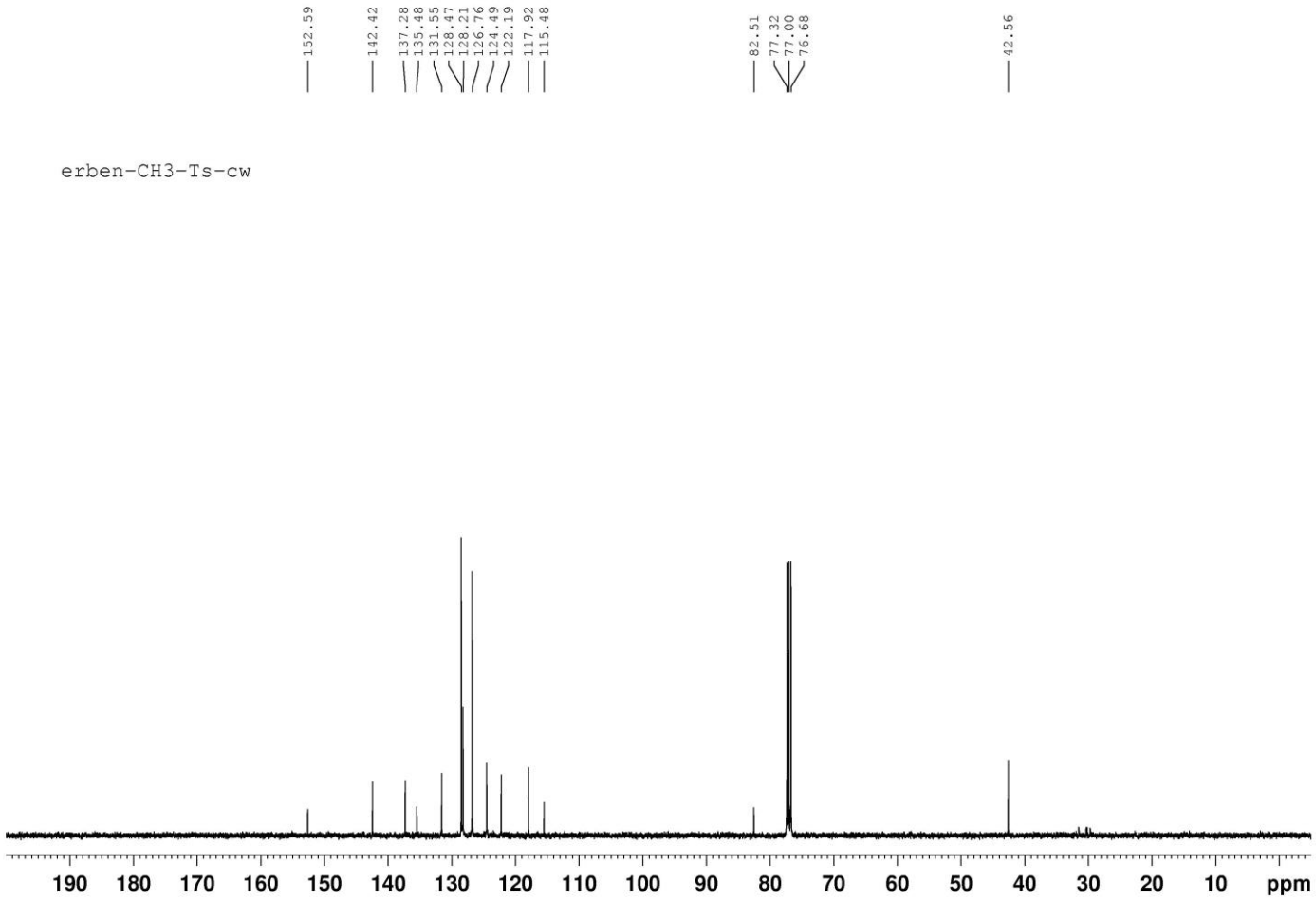

2.02
1.01
1.09
4.04
6.02
3.05
1.00
1.00
10
9
8
7
6
5
4
3
2
1
ppm
erben-p-F-Ts-cw
7.941
7.928
7.923
7.918
7.911
7.906
7.783
7.780
7.763
7.761
7.441
7.406
7.402
7.385
7.383
7.358
7.341
7.322
7.312
7.308
7.298
7.291
7.273
7.248
7.172
7.152
7.130
6.957
6.939
6.937
6.857
6.855
6.836
6.819
6.817
-0.000


erben-p-F-Ts-cw
166.93
164.38
152.55
142.49
137.68
135.91
135.67
131.35
130.63
130.54
128.50
128.25
126.80
124.88
121.82
117.70
116.77
116.54
115.16
82.71
77.32
77.00
76.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


O
O=S=O
CH3

3ad


erben-CH3-Ts-cw
7.879
7.860
7.407
7.404
7.386
7.348
7.345
7.328
7.309
7.293
7.282
7.276
7.259
7.250
7.243
7.063
7.042
6.986
6.967
6.948
1.01
4.01
8.20
1.00
1.01
3.05
3.055
0.000
ppm


152.59
142.42
137.28
135.48
131.55
128.47
128.21
126.76
124.49
122.19
117.92
115.48
82.51
77.32
77.00
76.68
42.56
erben-CH3-Ts-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm